Supporting information

Natural Products in Agarwood and *Aquilaria* Plants: Chemistry, Biological Activities and Biosynthesis

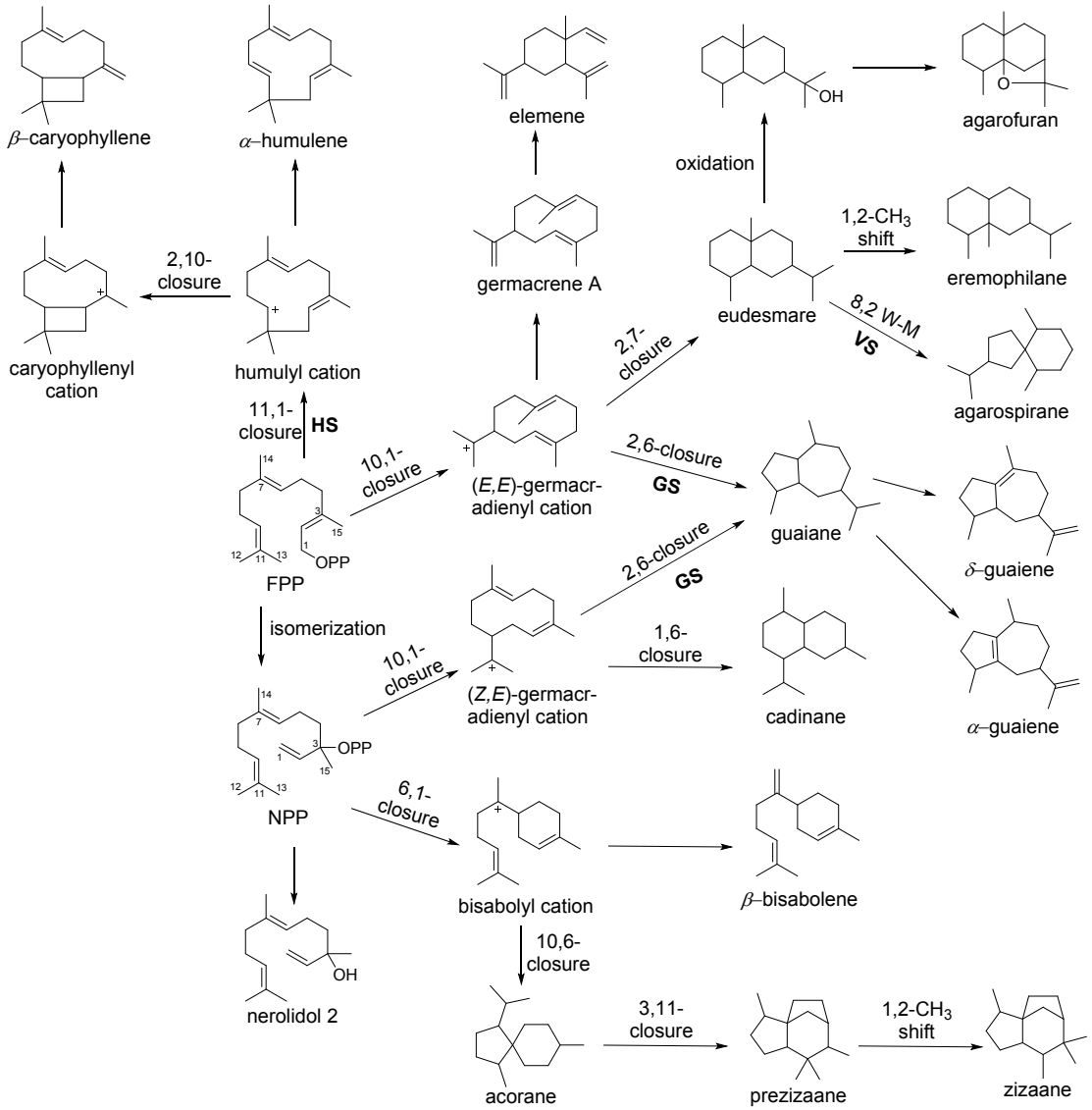
Wei Li[#abc], Hui-Qin Chen[#abc], Hao Wang[#abc], Wen-Li Mei*[abc] and Hao-Fu Dai*[abc]

[a]Hainan Engineering Research Center of Agarwood, Institute of Tropical Bioscience and Biotechnology, Chinese Academy of Tropical Agricultural Sciences, Haikou 571101, PR China. E-mail: meiwenli@itbb.org.cn; daihaofu@itbb.org.cn

[b]Hainan Key Laboratory for Research and Development of Natural Products from Li Folk Medicine, Haikou 571101, PR China.

[c]Hainan Institute for Tropical Agricultural Resources, CATAS, Haikou 571101, PR China.

[#]These authors contributed equally to this work.



Scheme 1 A simplified proposed biosynthetic pathway of sesquiterpenes from agarwood.

Table S1 Eudesmane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
E1	Agarol [11(13)-Eudesmen-12-ol]	$C_{15}H_{26}O$	222	*A. agallocha*	21
E2	(–)-Selina-3,11-dien-14-al	$C_{15}H_{22}O$	218	*A. agallocha*	23
E3	Selina-3,11-dien-14-oic acid	$C_{15}H_{22}O_2$	234	*A. agallocha*	23
E4	(4aβ,7β,8aβ)-3,4,4a,5,6,7,8,8a-Octahydro-7-[1-(hydroxymethyl) ethenyl]-4a-methylnaphthalene-1-carboxaldehyde	$C_{15}H_{22}O_2$	234	*A. malaccensis* *A. sinensis*	27 28-30
E5	12,15-Dioxo-*α*-selinen [Selina-3,11-diene-12,15-dial]	$C_{15}H_{20}O_2$	232	*A. sinensis* *G. salicifolia*	29,31,32 19
E6	Selina-3,11-dien-14-ol	$C_{15}H_{20}O$	220	*A. agallocha*	23
E7	15-Hydroxyl-12-oxo-*α*-selinen	$C_{15}H_{24}O_2$	236	*A. sinensis*	29
E8	(5*S*,7*S*,9*S*,10*S*)-(+)-9-Hydroxy-selina-3,11-dien-12-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	28,29
E9	(5*S*,7*S*,9*S*,10*S*)-(+)-9-Hydroxy-eudesma-3,11(13)-dien-12-methyl ester	$C_{16}H_{24}O_3$	264	*A. sinensis*	28,29
E10	(5*S*,7*S*,9*S*,10*S*)-(–)-9-Hydroxy-selina-3,11-dien-14-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	29
E11	(5*S*,7*S*,9*S*,10*S*)-(+)-Selina-3,11-dien-9-ol	$C_{15}H_{24}O$	220	*A. agallocha*	22
E12	(+)-8α-Hydroxyeudesma-3,11(13)-dien-14-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	28
E13	Petafolia A	$C_{15}H_{24}O_2$	236	*A. sinensis*	30
E14	Selina-3,11-dien-9,15-diol	$C_{15}H_{24}O_2$	236	*A. sinensis*	33
E15	(+)-Eudesma-3,11(13)-dien-8α,9β-diol	$C_{15}H_{24}O_2$	236	*A. sinensis*	28
E16	(5*S*,7*S*,10*S*)-(–)-Selina-3,11-dien-9-one	$C_{15}H_{22}O$	218	*A. agallocha*	22
E17	Selina-4,11-dien-14-al	$C_{15}H_{22}O$	218	*A. agallocha*	23
E18	Selina-4,11-dien-14-oic acid	$C_{15}H_{22}O_2$	234	*A. agallocha*	23

No.	Name	Formula	MW	Source or origin	Ref.
E19	12,15-Dioxo-selina-4,11-dine [Selina-4,11-diene-12,15-dial]	$C_{15}H_{20}O_2$	232	*A. malaccensis* *A. sinensis*	27 28,31
E20	Methyl-15-oxo-eudesmane-4,11(13)-dien-12-oate	$C_{16}H_{22}O_3$	262	*A. crassna*	34
E21	(–)-10-*Epi*-*γ*-eudesmol	$C_{15}H_{26}O$	222	*A. malaccensis*	24
E22	Eudesma-4-en-8,11-diol	$C_{15}H_{26}O_2$	238	*A. crassna*	34
E23	Eudesma-4-en-11,15-diol	$C_{15}H_{26}O_2$	238	*A. malaccensis* *A. sinensis* *A. crassna*	27 28 34
E24	12-Hydroxy-4(5),11(13)-eudesmadien-15-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	28,30
E25	(7*S*,8*R*,10*S*)-(+)-8,12-Dihydroxy-selina-4,11-dien-14-al	$C_{15}H_{22}O_3$	250	*A. sinensis*	29
E26	(7*S*,9*S*,10*S*)-(+)-9-Hydroxy-selina-4,11-dien-14-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	28-30
E27	9-Hydroxy-selina-4,11-dien-14-oic acid	$C_{15}H_{22}O_3$	250	*A. agallocha*	23
E28	(+)-9β-Hydroxyeudesma-4,11(13)-dien-12-al	$C_{15}H_{22}O_2$	234	*A. sinensis*	28
E29	(+)-Eudesma-4,11(13)-dien-8α,9β-diol	$C_{15}H_{24}O_2$	236	*A. sinensis*	28
E30	(+)-Eudesma-4(14),11(13)-dien-8α,9β-diol	$C_{15}H_{24}O_2$	236	*A. sinensis*	28
E31	5-Desoxylongilobol	$C_{15}H_{26}O_2$	238	*A. sinensis* *A.crassna*	28 35
E32	*Ent*-4(15)-eudesmen-1α,11-diol	$C_{15}H_{26}O_2$	238	*A. sinensis*	29
E33	Eudesmane-1β,5α,11-triol	$C_{15}H_{28}O_3$	256	*A. sinensis*	29
E34	(–)-7β-*H*-Eudesmane-4α,11-diol	$C_{15}H_{28}O_2$	240	*A. sinensis*	29
E35	(4*R*,5*R*,7*S*,9*S*,10*S*)-(–)-Eudesma-11(13)-en-4,9-diol	$C_{15}H_{26}O_2$	238	*A. sinensis*	28,30
E36	Selin-11-en-4α-ol	$C_{15}H_{26}O$	222	*A. sinensis*	28,30
E37	(2*R*,4a*S*)-2-(4a-Methyl-l,2,3,4,4a,5,6,7-octahydro-2-naphthyl)-propan-2-ol	$C_{14}H_{22}O$	208	*A. agallocha*	26

No.	Name	Formula	MW	Source or origin	Ref.
E38	(*S*)-4a-Methyl-2-(1-methylethy1)-3,4,4a,5,6,7-hexahydronapthalene	$C_{14}H_{22}$	190	*A. agallocha*	26
E39	(*S*)-4a-Methyl-2-(1-methylethylidene)-1,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{14}H_{22}$	190	*A. agallocha*	26
E40	(2*R*,4a*S*)-4a-Methyl-2-(1-methylethenyl)-l,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{14}H_{22}$	190	*A. agallocha*	26
E41	β-Agarofuran	$C_{15}H_{24}O$	220	*A. agallocha* *A. sinensis*	22,36 38,42,43
E42	Baimuxinol	$C_{15}H_{26}O_2$	238	*A. sinensis*	39,43
E43	4-Hydroxyl-baimuxinol	$C_{15}H_{26}O_3$	254	*A. sinensis*	41
E44	Dehydrobaimuxinol	$C_{15}H_{24}O_2$	236	*A. sinensis*	39,43
E45	Isobaimuxinol	$C_{15}H_{26}O_2$	238	*A. sinensis*	38
E46	Baimuxifuranic acid	$C_{15}H_{24}O_3$	252	*A. sinensis*	28,40
E47	(1*S*,2*R*,6*S*,9*R*)-6,10,10-Trimethyl-ll-oxatricyclo[7.2.1.$0^{1,6}$]dodecane-2-carbaldehyde	$C_{15}H_{24}O_2$	236	*A. agallocha*	44
E48	Dihydro-β-agarofuran	$C_{15}H_{26}O$	222	*A. agallocha*	36
E49	α-Agarofuran	$C_{15}H_{24}O$	220	*A. agallocha* *A. malaccensis*	36 24
E50	Epoxy-β-agarofuran	$C_{15}H_{24}O_2$	236	*A. agallocha*	44
E51	4-Hydroxy-dihydro-agarofuran	$C_{15}H_{26}O_2$	238	*A. agallocha*	37
E52	3,4-Dihydroxy-dihydro-agarofuran	$C_{15}H_{26}O_3$	254	*A. agallocha*	37
E53	(1*R*,6*S*,9*R*)-6,10,10-Trimethyl-11-oxatricyclo[7.2.1.$0^{1.6}$]dodecane	$C_{14}H_{24}O$	208	*A. agallocha*	26
E54	(1*R*,2*R*,6*S*,9*R*)-6,10,10-Trimethyl-11-oxatricyclo[7.2.1.$0^{1.6}$]dodecan-2-ol	$C_{14}H_{24}O_2$	224	*A. agallocha*	26
E55	Nor-ketoagarofuran	$C_{14}H_{22}O_2$	222	*A. agallocha*	37

Table S2 Eremophilane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
M1	(1β,4aβ,7β,8aβ)-Octahydro-7-[1-(hydroxymethyl)ethenyl]-1,8a-dimethylnaphthalen-4a(2*H*)-ol	$C_{15}H_{26}O_2$	238	*A. malaccensis* *A. sinensis*	27 28,45
M2	2-[(2β,4aβ,8β,8aβ)-Decahydro-4α-hydroxy-8,8a-dimethylnaphthalen-2-yl]prop-2-enal	$C_{15}H_{24}O_2$	236	*A. malaccensis* *A. sinensis*	27 28
M3	(+)-9β,10β-Epoxyeremophila-11(13)-en	$C_{15}H_{24}O$	220	*A. sinensis*	28
M4	(1a*β*,2*β*,3*β*,4a*β*,5*β*,8a*β*)-Octahydro-4a,5-dimethyl-3-(1-methylethenyl)-3*H*-naphth[1,8*a*-b]oxiren-2-ol	$C_{15}H_{24}O_2$	236	*A. malaccensis*	27
M5	(1β,3α,4aβ,5β,8aα)-4,4a-Dimethyl-6(prop-l-en-2-yl)octahydronaphtha-lene-1,8a(1*H*)-diol	$C_{15}H_{26}O_2$	238	*A. crassna*	34
M6	Eremophila-9,11(13)-dien-12-ol	$C_{15}H_{24}O$	220	*A. agallocha*	46
M7	Valenc- or eremophil-9-en-12-al (tentative)	$C_{15}H_{24}O$	220	*A. agallocha*	46
M8	Jinkoh-eremol	$C_{15}H_{26}O$	222	*A. malaccensis*	47
M9	Eremophil-9-ene-11,12,13-triol	$C_{15}H_{26}O_3$	254	*Aquilaria* spp.	48
M10	4β,7α-*H*-Eremophil-9(10)-ene-12,13-diol	$C_{15}H_{26}O_2$	238	*G. salicifolia*	20
M11	4β,7α-*H*-Eremophil-9(10)-ene-11,12,13-triol	$C_{15}H_{26}O_3$	254	*G. salicifolia*	20
M12	Eremophil-9(10)-ene-11,12-diol	$C_{15}H_{26}O_2$	238	*G. salicifolia*	20
M13	*rel*-4β,5β,7β-Eremophil-9-en-12,8α-olide	$C_{15}H_{22}O_2$	234	*G. salicifolia*	49
M14	8,12-Epoxy-eremophila-9,11(13)-diene	$C_{15}H_{22}O$	218	*A. agallocha*	46
M15	11,13-Dihydroxy-9(10)-ene-8β,12-epoxyemophilane	$C_{15}H_{24}O_3$	252	*A. crassna* *Aquilaria* spp.	35 48
M16	4β,7α,8α-*H*-Eremophil-9(10)-ene-8,12-epoxy-11α,13-diol	$C_{15}H_{24}O_3$	252	*G. salicifolia*	20
M17	Cyclodebneyol	$C_{15}H_{24}O_2$	236	*A. sinensis*	50
M18	(–)-Eremophila-9-en-8β,11-diol	$C_{15}H_{26}O_2$	238	*A. sinensis* *A. crassna*	28 34
M19	Ligudicin C	$C_{15}H_{24}O_2$	236	*A. sinensis*	32,51
M20	7β-*H*-9(10)-Ene-11,12-epoxy-8-oxoeremophilane	$C_{15}H_{22}O_2$	234	*A. sinensis*	41

No.	Name	Formula	MW	Source or origin	Ref.
M21	7α-*H*-9(10)-Ene-11,12-epoxy-8-oxoeremophilane	$C_{15}H_{22}O_2$	234	*A. sinensis* *A. crassna*	41,45,51 35
M22	Petafolia B	$C_{15}H_{22}O_2$	234	*A. sinensis*	30
M23	Neopetasane [Eremophila-9,11-dien-8-one]	$C_{15}H_{22}O$	218	*A. agallocha* *A. malaccensis* *A. sinensis*	23 52 30,32,41,45,51
M24	(+)-(4*S*,5*R*)-Dihydrokaranone [7(11)-Eremophilen-8-one]	$C_{15}H_{22}O$	218	*A. sinensis* *A. agallocha*	30,32,42,43,51 22,53
M25	(+)-(4*S*,5*R*)-Karanone	$C_{15}H_{20}O$	216	*A. agallocha*	22
M26	Dehydro-jinkoh-eremol	$C_{15}H_{24}O$	220	*A. agallocha*	23
M27	4β,7α-*H*-Eremophil-1(2),9(10)-dien-11,12,13-triol	$C_{15}H_{24}O$	220	*G. salicifolia*	20
M28	4β,7α-*H*-11,13-Dihydroxy-eremophil-1(10)-ene-11-methyl ester	$C_{16}H_{26}O_4$	282	*G. salicifolia*	20
M29	(+)-*trans*-Nootkatol	$C_{15}H_{24}O$	220	*G. salicifolia*	20
M30	Methyl crassicid	$C_{16}H_{26}O_4$	282	*A. crassna*	54
M31	2-[(2β,8β,8aα)-8,8a-Dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]-3-hydroxy-2-methoxypropanoic acid	$C_{16}H_{26}O_4$	282	*A. crassna*	34
M32	Kusunol [Valerianol]	$C_{15}H_{26}O$	222	*A. malaccensis* *A. agallocha* *A. sinensis*	46 22 43,45
M33	2-[(2β,8α,8aα)-8,8a-Dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propane-1,2-diol	$C_{15}H_{26}O_2$	238	*A. crassna*	34
M34	(4*S*,5*R*,7*R*)-11,12-Dihydroxy-eremophila-1(10)-ene-2-oxo-11-methylester	$C_{16}H_{24}O_5$	296	*A. crassna*	51
M35	11-Hydroxy-valenc-1(l0)-en-2-one	$C_{15}H_{24}O_2$	236	*A. sinensis*	28,30,45
M36	(+)-11-Hydroxyvalenc-1(10),8-dien-2-one	$C_{15}H_{22}O_2$	234	*A. sinensis*	28
M37	Valenca-1(10),8-dien-11-ol	$C_{15}H_{24}O$	220	*A. agallocha*	46
M38	2,*t*-3-dimethyl-*r*-2-(3-methyl-2-butenyl)-1-cyclohexanone [*rel*-(2*R*,3*S*)-2,3-Dimethyl-2-(3-methyl-2-butenyl)-1-cyclohexanone]	$C_{13}H_{22}O$	194	*A. agallocha*	44

Table S3 Guaiane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
G1	α-Guaiene	$C_{15}H_{24}$	204	*A. agallocha*	22
G2	α-Bulnesene	$C_{15}H_{24}$	204	*A. agallocha*	22
G3	(–)-Guaia-1(10),11-dien-15-al	$C_{15}H_{22}O$	218	*A. agallocha*	22,55
G4	(–)-Guaia-1(10),11-dien-15-ol	$C_{15}H_{24}O$	220	*A. agallocha*	55
G5	(–)-Guaia-1(10),11-diene-15-carboxylic acid	$C_{15}H_{22}O_2$	234	*A. agallocha*	55
G6	Methyl guaia-1(10),11-diene-15-carboxylate	$C_{16}H_{24}O_2$	248	*A. agallocha*	55
G7	(–)-1,10-Epoxyguai-11-ene	$C_{15}H_{24}O$	220	*A. agallocha*	55
G8	(+)-Guaia-1(10),11-dien-9-one	$C_{15}H_{22}O$	218	*A. agallocha*	55
G9	(–)-Guaia-1(10),11-dien-15,2-olide	$C_{15}H_{20}O_2$	232	*A. agallocha*	55
G10	(–)-2α-Hydroxyguaia-1(10),11-dien-15-oic acid	$C_{15}H_{22}O_3$	250	*A. agallocha*	56
G11	(–)-Rotundone	$C_{15}H_{22}O$	218	*A. agallocha*	55
G12	(+)-1,5-Epoxy-nor-ketoguaiene	$C_{14}H_{20}O_2$	220	*A. agallocha*	23
G13	Chamaejasmone E	$C_{16}H_{20}O_5$	292	*A. malaccensis*	57
G14	Chamaejasmone D	$C_{15}H_{22}O_3$	250	*A. malaccensis*	57
G15	Auranticanol A	$C_{15}H_{20}O_3$	248	*A. malaccensis*	57
G16	(+)-12,13-Dihydroxyguaiol	$C_{15}H_{26}O_3$	254	*Aquilaria* spp.	48
G17	*Epi*-guaidiol A	$C_{15}H_{26}O_2$	238	*A. sinensis*	50
G18	α-Kessyl alcohol	$C_{15}H_{26}O_2$	238	*A. sinensis*	58
G19	Qinan-guaiane-one	$C_{15}H_{20}O_3$	248	*A. sinensis*	58

No.	Name	Formula	MW	Source or origin	Ref.
G20	Qinanol A	$C_{15}H_{26}O_2$	238	*A. sinensis*	59
G21	Qinanol B	$C_{15}H_{26}O_2$	238	*A. sinensis*	59
G22	Qinanol C	$C_{15}H_{26}O_3$	254	*A. sinensis*	59
G23	Qinanol D	$C_{15}H_{26}O_3$	254	*A. sinensis*	59
G24	Qinanol E	$C_{15}H_{26}O_3$	254	*A. sinensis*	59
G25	Sinenofuranol	$C_{15}H_{26}O_2$	238	*A. sinensis*	42,59
G26	Sinenofuranal	$C_{15}H_{24}O_2$	236	*A. sinensis*	42
G27	3-Oxo-7-hydroxylholosericin A	$C_{15}H_{20}O_5$	280	*A. sinensis*	45
G28	1,5;8,12-Diepoxyguaia-12-one	$C_{15}H_{22}O_3$	250	*A. sinensis*	45
G29	1α-Hydroxy-4α,10α-dimethyl-5β*H*-octahydro-azulen-8-one	$C_{12}H_{20}O_2$	196	*A. sinensis*	31
G30	1α-Hydroxy-4β*H*-5β*H*-7β*H*-11α*H*-8,9-secoguaia-9(10)-en-8,12-olide	$C_{15}H_{24}O_4$	268	*A. sinensis*	31
G31	1,10-Dioxo-4α*H*-5α*H*-7β*H*-11α*H*-1,10-secoguaia-2(3)-en-12,8β-olide	$C_{15}H_{20}O_4$	264	*A. sinensis*	31
G32	7β*H*-Guaia-1(10)-en-12,8β-olide	$C_{15}H_{20}O_3$	248	*A. sinensis*	31
G33	Qinanlactone	$C_{15}H_{22}O_4$	266	*A. sinensis*	58
G34	1,8-Epoxy-5*H*-guaia-9-en-12,8-olide	$C_{15}H_{20}O_3$	248	*A. filaria*	60
G35	1(5)-Ene-7,10-epoxy-guaia-12-one	$C_{15}H_{20}O_3$	248	*A. filaria*	60
G36	4β,5α,7α,8α-*H*-3β-Hydroxy-1(10)-ene-8,12-epoxy-guaia-12-one	$C_{15}H_{22}O_3$	250	*G. salicifolia*	20
G37	Guaianolide	$C_{15}H_{22}O_2$	234	*G. salicifolia* *A. filaria*	20 60
G38	(−)-Gweicurculactone	$C_{15}H_{16}O_2$	228	*G. salicifolia*	20
G39	(4*R*,5*S*)-3-Oxo-5,6-dihydro-gweicurculactone	$C_{15}H_{16}O_3$	244	*A. filaria*	60

No.	Name	Formula	MW	Source or origin	Ref.
G40	(4*R*)-3-Oxo-gweicurculactone	$C_{15}H_{14}O_3$	242	*A. filaria*	60
G41	2-Oxoguaia-1(10),3,5,7(11),8-pentaen-12,8-olide	$C_{15}H_{12}O_3$	240	*G. salicifolia* *A. filaria*	20 60

Table S4 Agarospirane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
S1	Agarospirol	$C_{15}H_{26}O$	222	*A. agallocha* *A. malaccensis* *A. sinensis*	44,63 47 43,64
S2	Baimuxinol	$C_{15}H_{26}O_2$	238	*A. sinensis*	30
S3	Baimuxinic acid	$C_{15}H_{24}O_3$	252	*A. sinensis*	42,64
S4	Baimuxinal [Oxoagarospirol]	$C_{15}H_{24}O_2$	236	*A. sinensis* *A. malaccensis* *A. agallocha*	28,31,42,43,64 24,52 22
S5	(4*R*,5*R*,7*R*)-1(10)-spirovetiven-11-ol-2-one	$C_{15}H_{24}O_2$	236	Kyara 1st (Vietnam)	65
S6	2-Oxo-12-hydroxy-hinesol	$C_{15}H_{24}O_3$	252	*A. sinensis*	50
S7	Isoagarospirol	$C_{15}H_{26}O$	222		1
S8	Vetispira-2(11),6(14)-dien-7-ol	$C_{15}H_{24}O$	220	*A. agallocha*	46
S9	Vetispira-2(11),6-dien-14-al	$C_{15}H_{22}O$	218	*A. agallocha*	46
S10	2,14-Epoxy-vetispir-6-ene	$C_{15}H_{24}O$	220	*A. agallocha*	46
S11	2,14-Epoxy-vetispira-6(14),7-diene	$C_{15}H_{22}O$	218	*A. agallocha*	46
S12	*rel*-(2*R*,5*R*,10*S*)-6(7)-Spirovetiven-11,12,13-triol	$C_{15}H_{26}O_3$	254	*Aquilaria* spp.	48

Table S5 Acorane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
R1	4-*Epi*-10-hydroxyacoronene	$C_{15}H_{24}O_2$	236	*A. sinensis*	58
R2	4-*Epi*-15-hydroxyacorenone	$C_{15}H_{24}O_2$	236	*A. sinensis*	45,58
R3	15-Hydroxyacorenone	$C_{15}H_{24}O_2$	236	*A. snensis*	28

Table S6 Cadinane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
C1	*cis*-7-Hydroxycalamenen	$C_{15}H_{22}O$	218	*A. sinensis*	66
C2	(7β,8β,9β)-8,9-Epoxycalamenen-10-one	$C_{14}H_{16}O_2$	216	*A. crassna*	35

Table S7 Prezizaane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
P1	Agarozizanol B	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	68
P2	Jinkohol Ⅱ	$C_{15}H_{26}O$	222	*A. malaccensis* *Aquilaria* spp.	47 68
P3	Aquilarene D	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	69
P4	Aquilarene E	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	69
P5	Jinkoholic acid	$C_{15}H_{24}O_2$	236	*Aquilaria* spp.	68
P6	Agarozizanol D	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	68
P7	Jinkohol	$C_{15}H_{26}O$	222	*A. malaccensis* *Aquilaria* spp.	67 68
P8	Agarozizanol C	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	68
P9	Aquilarene A	$C_{15}H_{26}O_2$	238	*Aquilaria* spp.	69

No.	Name	Formula	MW	Source or origin	Ref.
P10	Aquilarene C	$C_{15}H_{26}O_3$	254	*Aquilaria* spp.	69
P11	Aquilarene B	$C_{15}H_{24}O_3$	252	*Aquilaria* spp.	69
P12	Agarozizanol A	$C_{15}H_{24}O_2$	236	*Aquilaria* spp.	68
P13	Aquilarene H	$C_{15}H_{24}O$	220	*Aquilaria* spp.	69
P14	Aquilarene I	$C_{15}H_{24}O_2$	236	*Aquilaria* spp.	69
P15	Aquilarene G	$C_{15}H_{24}O$	220	*Aquilaria* spp.	69
P16	Aquilarene J	$C_{15}H_{22}O_2$	234	*Aquilaria* spp.	69
P17	Aquilarene F	$C_{14}H_{20}O_2$	220	*Aquilaria* spp.	69

Table S8 Zizaane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
Z1	Agarozizanol E	$C_{15}H_{24}O$	220	*Aquilaria* spp.	68
Z2	Agarozizanol F	$C_{15}H_{24}O_2$	236	*Aquilaria* spp.	68
Z3	Isokhusenol	$C_{15}H_{24}O$	220	*Aquilaria* spp.	68

Table S9 Humulane-type sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
H1	Aquilanol A	$C_{15}H_{24}O_2$	236	*A. malaccensis*	57
H2	Aquilanol B	$C_{15}H_{24}O_3$	252	*A. malaccensis*	57
H3	12-Hydroxyhumula-2*Z*,6*E*,9*E*-triene	$C_{15}H_{24}O$	220	*A. malaccensis*	57
H4	14-Hydroxy-α-humulene	$C_{15}H_{24}O$	220	*A. sinensis*	28

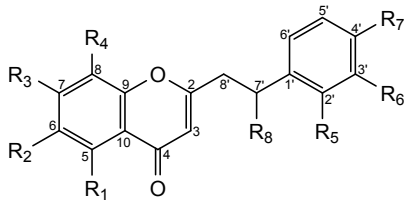
Table S10 Other sesquiterpenes identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
O1	Daphnauranol D	$C_{16}H_{22}O_4$	278	*A. malaccensis*	57
O2	Daphnauranol B	$C_{15}H_{20}O_3$	248	*A. malaccensis*	57
O3	Daphnauranol C	$C_{15}H_{20}O_2$	232	*A. malaccensis*	57
O4	12-Hydroxy-dihydrocyperolone	$C_{15}H_{26}O_3$	254	*G. salicifolia*	49
O5	Malacinone A	$C_{17}H_{24}O_5$	308	*A. malaccensis*	70
O6	Malacinone B	$C_{17}H_{24}O_5$	308	*A. malaccensis*	70
O7	1,5,9-Trimethyl-1,5,9-cyclododecatriene	$C_{15}H_{24}$	204	*A. sinensis*	45

Table S11 Distribution of sesquiterpenoids in agarwood from different origins

No.	Sesquiterpenoid skeleton		*A. sinensis*	*A. agallocha*	*A. malaccensis*	*A. crassna*	*A. filaria*	*A.* spp.	*G. salicifolia*
1	eudesmane	–	30	15	5	4	–	–	1
		nor-sesquiterpenes	–	7	–	–	–	–	–
2	eremophilane	–	14	9	6	8	–	–	8
		nor-sesquiterpenes	–	1	–	–	–	–	–
		(1) bearing 7-isopropenyl moiety	1	10	–	–	–	–	–
		(2) patchoulanes	–	–	3	–	–	–	–
		(3) possessing a 5,11-epoxy ring	7	–	–	–	–	–	–
3	guaiane	(4) bearing a five-membered lactone ring	3	–	–	–	3	–	2
			2	–	–	–	–	–	–
			–	–	–	–	3	–	2
		(5) nor-sesquiterpenes	1	1	–	–	–	–	–
		(6) others	3	1	–	–	–	1	–
4	agarospirane		5	6	2	–	–	1	–
5	acorane		3	–	–	–	–	–	–
6	cadinane		1	–	0	1	–	–	–
7	prezizaane		–	–	2	–	–	17	–
8	zizaane		–	–	–	–	–	3	–
9	humulane		1	–	3	–	–	–	–
10	others	with a rare 5/6/7 ring skeleton	–	–	3	–	–	–	–
		with a rearranged eudesmane skeleton	–	–	–	–	–	1	–
		with a 6/6/5 ring skeleton	–	–	2	–	–	–	–
		with a large ring	1	–	–	–	–	–	–
		total	72	50	26	13	6	23	13

Table S12 Flindersia 2-(2-phenylethyl)chromones identified in agarwood



No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
1	2-(2-Phenylethyl)chromone [flidersiachromone]									$C_{17}H_{14}O_2$	250	Vietnam *A. agallocha* *A. sinensis* *A. malaccensis* *A. crassna* *A. filaria* *G. salicifolia* *Aquilaria* spp.(Indonesia)	72 22 50,51,73-77 52,78,79 80 60,81 82 83
2	5-Hydroxy-2-(2-phenylethyl) chromone	OH								$C_{17}H_{14}O_3$	266	*A. sinensis* *A. malaccensis*	76 79
3	6-Hydroxy-2-(2-phenylethyl)chromone [AH_3]		OH							$C_{17}H_{14}O_3$	266	Kalimantan *A. sinensis* *A. malaccensis* *A. filaria* *G. salicifolia* *A. crassna* *Aquilaria* spp.(Indonesia)	84 32,73-75,77,85-87 52,79 81 88 89,90 83
4	7-Hydroxy-2-(2-phenylethyl)chromone			OH						$C_{17}H_{14}O_3$	266	*A. malaccensis*	78
5	8-Hydroxy-2-(2-phenylethyl)chromone				OH					$C_{17}H_{14}O_3$	266	*A. sinensis* *A. filaria* *A. malaccensis*	91 81 79
6	2-[2-(2-Hydroxyphenyl)ethyl]chromone [Qinanone F]					OH				$C_{17}H_{14}O_3$	266	*A. sinensis* *A. malaccensis*	75 79
7	2-[2-(3-Hydroxyphenyl)ethyl]chromone [Qinanone E]						OH			$C_{17}H_{14}O_3$	266	*A. sinensis*	75
8	2-[2-(4-Hydroxyphenyl)ethyl]chromone [Qinanone D]							OH		$C_{17}H_{14}O_3$	266	*A. sinensis*	75,92
9	(*R*)-2-(2-Hydroxy-2-phenylethyl)chromone								*R*-OH	$C_{17}H_{14}O_3$	266	*A. crassna* *A. sinensis* *A. filaria*	89 77,93 81
10	(*S*)-2-(2-Hydroxy-2-phenylethyl)chromone								*S*-OH	$C_{17}H_{14}O_3$	266	*A. crassna* *A. filaria*	89 81
11	6-Methoxy-2-(2-phenylethyl)chromone [AH_4]		OCH_3							$C_{18}H_{16}O_3$	280	Kalimantan *A. sinensis* *A. agallocha* *A. malaccensis* *A. crassna* *Aquilaria* spp.(Indonesia)	84 43,73,74 53 52,79 80 83
12	7-Methoxy-2-(2-phenylethyl)-4*H*-chromen-4-one			OCH_3						$C_{18}H_{16}O_3$	280	*A. malaccensis* *A. sinensis*	27,79 32,51,76

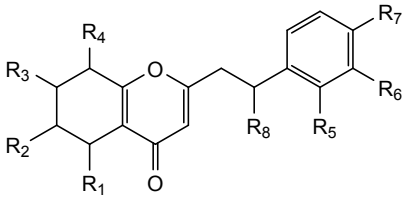
No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
13	2-[2-(4-Methoxyphenyl)ethyl]chromone							OCH_3		$C_{18}H_{16}O_3$	280	Vietnam *A. agallocha* *A. malaccensis* *A. sinensis* *A. crassna*	72 22,94 27,79 75,76,95 80
14	5,6-Dihydroxy-2-(2-phenylethyl)chromone	OH	OH							$C_{17}H_{14}O_4$	282	*A. crassna* *A. malaccensis*	96 79
15	5,8-Dihydroxy-2-(2-phenylethyl)chromone [AH_7]	OH			OH					$C_{17}H_{14}O_4$	282	Kalinantan *A. sinensis* *G. salicifolia*	97 76,95,98 82
16	5-Hydroxy-2-[2-(2-hydroxyphenyl)ethyl]chromone	OH				OH				$C_{17}H_{14}O_4$	282	*A. crassna*	99
17	6,7-Dihydroxy -2-(2-phenylethyl)chromone		OH	OH						$C_{17}H_{14}O_4$	282	*G. salicifolia* *Aquilaria* spp.(Indonesia) *A. sinensis*	19 100 50
18	6,8-Dihydroxy-2-(2-phenylethyl)chromone		OH		OH					$C_{17}H_{14}O_4$	282	*A. malaccensis* *A. sinensis* *A. filaria* *G. salicifolia* *Aquilaria* spp.(Indonesia)	78 77,87,95 81 82 100
19	6-Hydroxy-2-[2-(2-hydroxyphenyl)ethyl]chromone		OH			OH				$C_{17}H_{14}O_4$	282	*A. malaccensis* *A. sinensis*	78 75,77,85
20	6-Hydroxy-2-[2-(4-hydroxyphenyl)ethyl]chromone		OH					OH		$C_{17}H_{14}O_4$	282	*A. malaccensis* *A. sinensis* *A. filaria* *G. salicifolia* *A. crassna*	78 85,86,92 81 19 99
21	6-Hydroxy-2-(2-hydroxy-2-phenylethyl)chromone		OH						OH	$C_{17}H_{14}O_4$	282	*A. sinensis*	74,93
22	2-[2-Hydroxy-2-(4-hydroxyphenyl)ethyl]chromone							OH	OH	$C_{17}H_{14}O_4$	282	*A. sinensis*	91
23	5-Hydroxy-6-methoxy-2-(2-phenylethyl)chromone	OH	OCH_3							$C_{18}H_{16}O_4$	296	*A. sinensis* *A. malaccensis*	74 27,79
24	6-Hydroxy-5-methoxy-2-(2-phenylethyl)chromone	OCH_3	OH							$C_{18}H_{16}O_4$	296	*A. sinensis*	51
25	6-Hydroxy-7-methoxy-2-(2-phenylethyl)chromone		OH	OCH_3						$C_{18}H_{16}O_4$	296	*A. malaccensis* *A. sinensis* *A. filaria*	78 32,51,86 81
26	6-Methoxy-7-hydroxy-2-(2-phenylethyl) chromone		OCH_3	OH						$C_{18}H_{16}O_4$	296	*A. sinensis*	93,101
27	6-Methoxy-8-hydroxy-2-(2-phenylethyl) chromone		OCH_3		OH					$C_{18}H_{16}O_4$	296	*A. crassna*	102
28	6-Methoxy-2-[2-(2-hydroxyphenyl)ethyl]chromone		OCH_3			OH				$C_{18}H_{16}O_4$	296	*A. crassna*	96
29	6-Methoxy-2-[2-(3-hydroxyphenyl)ethyl]chromone		OCH_3				OH			$C_{18}H_{16}O_4$	296	*A. crassna*	96
30	6-Methoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone [Aquilarone H]		OCH_3					OH		$C_{18}H_{16}O_4$	296	*A. sinensis*	87,103
31	6-Hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone		OH					OCH_3		$C_{18}H_{16}O_4$	296	*A. sinensis* *A. crassna* *A. filarial* *G. salicifolia* *A. malaccensis*	73,75,86,87,92,95 80,90 81 88 79
32	7-Hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone			OH				OCH_3		$C_{18}H_{16}O_4$	296	*A. sinensis*	51
33	7-Methoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone			OCH_3				OH		$C_{18}H_{16}O_4$	296	*A. sinensis* *A. crassna*	51 104

No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
34	2-[2-(2-Hydroxy-4-methoxyphenyl)ethyl]chromone [Qinanone C]					OH		OCH_3		$C_{18}H_{16}O_4$	296	*A. sinensis*	75
35	2-[2-(3-Hydroxy-4-methoxyphenyl)ethyl]chromone [Qinanone A]						OH	OCH_3		$C_{18}H_{16}O_4$	296	*A. sinensis*	75
36	2-[2-(3-Methoxy-4-hydroxyphenyl)ethyl]chromone [Qinanone B]						OCH_3	OH		$C_{18}H_{16}O_4$	296	*A. sinensis* *A. crassna*	75,92 89
37	2-[2-Hydroxy -2-(4-methoxyphenyl)ethyl]chromone							OCH_3	OH	$C_{18}H_{16}O_4$	296	*A. sinensis* *A. crassna*	91 89
38	6-Hydroxy-8-chloro-2-(2-phenylethyl)chromone		OH		Cl					$C_{17}H_{13}ClO_3$	300	*A. sinensis* *A. filaria* *G. salicifolia* *A. crassna* *A. malaccensis*	76,93,105 81 88 54 79
39	6,7-Dimethoxy-2-(2-phenylethyl)chromone [AH_6]		OCH_3	OCH_3						$C_{19}H_{18}O_4$	310	Kalinantan *A. sinensis* *A. agallocha* Kyara 1st (Vietnam) *A. malaccensis* *A. crassna* *A. filaria* *Aquilaria* spp.(Indonesia)	84 32,43,51,73,74,77,87, 91,101 53 65 52,79 80,90 81 83
40	6-Methoxy-2-[2-(3-methoxyphenyl)ethyl]chromone [AH_5]		OCH_3				OCH_3			$C_{19}H_{18}O_4$	310	Kalimantan *A. sinensis* *A. malaccensis*	84 32,73,74,77,87 27,79
41	6-Methoxy-2-[2-(4-methoxyphenyl)ethyl]chromone		OCH_3					OCH_3		$C_{19}H_{18}O_4$	310	*A. agallocha* *A. sinensis* *A. malaccensis* *A. crassna*	22,94 43,73,87,95 27 80
42	5,8-Dihydroxy-6-methoxy-2-(2-phenylethyl)chromone	OH	OCH_3		OH					$C_{18}H_{16}O_5$	312	*A. sinensis*	106
43	5,8-Dihydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone	OH			OH			OCH_3		$C_{18}H_{16}O_5$	312	*A. sinensis* *G. salicifolia*	98 82
44	6-Hydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]chromone [Aquilarone I]		OH				OH	OCH_3		$C_{18}H_{16}O_5$	312	*A. sinensis* *A. crassna* *Aquilaria* spp.(Indonesia)	75,92,93,103,107 80 83
45	6-Hydroxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl]chromone		OH				OCH_3	OH		$C_{18}H_{16}O_5$	312	*A. sinensis* *G. salicifolia* *Aquilaria* spp.(Indonesia) *Aquilaria* spp.	75,93,107,108 82 100 68
46	6,7-Dihydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone		OH	OH				OCH_3		$C_{18}H_{16}O_5$	312	*A. sinensis* *G. salicifolia* *Aquilaria* spp.(Indonesia)	107,109 19 100
47	6-Hydroxy-7-methoxy-2-[2-(4-hydrxoyphenyl)ethyl] chromone		OH	OCH_3				OH		$C_{18}H_{16}O_5$	312	*A. sinensis* *G. salicifolia* *Aquilaria* spp.	93,109 82 110
48	6,8-Dihydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone		OH		OH			OCH_3		$C_{18}H_{16}O_5$	312	*A. sinensis* *Aquilaria* spp.(Indonesia) *G. salicifolia* *Aquilaria* spp.	95,107 100 88 68
49	7-Hydroxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl] chromone			OH			OCH_3	OH		$C_{18}H_{16}O_5$	312	*A. sinensis*	92

No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
50	6-Hydroxy-8-chloro-2-[2-(4-hydroxyphenyl)ethyl]chromone		OH		Cl			OH		$C_{17}H_{13}ClO_4$	316	*Aquilaria* spp.	110
51	5-Hydroxy-6-methoxy-2-[2-(3-methoxyphenyl)ethyl] chromone	OH	OCH_3				OCH_3			$C_{19}H_{18}O_5$	326	*A. sinensis*	32
52	5-Hydroxy-6-methoxy-2-[2-(4-methoxyphenyl)ethyl] chromone	OH	OCH_3					OCH_3		$C_{19}H_{18}O_5$	326	*A. malaccensis* *A. sinensis* *A. crassna*	27 87 80
53	6-Hydroxy-5-methoxy-2-[2-(4-methoxyphenyl)ethyl] chromone	OCH_3	OH					OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis*	32
54	5-Hydroxy-7-methoxy-2-[2-(4-methoxyphenyl)ethyl] chromone	OH		OCH_3				OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis*	106
55	5-Hydroxy-8-methoxy-2-[2-(4-methoxyphenyl)ethyl] chromone	OH			OCH_3			OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis*	95
56	6-Hydroxy-2-[2-(3,4-dimethoxyphenyl)ethyl]chromone		OH				OCH_3	OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis*	92,107
57	6-Methoxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl] chromone		OCH_3				OCH_3	OH		$C_{19}H_{18}O_5$	326	*A. malaccensis* *A. sinensis* *A. crassna* *Aquilaria* spp.(Indonesia) *G. salicifolia*	78 32,77,87,101 80,90 100 88
58	6-Methoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone		OCH_3				OH	OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis* *A. crassna* *Aquilaria* spp.(Indonesia)	87 80,90 83
59	6-Hydroxy-7-methoxy-2-[2-(4-methoxyphenyl)ethyl] chromone		OH	OCH_3				OCH_3		$C_{19}H_{18}O_5$	326	*A. sinensis* *G. salicifolia* *A. filaria*	107 19 81
60	6-Methoxy-7-hydroxy-2-[2-(4-methoxyphenyl)ethyl] chromone		OCH_3	OH				OCH_3		$C_{19}H_{18}O_5$	326	*A. malaccensis* *A. sinensis* *A. crassna*	52 92,95,107 99,102
61	6,7-Dimethoxy-2-[2-(2-hydroxyphenyl)ethyl]chromone		OCH_3	OCH_3		OH				$C_{19}H_{18}O_5$	326	*A. sinensis*	32,77
62	6,7-Dimethoxy-2-[2-(3-hydroxyphenyl)-ethyl]chromone		OCH_3	OCH_3			OH			$C_{19}H_{18}O_5$	326	*A. sinensis*	92
63	6,7-Dimethoxy-2-[2-(4-hydroxyphenyl)ethyl]chromone [Qinanone G]		OCH_3	OCH_3				OH		$C_{19}H_{18}O_5$	326	*A. sinensis*	77,91,92,107
64	(*R*)-6,7-Dimethoxy-2-(2-hydroxy-2-phenylethyl)chromone		OCH_3	OCH_3					*R*-OH	$C_{19}H_{18}O_5$	326	*A. sinensis*	93,107
65	(*S*)-6,7-Dimethoxy-2-(2-hydroxy-2-phenylethyl)chromone		OCH_3	OCH_3					*S*-OH	$C_{19}H_{18}O_5$	326	*A. sinensis*	93,107
66	7-Methoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone			OCH_3			OH	OCH_3		$C_{19}H_{18}O_5$	326	*A. crassna*	104
67	8-Chloro-6-hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone		OH		Cl			OCH_3		$C_{18}H_{15}ClO_4$	330	*A. sinensis* *A. crassna*	93,105 54,90
68	7-Chloro-8-hydroxy-2-[2-(4-methoxyphenyl)ethyl]chromone			Cl	OH			OCH_3		$C_{18}H_{15}ClO_4$	330	*A. sinensis*	32
69	6,7-Dimethoxy-2-[2-(4-methoxyphenyl)ethyl]chromone [AH_8]		OCH_3	OCH_3				OCH_3		$C_{20}H_{20}O_5$	340	Kalinantan *A. sinensis* *A. malaccensis* *A. crassna*	97 32,33,43,51,86,98,101 52 99
70	5,8-Dimethoxy-2-[2-(3-acetoxyphenyl)ethyl]chromone	OCH_3			OCH_3		$OCOCH_3$			$C_{21}H_{20}O_6$	368	*A. agallocha*	53
71	5,6-Dihydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone	OH	OH				OH	OCH_3		$C_{18}H_{16}O_6$	328	*A. sinensis*	51
72	5,8-Dihydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone	OH			OH		OH	OCH_3		$C_{18}H_{16}O_6$	328	*G. salicifolia*	19
73	6,8-Dihydrxoy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone		OH		OH		OH	OCH_3		$C_{18}H_{16}O_6$	328	*A. sinensis*	103,109

No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
74	6,8-Dihydroxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl] chromone		OH		OH		OCH_3	OH		$C_{18}H_{16}O_6$	328	*A. sinensis*	111
75	8-Chloro-6-hydroxy-2-[2-(3-hydroxy-4-methoxyphenyl) ethyl]chromone		OH		Cl		OH	OCH_3		$C_{18}H_{15}ClO_5$	346	*A. sinensis* *A. crassna*	77,93,107 90
76	6-Methoxy-2-[2-(3,4,5-trihydroxyphenyl)ethyl]chromone		OCH_3			OH	OH	OH		$C_{18}H_{16}O_6$	328	*A. sinensis*	106
77	5-Hydroxy-6-methoxy-2-[2-(3-hydroxy-4-methoxyphenyl) ethyl]chromone	OH	OCH_3				OH	OCH_3		$C_{19}H_{18}O_6$	342	*A. sinensis* *A. crassna*	87 99
78	5-Methoxy-6-hydroxy-2-[2-(3-hydroxy-4-methoxyphenyl) ethyl]chromone	OCH_3	OH				OH	OCH_3		$C_{19}H_{18}O_6$	342	*A. sinensis*	107
79	6-Hydroxy-7-methoxy-2-[2-(3-hydroxy-4-methoxyphenyl) ethyl]chromone		OH	OCH_3			OH	OCH_3		$C_{19}H_{18}O_6$	342	*A. sinensis* *G. salicifolia* *Aquilaria* spp.(Indonesia) *Aquilaria* spp.	92,103,107,109 82 83 68
80	6-Hydroxy-7-methoxy-2-[2-(3-methoxy-4-hydroxyphenyl) ethyl]chromone [Aquilarone G]		OH	OCH_3			OCH_3	OH		$C_{19}H_{18}O_6$	342	*A. sinensis* *Aquilaria* spp.(Indonesia)	103 83
81	6-Methoxy-7-hydroxy-2-[2-(3-hydroxy-4-methoxyphenyl) ethyl]chromone		OCH_3	OH			OH	OCH_3		$C_{19}H_{18}O_6$	342	*A. sinensis* *G. salicifolia* *Aquilaria* spp.	109 82 68
82	7-Hydroxyl-6-methoxyl-2-[2-(4-hydroxyl-3-methoxyl-phenyl)ethyl]chromone		OCH_3	OH			OCH_3	OH		$C_{19}H_{18}O_6$	342	*A. sinensis*	112
83	5-Hydroxy-6,7-dimethoxy-2-[2-(4-methoxyphenyl)ethyl] chromone	OH	OCH_3	OCH_3				OCH_3		$C_{20}H_{20}O_6$	356	*A. sinensis*	76
84	6,7-Dimethoxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl] chromone		OCH_3	OCH_3			OH	OCH_3		$C_{20}H_{20}O_6$	356	*A. sinensis* *A. crassna*	92,107,109 99
85	6,7-Dimethoxy-2-[2-(3-methoxy-4-hydroxylphenyl)ethyl] chromone		OCH_3	OCH_3			OCH_3	OH		$C_{20}H_{20}O_6$	356	*A. sinensis* *Aquilaria* spp.(Indonesia)	92,107,109 83
86	2-[2-(4-Glucosyloxy-3-methoxyphenyl)ethyl]chromone						OCH_3	Glu		$C_{24}H_{26}O_9$	458	*A. sinensis*	113

Table S13 5,6,7,8-Tetrahydro-2-(2-phenylethyl)chromones identified in agarwood



No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
87	6,7-Dihydroxy-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromone		*α*-OH	*α*-OH						$C_{17}H_{18}O_6$	286	*A. sinensis* *Aquilaria* spp.(Indonesia)	74 83
88	6,7-Dihydroxy-5,6,7,8-tetrahydro-2-(2-(4-methoxy phenyl)ethyl)chromone		*α*-OH	*α*-OH				OCH_3		$C_{18}H_{20}O_5$	316	*A. crassna*	116
89	(6*S*,7*S*,8*S*)-6,7,8-Trihydroxyl-2-(4-hydroxyl-3-methoxylphenylethyl)-5,6,7,8-tetrahydro-4*H*-chromen-4-one		*α*-OH	*α*-OH	*α*-OH		OCH_3	OH		$C_{18}H_{20}O_7$	348	*A. sinensis*	112
90	(6*S*,7*S*,8*S*)-6,7,8-Trihydroxyl-2-(3-hydroxyl-4-methoxylphenylethyl)-5,6,7,8-tetrahydro-4*H*-chromen-4-one.		*α*-OH	*α*-OH	*α*-OH		OH	OCH_3		$C_{18}H_{20}O_7$	348	*A. sinensis*	112
91	(6*S*,7*S*,8*R*)-6,7-Dihydroxy-8-chloro-5,6,7,8-tetra hydro-2-(2-(3-hydroxy-4-methoxyphenyl)ethyl) chromone		*α*-OH	*α*-OH	*β*-Cl		OH	OCH_3		$C_{18}H_{19}ClO_6$	366	*A. crassna*	116
92	*rel*-(5*R*,6*S*,7*R*)-5,6,7,8-Tetrahydro-5,6,7-trihydroxy-2-(2-phenylethyl)-4*H*-1-benzopyran-4-one	*α*-OH	*α*-OH	*β*-OH						$C_{17}H_{18}O_5$	302	*A. malaccensis*	52
93	(5*S*,6*S*,7*R*)-5,6,7-Trihydroxy-2-[2-(hydroxylphenyl) ethyl]-5,6,7,8-tetrahydrochromone [AH_9]	*α*-OH	*β*-OH	*α*-OH		OH				$C_{17}H_{18}O_6$	318	Kalimantan	97
94	*rel*-(5*R*,6*S*,7*R*)-5,6,7,8-Tetrahydro-5,6,7-trihydroxy-2-[2-(4-methoxyphenyl)ethyl]-4*H*-1-benzopyran-4-one	*α*-OH	*α*-OH	*β*-OH				OCH_3		$C_{18}H_{20}O_6$	332	*A. malaccensis*	52
95	(5*S*,6*R*,7*S*)-5,6,7-trihydroxy-2-(3-hydroxy-4-methoxy phenylethyl)-5,6,7,8-tetrahydro-4*H*-chromen-4-one	*α*-OH	*α*-OH	*β*-OH			OH	OCH_3		$C_{18}H_{20}O_7$	348	*A. sinensis*	117
96	(5*S*,6*R*,7*R*)-5,6,7-trihydroxy-2-(3-hydroxy-4-methoxy phenylethyl)-5,6,7,8-tetrahydro-4H-chromen-4-one	*α*-OH	*α*-OH	*α*-OH			OH	OCH_3		$C_{18}H_{20}O_7$	348	*A. sinensis*	76,117
97	(6*R*,7*S*,8*S*)-6,7,8-Trihydroxy-2-(4-hydroxyl-3methoxylphenethyl)-5,6,7,8-tetrahydro-4*H*-chromen-4-one.	*β*-OH	*β*-OH	*β*-OH			OCH_3	OH		$C_{18}H_{20}O_7$	348	*A. sinensis*	76
98	Aquilarone B	*α*-OH	*α*-OH	*α*-OH	*β*-OH					$C_{17}H_{18}O_6$	318	*A. sinensis* *Aquilaria* spp.(Indonesia)	76,103,118 83
99	Agarotetrol [AH_1]	*α*-OH	*β*-OH	*β*-OH	*α*-OH					$C_{17}H_{18}O_6$	318	*A. agallocha* Kalimantan *Aquilaria* spp.(Indonesia) *A. sinensis* *Aquilaria* spp.	119 120 100 10, 118 110
100	Isoagarotetrol [AH_2]	*α*-OH	*β*-OH	*α*-OH	*β*-OH					$C_{17}H_{18}O_6$	318	Kalimantan *A. sinensis* *Aquilaria* spp.(Indonesia)	120 74 83
101	(5*R*,6*R*,7*S*,8*R*)-2-(2-Phenylethyl)-tetrahydroxy-5,6,7,8-tetrahydrochromone [AH_{16}]	*β*-OH	*β*-OH	*α*-OH	*β*-OH					$C_{17}H_{18}O_6$	318	Kalimantan *A. sinensis* *G. salicifolia*	121 10 88

No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
102	5α,6β,7β-Trihydroxy-8α-methoxy-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromone [AH_{17}]	α-OH	β-OH	β-OH	α-OCH_3					$C_{18}H_{20}O_6$	332	Kalimantan *A. sinensis* *G. salicifolia*	122 118 88
103	Tetrahydrochromone B	β-OCH_3	α-OH	α-OH	β-OH					$C_{18}H_{20}O_6$	332	*A. sinensis*	118
104	5α,6β,7β,8α-Tetrahydroxy-2-[2-(2-hydroxyphenyl) ethyl]-5,6,7,8-tetrahydrochromone (AH_{23})	α-OH	β-OH	β-OH	α-OH	OH				$C_{17}H_{18}O_7$	334	Kalimantan	122
105	5α,6β,7α,8β-Tetrahydroxy-2-[2-(2-hydroxyphenyl) ethyl]-5,6,7,8-tetrahydrochromone [AH_{2b}]	α-OH	β-OH	α-OH	β-OH	OH				$C_{17}H_{18}O_7$	334	Kalimantan *A. sinensis* *Aquilaria* spp.(Indonesia)	123 33 83
106	Aquilarone F	α-OH	β-OH	β-OH	α-OH			OH		$C_{17}H_{18}O_7$	334	*A. sinensis* *Aquilaria* spp.(Indonesia)	103 83
107	(5*S*,6*R*,7*S*,8*R*,7'*R*)-7'-Hydroxyisoagarotetrol	α-OH	β-OH	α-OH	β-OH				*R*-OH	$C_{17}H_{18}O_7$	334	Kalimantan	124
108	(5*S*,6*R*,7*S*,8*R*,7'*S*)-7'-Hydroxyisoagarotetrol	α-OH	β-OH	α-OH	β-OH				*S*-OH	$C_{17}H_{18}O_7$	334	Kalimantan	124
109	(5*S*,6*S*,7*S*,8*S*)-8-Chloro-5,6,7-trihydroxy-2-(phenyl ethyl)-5,6,7,8-tetrahydrochromone	α-OH	α-OH	α-OH	α-Cl					$C_{17}H_{17}ClO_5$	336	*A. sinensis*	76
110	8-Chloro-2-(2-phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydrochromone	α-OH	α-OH	α-OH	β-Cl					$C_{17}H_{17}ClO_5$	336	*A. sinensis* *Aquilaria* spp.(Indonesia) *Aquilaria* spp.	32,74,76 83 68
111	5α,6β,7α,8β-Tetrahydroxy-2-[2-(4-methoxyphenyl) ethyl]-5,6,7,8-tetrahydrochromone [AH_{2a}]	α-OH	β-OH	α-OH	β-OH			OCH_3		$C_{18}H_{20}O_7$	348	Kalimantan *A. sinensis* *Aquilaria* spp.(Indonesia)	123 50,85 83
112	5α,6β,7β,8α-Tetrahydroxy-2-[2-(4-methoxyphenyl) ethyl]-5,6,7,8-tetrahydrochromone [AH_{1A}] [4'-Methoxy-agarotetrol]	α-OH	β-OH	β-OH	α-OH			OCH_3		$C_{18}H_{20}O_7$	348	Kalimantan *A. sinensis* *Aquilaria* spp.	123 118,125 110
113	Aquilarone C	α-OH	α-OH	α-OH	β-OH			OCH_3		$C_{18}H_{20}O_7$	348	*A. sinensis* *Aquilaria* spp.(Indonesia)	76,103,118 83
114	(5*R*,6*S*,7*S*,8*R*)-2-[2-(4-Methoxyphenyl)ethyl]-5,6,7,8-tetrahydroxy-5,6,7,8-tetrahydrochromone	β-OH	α-OH	α-OH	β-OH			OCH_3		$C_{18}H_{20}O_7$	348	*Aquilaria* spp.(Indonesia)	83
115	Tetrahydrochromone E	α-OH	β-OH	β-OH	α-OCH_3			OCH_3		$C_{19}H_{22}O_7$	362	*A. sinensis*	118
116	(5*R*,6*S*,7*S*,8*R*)-5,6,7-Trihydroxy-8-methoxy-5,6,7,8-tetrahydro-2-(2-(4-methoxyphenyl)ethyl)chromone	β-OH	α-OH	α-OH	β-OCH_3			OCH_3		$C_{19}H_{22}O_7$	362	*A. crassna*	116
117	Tetrahydrochromone F	α-OCH_3	α-OH	α-OH	β-OH			OCH_3		$C_{19}H_{22}O_7$	362	*A. sinensis* *A. crassna*	118 99
118	Tetrahydrochromone A	α-OCH_3	β-OH	β-OH	α-OH			OCH_3		$C_{19}H_{22}O_7$	362	*A. sinensis*	118
119	Tetrahydrochromone G	β-OCH_3	β-OH	β-OH	α-OH			OCH_3		$C_{19}H_{22}O_7$	362	*A. sinensis*	118
120	5,6,7,8-Tetrahydroxy-2-(3-hydroxy-4-methoxy phenethyl)-5,6,7,8-tetrahydro-4*H*-chromen-4-one	α-OH	α-OH	β-OH	α-OH		OH	OCH_3		$C_{18}H_{20}O_8$	364	*A. sinensis*	126
121	Aquilarone A	α-OH	α-OH	α-OH	β-OH		OH	OCH_3		$C_{18}H_{20}O_8$	364	*A. sinensis* *Aquilaria* spp.(Indonesia)	103,118 83
122	Aquilarone D	α-OH	β-OH	α-OH	β-OH		OH	OCH_3		$C_{18}H_{20}O_8$	364	*A. sinensis* *Aquilaria* spp.(Indonesia)	33,103 83
123	Aquilarone E	α-OH	β-OH	β-OH	α-OH		OH	OCH_3		$C_{18}H_{20}O_8$	364	*A. sinensis*	103,118
124	(5*R*,6*S*,7*S*,8*R*)-2-[2-(3-Hydroxy-4-methoxyphenyl) ethyl]-5,6,7,8-tetrahydroxy-5,6,7,8-tetrahydro chromone	β-OH	α-OH	α-OH	β-OH		OH	OCH_3		$C_{18}H_{20}O_8$	364	*Aquilaria* spp.(Indonesia)	83
125	(5*R*,6*S*,7*S*,8*R*)-2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]-5,6,7,8-tetrahydroxy-5,6,7,8-tetrahydrochromone	β-OH	α-OH	α-OH	β-OH		OCH_3	OH		$C_{18}H_{20}O_8$	364	*Aquilaria* spp.(Indonesia)	83

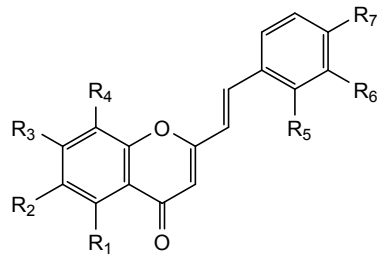
No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	Formula	MW	Source or origin	Ref.
126	*rel*-(5*R*,6*S*,7*S*,8*R*)-8-Chloro--5,6,7,8-tetrahydro-5,6,7-trihydroxy-2-[2-(4-methoxyphenyl)ethyl]-4*H*-1-benzopyran-4-one	*α*-OH	*β*-OH	*β*-OH	*α*-Cl			OCH_3		$C_{18}H_{19}ClO_6$	366	*A. malaccensis* *A. sinensis*	52 118
127	(5*R*,6*R*,7*R*,8*S*)-8-Chloro-5,6,7-trihydroxy-2-(4-methoxy phenethyl)-5,6,7,8-tetrahydrochromone	*β*-OH	*β*-OH	*β*-OH	*α*-Cl			OCH_3		$C_{18}H_{19}ClO_6$	366	*A. sinensis* *Aquilaria* sp	76 68
128	(5*R*,6*R*,7*R*,8*R*)-8-Chloro-5,6,7-trihydroxy-2-(4-methoxyphenethyl)-5,6,7,8-tetrahydrochromone	*β*-OH	*β*-OH	*β*-OH	*β*-Cl			OCH_3		$C_{18}H_{19}ClO_6$	366	*A. sinensis*	76
129	Tetrahydrochromone H	*α*-OCH_3	*α*-OH	*α*-OH	*β*-OH		OH	OCH_3		$C_{19}H_{22}O_8$	378	*A. sinensis*	118
130	Tetrahydrochromone C	*α*-OCH_3	*β*-OH	*β*-OH	*α*-OH		OH	OCH_3		$C_{19}H_{22}O_8$	378	*A. sinensis*	118
131	Tetrahydrochromone D	*α*-OCH_3	*β*-OH	*β*-OH	*α*-Cl			OCH_3		$C_{19}H_{21}ClO_6$	380	*A. sinensis*	118
132	Tetrahydrochromone I	*α*-OCH_3	*α*-OH	*α*-OH	*β*-Cl			OCH_3		$C_{19}H_{21}ClO_6$	380	*A. sinensis*	118
133	8-Chloro-5,6,7-trihydroxy-2-(3-hydroxy-4-methoxy phenethyl)-5,6,7,8-tetrahydro-4*H*-chromon-one	*α*-OH	*α*-OH	*α*-OH	*β*-Cl		OH	OCH_3		$C_{18}H_{19}ClO_7$	382	*A. sinensis*	127
134	*rel*-(5*R*,6*S*,7*S*,8*R*)-8-Chloro-5,6,7,8-tetrahydro-5,6,7-trihydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-4*H*-1-benzopyran-4-one	*α*-OH	*β*-OH	*β*-OH	*α*-Cl		OH	OCH_3		$C_{18}H_{19}ClO_7$	382	*A. malaccensis* *A. sinensis*	52 50
135	Tetrahydrochromone J	*α*-OCH_3	*α*-OH	*α*-OH	*β*-Cl		OH	OCH_3		$C_{19}H_{21}ClO_7$	396	*A. sinensis*	118

Table S14 Mono- and diepoxy-5,6,7,8-tetrahydro-2-(2-phenylethyl)chromones identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
136	*rel*-(1a*R*,2*R*,3*R*,7b*S*)-1a,2,3,7b-Tetrahydro-2,3-dihydroxy-5-(2-phenylethyl)-7*H*-oxireno[*f*] [1]benzopyran-7-one	$C_{17}H_{16}O_5$	300	*A. malaccensis* *A. sinensis*	52,79 32,87
137	*rel*-(1a*R*,2*R*,3*R*,7b*S*)-1a,2,3,7b-Tetrahydro-2,3-dihydroxy-5-[2-(4-methoxyphenyl)ethyl]-7*H*-oxireno[*f*] [1]benzopyran-7-one	$C_{18}H_{18}O_6$	330	*A. malaccensis* *A. sinensis* *A. crassna*	52 76 102
138	*rel*-(1a*R*,2*R*,3*R*,7b*S*)-1a,2,3,7b-Tetrahydro-2,3-dihydroxy-5-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-7*H*-oxireno[*f*][1]benzopyran-7-one	$C_{18}H_{18}O_7$	346	*A. malaccensis* *A. sinensis*	52 87
139	5α,6α-Epoxy-7β,8α,3′-trihydroxy-4′-methoxy-2-(2-phenylethyl)chromone	$C_{18}H_{18}O_7$	346	*A. sinensis*	106
140	5,6-Epoxy-7β-hydroxy-8β-methoxy-2-(2-phenylethyl)chromone	$C_{18}H_{18}O_5$	314	*A. sinensis*	87
141	Tetrahydrochromone K	$C_{17}H_{16}O_5$	300	*A. sinensis*	118
142	Tetrahydrochromone L	$C_{18}H_{18}O_6$	330	*A. sinensis*	118

No.	Name	Formula	MW	Source or origin	Ref.
143	(5*R*,6*S*,7*S*,8*S*)-2-[2-(4′-Methoxyphenyl)ethyl]-7,8-epoxy-5-methoxy-6-hydroxy-5,6,7,8-tetrahydrochromone	$C_{19}H_{20}O_6$	344	*A. sinensis* *A. crassna*	128 102
144	Tetrahydrochromone M	$C_{18}H_{18}O_7$	346	*A. sinensis*	118
145	(5*S*,6*S*,7*S*,8*S*)-2-[2-(4′-Methoxyphenyl)ethyl]-7,8-epoxy-5,6-dihydroxy-5,6,7,8-tetrahydrochromone	$C_{18}H_{18}O_6$	330	*A. sinensis*	128
146	(5*S*,6*S*,7*S*,8*S*)-2-[2-(4′-Methoxyphenyl)ethyl]-7,8-epoxy-5-methoxy-6-hydroxy-5,6,7,8-tetrahydrochromone	$C_{19}H_{20}O_6$	344	*A. sinensis*	128
147	(5*S*,6*S*,7*S*,8*S*)-2-[2-(3′-Hydroxy-4′-methoxyphenyl)ethyl]-7,8-epoxy-5-methoxy-6-hydroxy-5,6,7,8- tetrahydrochromone	$C_{19}H_{20}O_7$	360	*A. sinensis*	128
148	(5*S*,6*R*,7*S*,8*S*)-2-[2-(4′-Methoxyphenyl)ethyl]-6,7-epoxy-5,8-dihydroxy-5,6,7,8-tetrahydrochromone	$C_{18}H_{18}O_6$	330	*A. sinensis*	128
149	Oxidoagarochromone A	$C_{17}H_{14}O_4$	282	*A. crassna* *A. malaccensis* *A. sinensis*	129 52 32,87
150	Oxidoagarochromone B	$C_{18}H_{16}O_5$	312	*A. crassna* *A. malaccensis* *A. sinensis*	90,129 52 32,87
151	Oxidoagarochromone C	$C_{18}H_{16}O_6$	328	*A. crassna* *A. malaccensis* *A. sinensis*	129 52 118

Table S15 2-(2-Phenylethenyl)chromones identified in agarwood



No.	Name	R_1	R_2	R_3	R_4	R_5	R_6	R_7	Formula	MW	Source or origin	Ref.
152	5-Hydroxy-2-[2-(4-methoxy phenyl)ethenyl]chromone	OH						OCH_3	$C_{18}H_{14}O_4$	294	*G. salicifolia* *A. filaria*	19 60
153	5-Hydroxy-2-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]chromone	OH					OH	OCH_3	$C_{18}H_{14}O_5$	310	*G. salicifolia*	13
154	6-Hydroxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethenyl]chromone		OH				OCH_3	OH	$C_{18}H_{14}O_5$	310	*A. sinensis* *Aquilaria* spp.	50,109 110
155	6,7-Dimethoxy-2-[2-(4-hydroxy phenyl)ethenyl]-4H-chromen-4-one		OCH_3	OCH_3				OH	$C_{19}H_{16}O_5$	324	*A. sinensis*	77
156	(*E*)-2-[2-(3-Methoxy-4-hydroxy phenyl)ethenyl]chromone						OCH_3	OH	$C_{18}H_{14}O_4$	294	*A. crassna*	104
157	(*E*)-6-Methoxy-2-[2-(4-hydroxy phenyl)ethenyl]chromone		OCH_3					OH	$C_{18}H_{14}O_4$	294	*A. crassna*	104
158	(*E*)-6-Methoxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethenyl] chromone		OCH_3				OCH_3	OH	$C_{19}H_{16}O_5$	324	*A. crassna*	104

Table S16 Bi-2-(2-phenylethyl)chromones with C–C bond identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
159	2,2′-Di-(2-phenylethyl)-8,6′-dihydroxy-5,5′-bichromone [AH_{11}]	$C_{34}H_{26}O_6$	530	Kalimantan *A. sinensis*	135 140
160	Aquisinenone O	$C_{35}H_{28}O_7$	560	*A. sinensis*	140
161	Crassin A	$C_{36}H_{30}O_8$	590	*A. crassna* *A. sinensis*	139 140
162	7,4′-Dimethoxyaquisinenone O	$C_{37}H_{32}O_9$	620	*A. sinensis*	140

Table S17 Bi-2-(2-phenylethyl)chromones with C–O–C bond identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
163	(5*S*,6S,7*R*,8*S*)-2-(2-Phenylethyl)-6,7,8-trihydroxy-5,6,7,8-tetrahydro-5-[2-(2-phenylethy)chromonyl-6-oxy]chromone [AH_{10}]	$C_{34}H_{30}O_8$	566	Kalimantan *A. sinensis*	135 74
164	(5*S*,6*R*,7*S*,8*S*)-2-(2-Phenylethyl)-6,7,8-trihydroxy-5,6,7,8-tetrahydro-5-[2-(2-phenylethy)chromonyl-6-oxy]chromone [AH_{14}]	$C_{34}H_{30}O_8$	566	Kalimantan *A. sinensis*	137 66,74
165	(5*S*,6*S*,7*R*,8*S*)-2-(2-Phenylethyl)-6,7,8-trihydroxy-5,6,7,8-tetrahydro-5-[2-(2-phenylethyl)-7-hydroxy-chromonyl-6-oxy]chromone [AH_{15}]	$C_{34}H_{30}O_9$	582	Kalimantan	136
166	Aquilasinenone K	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
167	(5*S*,6*R*,7*R*,8*S*)-2-(2-Phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-[2-(2-phenylethy)chromonyl-6-oxy]chromone [AH_{13}]	$C_{34}H_{30}O_8$	566	Kalimantan	137

No.	Name	Formula	MW	Source or origin	Ref.
168	(5*R*,6*R*,7*R*,8*S*)-2-(2-Phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-[2-(2-phenylethy)-7-methoxychromonyl-6-oxy]chromone [AH_{12}]	$C_{35}H_{32}O_9$	596	Kalimantan	137
169	(5*R*,6*R*,7*R*,8*S*)-2-(2-Phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-[2-(2-phenylethyl)chromonyl-6-oxy]chromone	$C_{34}H_{30}O_8$	566	*A. sinensis*	142
170	Aquilasinenone J	$C_{35}H_{32}O_{10}$	612	*A. sinensis*	141
171	(5*S*,6*R*,7*S*,8*R*)-2-(2-Phenylethyl)-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-[2-(2-phenylethyl)chromonyl-6-oxy]chromone	$C_{34}H_{30}O_8$	566	*A. sinensis*	142
172	(5*S*,6*R*,7*S*,8*R*)-2-[2-(4-Methoxyphenyl)ethyl]-5,6,7-trihydroxy5,6,7,8-tetrahydro-8-{2-[2-(4‴-methoxyphenyl)ethyl]chromonyl-6-oxy}chromone	$C_{36}H_{34}O_{10}$	626	*A. sinensis*	142
173	Aquisinenone N	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	140
174	Crassin B	$C_{35}H_{32}O_9$	596	*A. crassna*	139
175	Crassin D	$C_{37}H_{36}O_{11}$	656	*A. crassna*	139
176	Aquisinenone M	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	140
177	Crassin C	$C_{37}H_{36}O_{11}$	656	*A. crassna*	139
178	Aquilasinenone I	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	141
179	(5*S*,6*R*,7*S*,8*R*)-2-[2-(4-Methoxyphenyl)ethyl]-5,6,7-trihydroxy-5,6,7,8-tetrahydro-8-{6-methoxy-2-[2-(3‴-methoxy-4‴-hydroxyphenyl)ethyl]chromonyl-7-oxy}chromone	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	142
180	Aquilasinenone F	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
181	Aquilasinenone G	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
182	Aquilasinenone H	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
183	Aquilasinenone E	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	141
184	Aquilasinenone D	$C_{37}H_{36}O_{12}$	672	*A. sinensis*	141

No.	Name	Formula	MW	Source or origin	Ref.
185	Aquilasinenone A	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
186	Aquilasinenone B	$C_{37}H_{36}O_{13}$	688	*A. sinensis*	141
187	Aquilasinenone C	$C_{36}H_{34}O_{13}$	674	*A. sinensis*	141
188	Aquisinenone L	$C_{34}H_{29}ClO_7$	584	*A. sinensis*	140
189	Aquisinenone I	$C_{34}H_{28}O_7$	548	*A. sinensis*	140
190	7″-Methoxyaquisinenone I	$C_{35}H_{30}O_8$	578	*A. sinensis*	140
191	4′,7″-Dimethoxyaquisinenone I	$C_{36}H_{32}O_9$	608	*A. sinensis*	140
192	4′,7″,4‴-Trimethoxyaquisinenone I	$C_{37}H_{34}O_{10}$	638	*A. sinensis*	140
193	Aquisinenone H	$C_{35}H_{30}O_8$	578	*A. sinensis*	140
194	4′-Methoxyaquisinenone	$C_{36}H_{32}O_9$	608	*A. sinensis*	140
195	Aquisinenone J	$C_{36}H_{32}O_9$	608	*A. sinensis*	140
196	4′-Methoxyaquisinenone J	$C_{37}H_{34}O_{10}$	638	*A. sinensis*	140
197	Aquisinenone K	$C_{34}H_{30}O_9$	582	*A. sinensis*	140
198	4′,4‴-Dimethoxyaquisinenone K	$C_{36}H_{34}O_{11}$	642	*A. sinensis*	140

Table S18 Bi-2-(2-phenylethyl)chromones with double C–O–C bonds identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
199	AH_{21}	$C_{34}H_{28}O_8$	564	Kalimantan	138
200	(−)-Aquisinenone G	$C_{34}H_{28}O_8$	564	*A. sinensis*	143

201	(+)-4′-Methoxyaquisinenone G	$C_{35}H_{30}O_9$	594	*A. sinensis*	143
202	Crassin E	$C_{35}H_{30}O_9$	594	*A. crassna*	144
203	Crassin F	$C_{35}H_{30}O_9$	594	*A. crassna*	144
204	Crassin G	$C_{36}H_{32}O_{10}$	624	*A. crassna*	144

Table S19 Bi-2-(2-phenylethyl)chromones with C–O–C and C–C bond identified in agarwood

No.	**Name**	**Formula**	**MW**	**Source or origin**	**Ref.**
205	(+)-Aquisinenone A	$C_{34}H_{28}O_7$	548	*A. sinensis* *A. crassna*	143 12
206	(−)-Aquisinenone A	$C_{34}H_{28}O_7$	548	*A. sinensis* *A. crassna*	143 12
207	(−)-4′-Methoxyaquisinenone A	$C_{35}H_{30}O_8$	578	*A. sinensis*	143
208	Aquisinenone Q	$C_{36}H_{32}O_9$	608	*A. crassna*	12
209	(+)-Aquisinenone B	$C_{34}H_{28}O_7$	548	*A. sinensis*	143
210	(−)-Aquisinenone B	$C_{34}H_{28}O_7$	548	*A. sinensis*	143
211	(−)-6″-Hydroxyaquisinenone B	$C_{34}H_{28}O_8$	564	*A. sinensis*	143
212	(+)-6″-Hydroxy-4′,4‴-dimethoxyaquisinenone B	$C_{36}H_{32}O_{10}$	624	*A. sinensis*	143
213	(+)-Aquisinenone C	$C_{34}H_{28}O_8$	564	*A. sinensis*	143
214	(−)-Aquisinenone C	$C_{34}H_{28}O_8$	564	*A. sinensis*	143
215	Aquisinenone P	$C_{37}H_{34}O_{10}$	638	*A. crassna*	12
216	(+)-Aquisinenone E	$C_{36}H_{32}O_9$	608	*A. sinensis*	143
217	(−)-Aquisinenone F	$C_{35}H_{30}O_8$	578	*A. sinensis*	143
218	(−)-Aquisinenone D	$C_{37}H_{34}O_{10}$	638	*A. sinensis* *A. crassna*	143 12

No.	Name	Formula	MW	Source or origin	Ref.
219	(+)-4′-Demethoxyaquisinenone D	$C_{36}H_{32}O_9$	608	*A. sinensis* *A. crassna*	143 90
220	(−)-4′-Demethoxyaquisinenone D	$C_{36}H_{32}O_9$	608	*A. sinensis* *A. crassna*	143 90
221	Aquisinenone R	$C_{35}H_{30}O_8$	578	*A. crassna*	12
222	(+)-Aquisinenone D	$C_{37}H_{34}O_{10}$	638	*A. crassna*	12
223	3′-Hydroxyaquisinenone D	$C_{37}H_{34}O_{11}$	654	*A. crassna*	116
224	Crassin H	$C_{37}H_{34}O_{11}$	654	*A. crassna*	144

Table S20 Sesquiterpenoid-4*H*-chromone derivatives identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
225	Aquilacrassnin A	$C_{32}H_{38}O_7$	534	*A. crassna*	11
226	Aquilacrassnin B	$C_{32}H_{38}O_7$	534	*A. crassna*	11
227	Aquilacrassnin C	$C_{33}H_{40}O_8$	564	*A. crassna*	11
228	Aquilacrassnin D	$C_{33}H_{40}O_8$	564	*A. crassna*	11
229	Aquilacrassnin E	$C_{32}H_{38}O_7$	534	*A. crassna*	11
230	Aquilacrassnin F	$C_{32}H_{32}O_7$	528	*A. crassna*	11
231	Qinanmer	$C_{32}H_{38}O_8$	550	*A. sinensis*	10

232	Xcrassin A	$C_{33}H_{42}O_7$	550	*A. crassna*	12
233	Xcrassin B	$C_{33}H_{42}O_7$	550	*A. crassna*	12
234	Xcrassin C	$C_{33}H_{38}O_7$	546	*A. crassna*	12

Table S21 Benzylacetone-4*H*-chromone derivatives identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
235	Gyrinone A	$C_{28}H_{28}O_7$	476	*G. salicifolia*	13
236	Gyrinone B	$C_{29}H_{30}O_8$	506	*G. salicifolia*	13

Table S22 Tri-2-(2-phenylethyl)chromones identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
237	(5*S*,6*S*,7*R*,8*S*)-2-(2-Phenylethyl)-6,7,8-trihydroxy-5,6,7,8-tetrahydro-5-[2-(2-phenylethyl)chromonyl-6,7-dioxy]chromone [AH_{18}]	$C_{51}H_{46}O_{14}$	882	Kalimantan	136
238	AH_{19a}	$C_{51}H_{46}O_{14}$	882	Kalimantan	145
239	AH_{19b}	$C_{51}H_{46}O_{14}$	882	Kalimantan	145
240	AH_{20}	$C_{51}H_{46}O_{14}$	882	Kalimantan	122

Table S23 Simple phenolic and miscellaneous compounds identified in agarwood

No.	Name	Formula	MW	Source or origin	Ref.
X1	Benzylacetone	$C_{10}H_{12}O$	148	*A. sinensis*	38,43

No.	Name	Formula	MW	Source or origin	Ref.
X2	*p*-Methoxybenzylacetone [4-(4-Methoxyphenyl)butan-2-one] [Anisyl acetone]	$C_{11}H_{14}O_2$	178	*A. sinensis*	38,43,152
X3	Zingerone	$C_{11}H_{14}O_3$	194	*A. sinensis*	153
X4	Guaiacylacetone	$C_{10}H_{12}O_3$	180	*A. sinensis*	85
X5	*p*-Methoxy phenylpropionic acid	$C_{10}H_{12}O_3$	180	*A. sinensis*	153
X6	4'-Methoxycinnamic acid	$C_{10}H_{10}O_3$	178	*A. sinensis*	33
X7	Methyl (*Z*)-*p*-coumarate	$C_{10}H_{10}O_3$	178	*A. sinensis*	33
X8	Benzenepropanoic acid, 3-hydroxy-4-methoxy-methyl ester	$C_{11}H_{14}O_4$	210	*A. sinensis*	153
X9	Syringin	$C_{17}H_{24}O_9$	372	*A. sinensis*	33
X10	Anisic acid	$C_8H_8O_3$	152	*A. sinensis*	38
X11	5-Hydroxy-7,4′-dimethoxyflavone	$C_{17}H_{14}O_5$	298	*A. sinensis*	153
X12	1-Hydroxy-1,5-diphenylpentan-3-one	$C_{17}H_{18}O_2$	254	*A. malaccensis* *A. sinensis*	27 66
X13	3,3'-(3-Hydroxypropane-1,2-diyl)diphenol	$C_{15}H_{16}O_3$	244	*A. sinensis*	85
X14	Syringaresinol-glycoside	$C_{28}H_{36}O_{13}$	580	*A. sinensis*	66
X15	3-Oxo-22-hydroxyhopane	$C_{30}H_{50}O_2$	442	*A. sinensis*	43
X16	(3β)-Olean-12-ene-3,23-diol	$C_{30}H_{50}O_2$	442	*A. sinensis*	66
X17	(20*R*)-24-Ethylcholest-4-en-3-one	$C_{29}H_{48}O$	412	*A. sinensis*	153

Table S24 Inhibition of LPS induced NO production activity of compounds from agarwood

Compound	Activity (IC_{50}, μM)	Ref.	Compound	Activity (IC_{50}, μM)	Ref.
E4	7.2 ± 0.7	28	**128**	7.3 ± 0.6	76
E8	7.1 ± 0.4	28	**137**	1.6 ± 0.2	76
E13	3.20 ± 0.20	30	**139**	84 ± 2	106
E19	12.8 ± 0.4	28	**159**	7.4 ± 0.1	140
E24	14.20 ± 0.18	30	**160**	7.6 ± 0.2	140
E42	2.50 ± 0.35	30	**162**	2.3 ± 0.4	140
M2	9.3 ± 0.5	28	**176**	37.1 ± 0.5	140
M3	53.8 ± 5.1	28	**188**	8.0 ± 0.3	140
M24	12.50 ± 0.23	30	**189**	1.9 ± 0.2	140
M35	17.3 ± 0.65	30	**190**	1.6 ± 0.1	140
G31	8.1	31	**191**	5.8 ± 0.3	140
15	6.4 ± 0.3	76	**193**	4.3 ± 0.3	140
30	5.95	103	**197**	0.7 ± 0.1	140
44	7.59	103	**198**	0.6 ± 0.1	140
54	4.6 ± 0.1	106	**200**	11.4 ± 0.3	143
73	7.94	103	**201**	8.0 ± 0.4	143
79	6.59	103	**205**	11.5 ± 0.6	143
80	7.94	103	**206**	7.6 ± 0.1	143
98	5.12	103	**207**	9.3 ± 0.3	143
106	13.09	103	**209**	8.8 ± 0.2	143
109	3.8 ± 0.4	76	**210**	8.6 ± 0.2	143
110	4.5 ± 0.9	76	**212**	10.5 ± 0.2	143
113	7.71	103	**217**	12.0 ± 0.5	143
121	9.03	103	**218**	7.0 ± 0.1	143
122	7.49	103	**219**	8.5 ± 0.1	143
123	22.26	103	**220**	8.5 ± 0.4	143
127	4.5 ± 0.5	76			

Table S25 Cytotoxicity of compounds from agarwood

Compound	IC_{50} (cell line)	Ref.
M13	17.85 ± 0.04 μg/mL (K562), 21.82 ± 0.07 μg/mL (BEL-7402)	49
G34	33.8 ± 1.5 μM (K562)	60
G35	48.6 ± 0.7 μM (K562)	60
G39	45.1 ± 1.2 μM (K562)	60
3	26.2 ± 4.8 μM (A549), 19.2 ± 3.2 μM (KB-VIN)	81
17	18.1 μM (K562), 20.1 μM (BEL-7402)	19
20	47.0 μM (K562), 37.95 μg/mL (SMMC-7721), 35.25 μg/mL (MGC-803), 26.98 μg/mL (OV-90), 33.8 ± 0.4 μM (A549), 36.6 ± 0.7 μM (KB-VIN), 29.0 ± 0.5 μM (MCF-7)	19,81,92
36	31.59 μg/mL (SMMC-7721), 33.12 μg/mL (MGC-803), 30.77 μg/mL (OV-90)	92
45	13.20 ± 0.80 μM (K562), 25.91 ± 0.41 μM (BEL-7402), 23.51 ± 0.14 μM (SGC-7901), 22.00 ± 0.90 μM (A549), 30.55±3.04 μM (HeLa)	110
46	22.21 μM (SGC-7901), 8.36 μM (K562), 5.76 μM (BEL-7402)	19,107
47	45.38 ± 1.84 μM (K562), 35.42 ± 1.44 μM (SGC-7901), 33.31 ± 0.68 μM (A549)	110
49	18.82 μg/mL (SMMC-7721), 25.35 μg/mL (MGC-803), 31.60 μg/mL (OV-90)	92
56	21.40 μg/mL (SMMC-7721), 36.42 μg/mL (MGC-803), 35.38 μg/mL (OV-90)	92
57	43.65 μg/mL, 14. 96 ± 0.13 μM (K562)	90,99
58	61.31 ± 0.92 μM (K562), 28.53 ± 0.36 μM (BEL-7402), 17.63 ± 0.70 μM (SGC-7901), 49.42 ± 0.59 μM (HeLa)	99
59	17.8 μM (SGC-7901), 13.9 μM (K562), 31.9 μM (BEL-7402), 25.8 ± 0.7 μM (A549), 26.1 ± 0.7 μM (KB), 21.9 ± 0.4 μM (KB-VIN), 38.1 ± 0.7 μM (MDA-MB-231), 28.7 ± 0.2 μM (MCF-7)	19,81
60	37.64 μM (SGC-7901), 27.08 μg/mL (SMMC-7721), 31.17 μg/mL (MGC-803), 33.51 μg/mL (OV-90)	92,107
62	30.01 μg/mL (SMMC-7721), 35.25 μg/mL (MGC-803), 26.98 μg/mL (OV-90)	92
63	20.01 μg/mL (SMMC-7721), 31.34 μg/mL (MGC-803), 36.64 μg/mL (OV-90)	92
77	11.83 ± 0.15 μM (K562), 25.02 ± 0.09 μM (BEL-7402), 29.29 ± 0.34 μM (SGC-7901), 44.11 ± 0.35 μM (HeLa)	99
84	31.06 μg/mL (SMMC-7721), 28.24 μg/mL (MGC-803), 22.54 μg/mL (OV-90)	92
85	24.85 μg/mL (SMMC-7721), 28.60 μg/mL (MGC-803), 30.40 μg/mL (OV-90)	92

Compound	IC_{50} (cell line)	Ref.
91	49.8 ± 1.2 μM (HeLa)	114
112	35.11 ± 0.43 μM (BEL-7402), 32.95 ± 0.87 μM (SGC-7901)	110
116	42.66 ± 0.47 μM (K562)	114
133	14.6 mg/mL (SGC-7901)	127
137	46.1 μM (SGC-7901), 43.8 μM (A549)	102
154	2.87 ± 0.01 μM (K562), 4.75 ± 0.19 μM (BEL-7402), 9.91 ± 0.09 μM (SGC-7901), 22.43 ± 0.40 μM (A549), 13.86 ± 0.13 μM (HeLa)	110
157	40.81 ± 0.64 μM (K562), 44.18 ± 0.34 μM (BEL-7402)	104
175	73.5 μM (K562)	139
177	70.9 μM (K562)	139
202	44.68 ± 0.10 μM (BEL-7402)	144
204	42.10 ± 0.12 μM (BEL-7402)	144
205	34.20 ± 0.29 μM (SGC-7901), 37.99 ± 0.31 μM (K562), 36.26 ± 0.09 μM (HeLa)	12
206	11.59 ± 0.09 μM (SGC-7901), 22.97 ± 0.13 (A549), 10.93 ± 0.01 μM (K562), 12.88 ± 0.15 μM (HeLa)	12
225	33.9 μM (K562), 29.9 μM (BEL-7402), 26.7 μM (HeLa), 46.3 μM (A549)	11
226	25.7 μM (BEL-7402), 30.6 μM (HeLa)	11
229	24.8 μM (BEL-7402), 30.9 μM (SGC-7901), 17.6 μM (HeLa), 32.0 μM (A549)	11
233	39.95 ± 0.11 μM (SGC-7901), 28.67 ± 0.38 μM (K562), 29.34 ± 0.53 μM (HeLa)	12
234	31.50 ± 0.24 μM (SGC-7901), 49.00 ± 0.57 (A549), 22.12 ± 0.14 μM (K562), 30.75 ± 0.11 μM (HeLa)	12

Table S26 AChE inhibitory activity of compounds from agarwood at 50 μg/mL

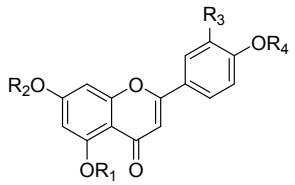
Compound	Inhibition rate (%)	Ref.	Compound	Inhibition rate (%)	Ref.
E22	21.2 ± 0.9	34	**36**	14.9 ± 2.6	75
M10	33.3 ± 1.0	20	**37**	25.4 ± 0.5	91
M18	32.7 ± 1.3	34	**38**	26.9 ± 0.8	88
M20	274.8 μM (IC_{50})	41	**39**	10.8 ± 0.9	87
M21	491.4 μM (IC_{50})	41	**40**	10.1 ± 0.9	87
M23	158.3 μM (IC_{50})	41	**43**	24.0 ± 0.6	20
M31	15.2 ± 0.8	34	**45**	15.0 ± 0.8	75
M34	42.9 ± 0.6	35	**48**	12.2 ± 0.8	107
G18	19.5 ± 0.4	58	**57**	22.0 ± 0.04	90
G19	19.4 ± 2.5	58	**63**	10.0 ± 1.2	91
G20	63.1 ± 1.2	59	**66**	35.0 ± 2.19	104
G21	15.0 ± 1.5	59	**77**	33.6 ± 0.6	87
G22	19.1 ± 2.0	59	**79**	21.6 ± 0.9	20
G25	24.1 ± 1.4	59	**82**	41.47 ± 0.12	112
G33	31.0 ± 0.8	58	**84**	19.6 ± 0.9	107
G36	35.3 ± 1.2	20	**89**	32.11 ± 1.02	112
G38	46.2 ± 0.9	20	**90**	41.27 ± 0.65	112
G41	54.2 ± 1.4	20	**103**	17.5 ± 0.8	118
S6	16.35 ± 3.66	50	**111**	10.61 ± 1.59	50
C1	49.9 ± 1.4	66	**118**	19.1 ± 0.9	118
R1	44.5 ± 2.7	58	**134**	21.10 ± 2.92	50
R2	20.8 ± 2.5	58	**140**	31.5 ± 0.9	87
3	19.3 ± 0.8	87	**141**	47.4 ± 0.9	118
6	14.3 ± 0.9	75	**142**	35.9 ± 0.9	118
7	24.1 ± 0.9	75	**144**	15.8 ± 0.6	118

Compound	Inhibition rate (%)	Ref.	Compound	Inhibition rate (%)	Ref.
8	18.6 ± 0.9	75	**146**	441.6 μM (IC_{50})	128
9	17.4 ± 0.6	89	**147**	155.6 μM (IC_{50})	128
10	15.8 ± 0.7	89	**149**	47.9 ± 0.8	118
15	38.0 ± 1.0	82	**166**	16.82	141
18	11.4 ± 0.5	20	**169**	44.01 ± 4.30	142
22	20.3 ± 1.2	91	**170**	16.80	141
30	23.5 ± 0.8	87	**171**	24.57 ± 3.63	142
31	16.3 ± 0.9	75	**172**	10.85 ± 3.37	142
34	17.0 ± 2.0	75	**178**	15.66	141
35	10.0 ± 2.9	75			

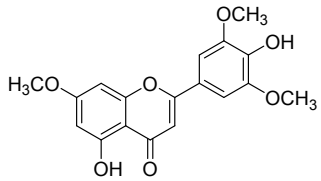
Table S27 Diameters of the inhibition zone (mm) of isolated compounds from agarwood against *S. aureus* and *R. solanacearum*

Compound	*S. aureus*	*R. solanacearum*	Ref.
E4	9.12 ± 0.06	8.98 ± 0.11	29
E5	20.02 ± 0.12	11.02 ± 0.08	29
E8	12.90 ± 0.26	18.20 ± 0.07	29
E9	14.20 ± 0.10	10.15 ± 0.25	29
E10	8.10 ± 0.15	–	29
E31	12.35 ± 0.11	16.90 ± 0.09	35
3	ND	6.80 ± 0.08	89
52	9.10 ± 0.06	–	87
58	10.01 ± 0.08	–	87
149	12.75 ± 0.09	15.40 ± 0.10	87
150	14.95 ± 0.05	12.09 ± 0.06	87
X3	11.20±0.10	7.82 ± 0.09	153

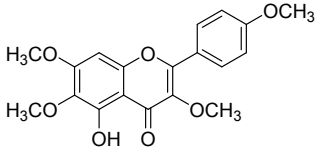
–inactive



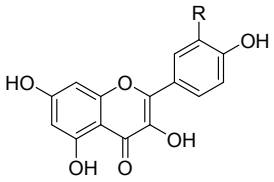
AF1 R_1 = H, R_2 = H, R_3 = H, R_4 = H
AF2 R_1 = H, R_2 = H, R_3 = H, R_4 = CH_3
AF3 R_1 = H, R_2 = H, R_3 = OH, R_4 = H
AF4 R_1 = H, R_2 = CH_3, R_3 = H, R_4 = H
AF5 R_1 = H, R_2 = CH_3, R_3 = H, R_4 = CH_3
AF6 R_1 = H, R_2 = CH_3, R_3 = OH, R_4 = H
AF7 R_1 = H, R_2 = CH_3, R_3 = OH, R_4 = CH_3
AF8 R_1 = H, R_2 = CH_3, R_3 = OCH_3, R_4 = H
AF9 R_1 = H, R_2 = CH_3, R_3 = OCH_3, R_4 = CH_3
AF10 R_1 = CH_3, R_2 = H, R_3 = H, R_4 = CH_3
AF11 R_1 = CH_3, R_2 = CH_3, R_3 = H, R_4 = CH_3
AF12 R_1 = CH_3, R_2 = CH_3, R_3 = OCH_3, R_4 = CH_3



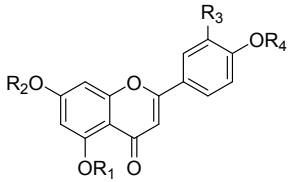
AF13



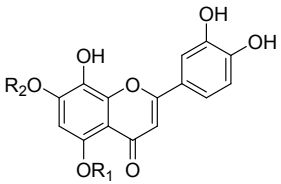
AF14



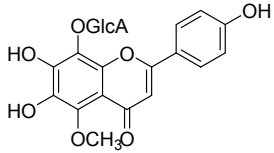
AF15 R = H
AF16 R = OH



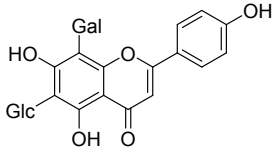
AF17 R_1 = CH_3, R_2 = Glc, R_3 = H, R_4 = H
AF18 R_1 = Glc, R_2 = H, R_3 = H, R_4 = CH_3
AF19 R_1 = Glc, R_2 = CH_3, R_3 = H, R_4 = H
AF20 R_1 = Glc, R_2 = CH_3, R_3 =H, R_4 = CH_3
AF21 R_1 = Glc, R_2 = CH_3, R_3 = OCH_3, R_4 = H
AF22 R_1 = Glc, R_2 = CH_3, R_3 = OCH_3, R_4 = CH_3
AF23 R_1 = Glc(6-1)Xyl, R_2 = H, R_3 =H, R_4 = CH_3
AF24 R_1 = Glc(6-1)Xyl, R_2 = CH_3, R_3 = H, R_4 = H
AF25 R_1 = Glc(6-1)Xyl, R_2 = CH_3, R_3 = H, R_4 = CH_3
AF26 R_1 = Glc(6-1)Xyl, R_2 = CH_3, R_3 = OCH_3, R_4 = H
AF27 R_1 = Glc(6-1)Xyl, R_2 = CH_3, R_3 = OCH_3, R_4 = CH_3



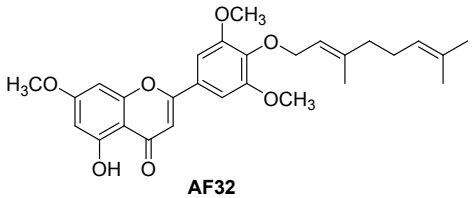
AF28 R_1 = H, R_2 = Glc
AF29 R_1 = GlcA, R_2 = H



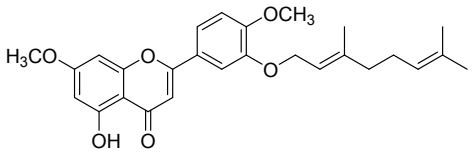
AF30



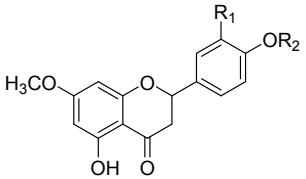
AF31



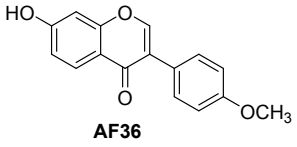
AF32



AF33



AF34 R_1 = H, R_2 = H
AF35 R_1 = OH, R_2 = CH_3



AF36

Fig. S1 Flavonoids identified from *Aquilaria* plants

Table S28 Flavonoids identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AF1	Apigenin	*A. agallocha*	bark flower	$C_{15}H_{10}O_5$	270	186-187
AF2	5,7-Dihydroxy-4'-methoxyflavone	*A. sinensis*	leaf stem	$C_{16}H_{12}O_5$	284	164-166
AF3	Luteolin	*A. sinensis* *A. agallocha*	leaf flower	$C_{15}H_{10}O_6$	286	164,167-168,187
AF4	Genkwanin	*A. sinensis* *A. crassna* *A. agallocha*	bark fruit leaf stem flower	$C_{16}H_{12}O_5$	284	164-165,167-171,179-182,187
AF5	5-Hydroxy-4',7-dimethoxyflavone	*A. sinensis* *A. crassna* *A. agallocha*	bark seed leaf stem bark flower	$C_{17}H_{14}O_5$	298	164-166,169,171-174,183,186-189
AF6	3'-Hydroxygenkwanin	*A. sinensis*	leaf stem	$C_{16}H_{12}O_6$	300	166-168,170,174
AF7	Luteolin-7,4'-dimethyl [Pilloin]	*A. sinensis* *A. agallocha*	leaf bark seed flower	$C_{17}H_{14}O_6$	314	165,168-169,173-174,186-189
AF8	5,4'-Dihyroxy-7,3'-dimethoxyflavone [Velutin]	*A. sinensis* *A. agallocha*	leaf stem flower	$C_{17}H_{14}O_6$	314	171,173-174,180,187

No.	Compound	Source	Part	Formula	MW	Ref.
AF9	5-Hydroxy-7,3',4'-trimethoxyflavone [Luteolin-7,3',4'-trimethyl]	*A. sinensis* *A. agallocha*	bark seed leaf stem flower	$C_{18}H_{16}O_6$	328	165-166,168-174,186-189
AF10	7-Hydroxy-5,4'-dimethoxyflavone	*A. sinensis*	leaf	$C_{17}H_{14}O_5$	298	171
AF11	5,7,4'-Trimethoxyflavone	*A. sinensis*	leaf	$C_{18}H_{16}O_5$	312	165
AF12	5,7,3',4'-Tetramethoxyflavone	*A. sinensis*	leaf	$C_{19}H_{18}O_6$	342	165
AF13	Tricin	*A. sinensis*	stem	$C_{18}H_{16}O_7$	344	174
AF14	5-Hydroxy-3,6,7,4'-tetramethoxyflavone	*A. sinensis*	leaf	$C_{19}H_{18}O_7$	358	165
AF15	Kaempferol	*A. sinensis* *A. agallocha*	leaf flower	$C_{15}H_{10}O_6$	286	172,187
AF16	Quercetin	*A. sinensis*	leaf	$C_{15}H_{10}O_7$	302	172
AF17	7-β-D-Glucoside of 5-*O*-methylapigenin	*A. sinensis*	leaf	$C_{22}H_{22}O_{10}$	446	167
AF18	7-Hydroxy-4'-methyl-5-*O*-glucosideflavonoid	*A. sinensis*	stem	$C_{22}H_{22}O_{10}$	446	166
AF19	Genkwanin-5-*O*-β-glucoside	*A. sinensis* *A. crassna*	fruit leaf	$C_{22}H_{22}O_{10}$	446	164,171,179
AF20	7,4'-Dimethyl-5-*O*-glucosideflavonoide	*A. sinensis*	stem	$C_{23}H_{24}O_{10}$	460	166
AF21	7,3'-Dimethyl-4'-hydroxy-5-*O*-glucosideflavonoide 5-β-D-Glucoside of 7,3'-di-*O*-methylluteodin	*A. sinensis*	leaf stem	$C_{23}H_{24}O_{11}$	476	166-167
AF22	Lethedoside A	*A. sinensis*	stem	$C_{24}H_{26}O_{11}$	490	166
AF23	Aquilarinoside A_1	*A. sinensis*	stem	$C_{27}H_{30}O_{14}$	578	166
AF24	Genkwanin-5-*O*-β-D-primeveroside	*A. sinensis* *A. crassna*	fruit leaf stem	$C_{27}H_{30}O_{14}$	578	167,176,179,181,184-185
AF25	7,4'-Dimethylapigenin-5-*O*-xylosylglucoside	*A. sinensis* *A. crassna*	leaf stem	$C_{28}H_{32}O_{14}$	592	166-167,170
AF26	Aquisiflavoside	*A. sinensis*	leaf	$C_{28}H_{32}O_{15}$	608	177

No.	Compound	Source	Part	Formula	MW	Ref.
AF27	Lethedioside A	*A. sinensis*	stem	$C_{29}H_{34}O_{15}$	622	166
AF28	Hypolaetin-7-*O*-β-D-glucopyranoside	*A. sinensis*	leaf	$C_{21}H_{20}O_{12}$	464	164
AF29	Hypolaetin 5-*O*-β-D-glucuronopyranoside	*A. sinensis*	leaf	$C_{21}H_{18}O_{13}$	478	178
AF30	Aquilarisin	*A. sinensis*	leaf	$C_{22}H_{20}O_{13}$	492	178
AF31	8-*C*-β-D-galactopyranosylisovitexin	*A. sinensis*	leaf	$C_{27}H_{30}O_{15}$	594	164
AF32	4'-*O*-Geranyltricin	*A. sinensis*	stem	$C_{28}H_{32}O_{7}$	480	174
AF33	3'-*O*-Geranylpolloin	*A. sinensis*	stem	$C_{27}H_{30}O_{6}$	450	174
AF34	Sakuranetin	*A. sinensis*	stem	$C_{16}H_{14}O_{5}$	286	174
AF35	Persicogenin	*A. sinensis* *A. agallocha*	bark seed	$C_{17}H_{16}O_{6}$	316	169,186,189
AF36	Formononetin	*A. sinensis*	stem	$C_{16}H_{12}O_{4}$	268	166

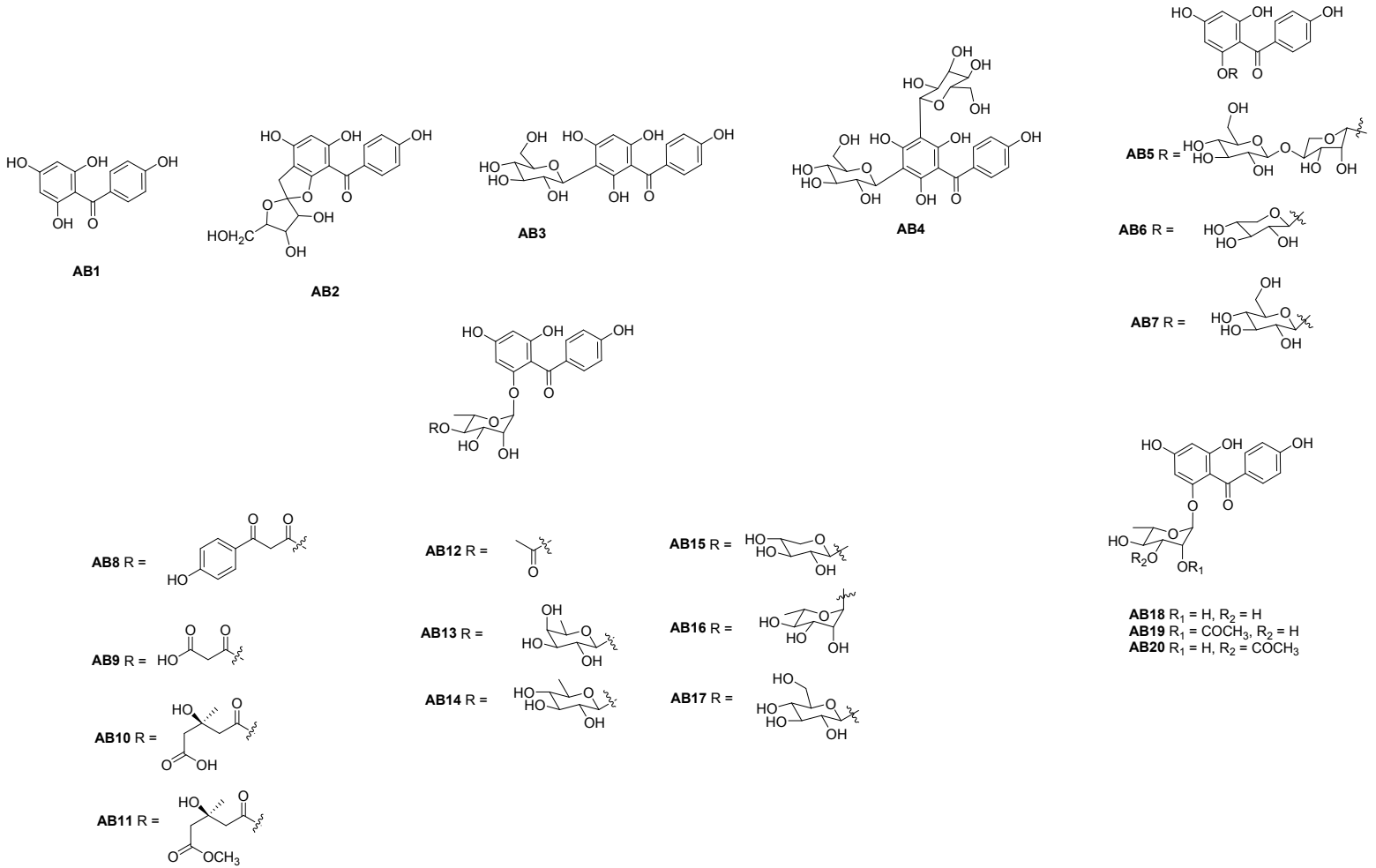
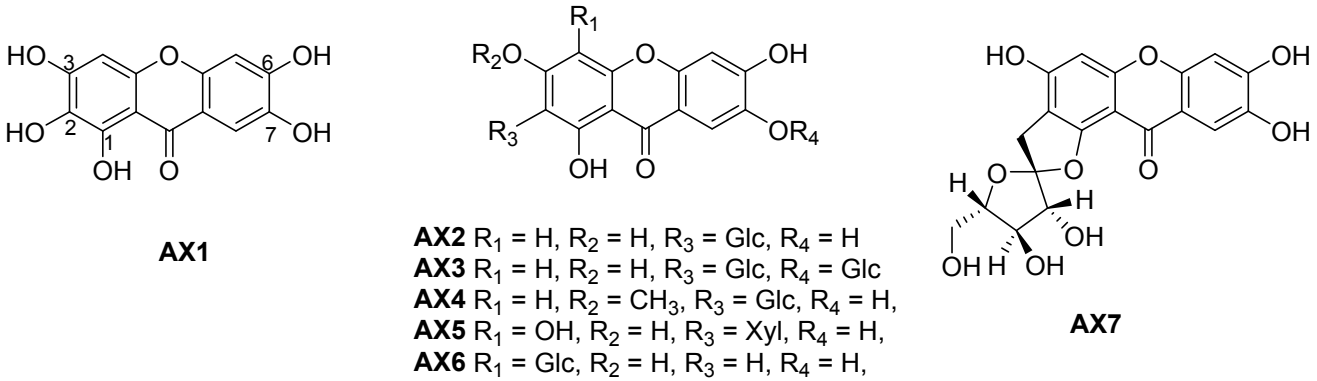


Fig. S2 Benzophenones identified from *Aquilaria* plants

Table S29 Benzophenoes identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AB1	Iriflophenone	*A. sinensis*	leaf	$C_{13}H_{10}O_5$	246	167,170
AB2	Aquilarinoside A	*A. sinensis*	leaf	$C_{19}H_{18}O_9$	390	167
AB3	Iriflophenone 3-*C*-β-D-glucoside	*A. sinensis* *A. crassna*	leaf petiole	$C_{19}H_{20}O_{10}$	408	170,178,181,184-185,190-191
AB4	Iriflophenone 3,5-*C*-β-D-diglucoside	*A.sinensis,* *A. crassna*	leaf petiole	$C_{25}H_{30}O_{15}$	570	170,176,178,181,184-185,190
AB5	Aquilarisinin	*A. sinensis*	stem	$C_{24}H_{28}O_{14}$	540	191
AB6	Aqulaside D	*A. sinensis,* *A. yunanensis*	flower bud pericarp	$C_{18}H_{18}O_9$	378	192,194
AB7	Iriflophenone 2-*O*-β-D-glucopyranoside	*A. yunanensis*	pericarp	$C_{19}H_{20}O_{10}$	408	194
AB8	Aqulaside A	*A. sinensis* *A. yunanensis*	flower bud pericarp	$C_{28}H_{26}O_{12}$	554	192,194
AB9	Aqulaside B	*A. sinensis*	flower bud	$C_{22}H_{22}O_{12}$	478	192
AB10	Aqulaside C	*A. sinensis* *A. yunanensis*	flower bud pericarps	$C_{25}H_{28}O_{13}$	536	192,194
AB11	Aquilariside B	*A. yunanensis*	pericarps	$C_{26}H_{30}O_{13}$	550	194
AB12	Aquilarinenside E	*A. sinensis* *A. yunanensis*	leaf pericarp	$C_{21}H_{22}O_{10}$	434	193-194
AB13	Aquilarinenside B	*A. sinensis*	leaf	$C_{25}H_{30}O_{13}$	538	193
AB14	Aquilarinenside C	*A. sinensis*	leaf	$C_{25}H_{30}O_{13}$	538	193
AB15	Aquilarinenside D	*A. sinensis*	leaf	$C_{24}H_{28}O_{13}$	524	193
AB16	Aquilarinenside A	*A. sinensis*	leaf	$C_{25}H_{30}O_{13}$	538	193
AB17	Aquilarisinin	*A. sinensis*	leaf	$C_{25}H_{30}O_{14}$	554	178,190
AB18	Iriflophenone 2-*O*-α-L-rhamnoside	*A. sinensis* *A. crassna* *A. yunanensis*	leaf pericarp	$C_{19}H_{20}O_9$	392	165,168,170,176,178,181,194
AB19	Iriflophenone, [2-(2-*O*-acty-L-rhamnopyranosyl)oxy]	*A. sinensis*	leaf	$C_{21}H_{22}O_{10}$	434	170
AB20	Iriflophenone, [2-(3-*O*-acty-L-rhamnopyranosyl)oxy]	*A. sinensis*	leaf	$C_{21}H_{22}O_{10}$	434	170



AX1

AX2 R_1 = H, R_2 = H, R_3 = Glc, R_4 = H
AX3 R_1 = H, R_2 = H, R_3 = Glc, R_4 = Glc
AX4 R_1 = H, R_2 = CH_3, R_3 = Glc, R_4 = H,
AX5 R_1 = OH, R_2 = H, R_3 = Xyl, R_4 = H,
AX6 R_1 = Glc, R_2 = H, R_3 = H, R_4 = H,

AX7

Fig. S3 Xanthones identified from *Aquilaria* plants

Table S30 Xanthones identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AX1	9*H*-Xanthen-9-one, 1,2,3,6,7-pentahydroxy	*A. sinensis*	leaf	$C_{13}H_8O_7$	276	170
AX2	Mangiferin	*A. sinensis* *A. crassna*	fruit leaf	$C_{19}H_{18}O_{11}$	422	167,170,176,178-179, 181-182,185,195
AX3	Neomangiferin	*A. sinensis*	leaf	$C_{25}H_{28}O_{16}$	584	170
AX4	Homomangiferin	*A. sinensis*	leaf	$C_{20}H_{20}O_{11}$	436	170
AX5	Aquilarixanthone	*A. sinensis*	leaf	$C_{18}H_{16}O_{11}$	408	170,178
AX6	Isomangiferin	*A. sinensis*	leaf	$C_{19}H_{18}O_{11}$	422	170
AX7	Aquilariside A	*A. yunanensis*	pericarp	$C_{19}H_{16}O_{10}$	404	194

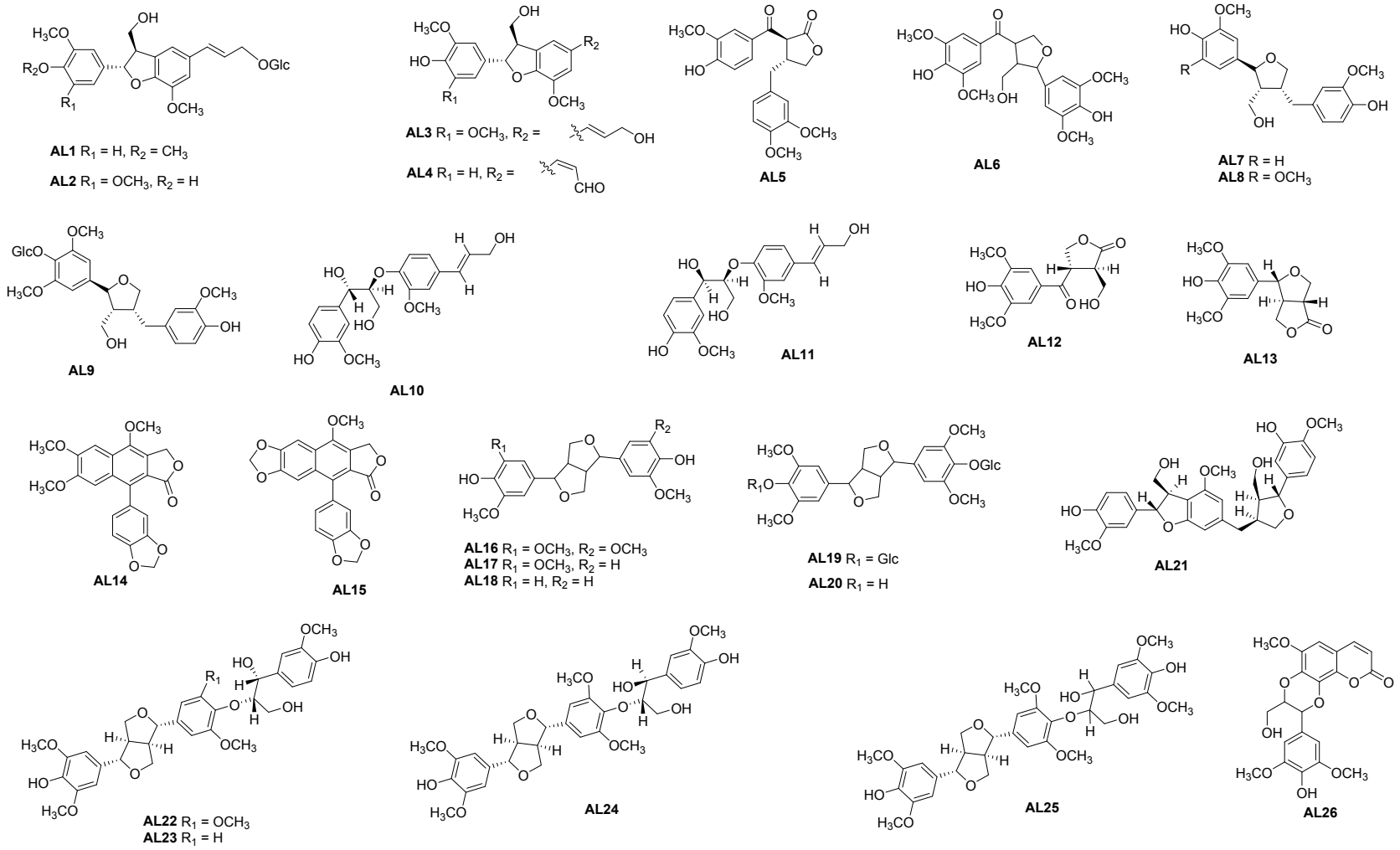
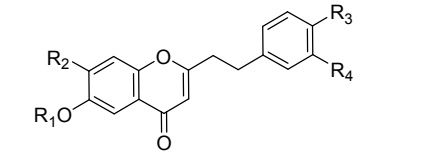


Fig. S4 Lignans identified from *Aquilaria* plants

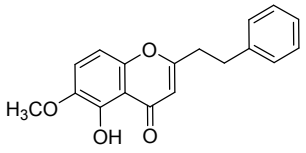
Table S31 Lignans identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AL1	Longifloroside A	*A. sinensis*	stem	$C_{27}H_{34}O_{11}$	534	191
AL2	(+)-Aquilaroside A	*A. sinensis*	stem	$C_{27}H_{34}O_{12}$	550	191
AL3	(-)-Simulanol	*A. sinensis*	stem	$C_{21}H_{24}O_{7}$	388	191
AL4	Balanophonin	*A. sinensis*	stem	$C_{21}H_{22}O_{7}$	386	197
AL5	Conicaol B	*A. sinensis*	stem	$C_{21}H_{22}O_{7}$	386	191
AL6	Ciwujiatone	*A. sinensis*	stem	$C_{22}H_{26}O_{9}$	434	196,198
AL7	(+)-Lariciresinol	*A. sinensis*	stem	$C_{20}H_{24}O_{6}$	360	197
AL8	5'-Methoxy lariciresinol	*A. sinensis*	stem	$C_{21}H_{26}O_{7}$	390	198
AL9	Conicaoside	*A. sinensis*	stem	$C_{27}H_{36}O_{12}$	552	191
AL10	*erythro*-Guaiacylglycerol-β-coniferyl ether	*A. sinensis*	stem	$C_{20}H_{24}O_{7}$	376	198
AL11	*threo*-Guaiacylglycerol-β-coniferyl ether	*A. sinensis*	stem	$C_{20}H_{24}O_{7}$	376	198
AL12	Aquilarin A	*A. sinensis*	stem	$C_{14}H_{16}O_{7}$	296	197
AL13	Curuilignan D	*A. sinensis*	stem	$C_{14}H_{16}O_{6}$	280	196
AL14	Justicidin A	*A. sinensis*	stem	$C_{22}H_{18}O_{7}$	394	196
AL15	Justidin F	*A. sinensis*	stem	$C_{21}H_{14}O_{7}$	378	196
AL16	Syringaresinol	*A. sinensis*	bark stem cell culture	$C_{22}H_{26}O_{8}$	418	169,174,189,191, 196,198-199
AL17	(-)-Medioresinol	*A. sinensis*	stem	$C_{21}H_{24}O_{7}$	388	198
AL18	(-)-Pinoresinol	*A. sinensis*	stem	$C_{20}H_{22}O_{6}$	358	198

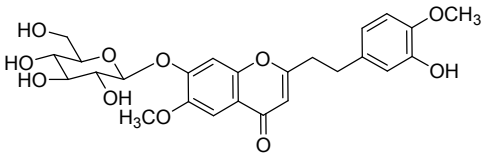
No.	Compound	Source	Part	Formula	MW	Ref.
AL19	Liriodendrin	*A. sinensis*	stem	$C_{34}H_{46}O_{18}$	742	191,196
AL20	Syringaresinol-4'-*O*-β-D-glucopyranoside	*A. sinensis*	stem	$C_{28}H_{36}O_{13}$	580	196
AL21	Herpetin	*A. sinensis*	stem	$C_{30}H_{34}O_{19}$	538	198
AL22	*threo*-Buddlenol C	*A. sinensis*	stem	$C_{32}H_{38}O_{12}$	614	198
AL23	*threo*-Ficusesquilignan A	*A. sinensis*	stem	$C_{31}H_{36}O_{11}$	584	198
AL24	*erythro*-Buddlenol C	*A. sinensis*	stem	$C_{32}H_{38}O_{12}$	614	198
AL25	(±)-Buddlenol D	*A. sinensis*	stem	$C_{33}H_{40}O_{13}$	644	198
AL26	Aquillochin	*A. agallocha*	whole plant	$C_{21}H_{20}O_{10}$	416	200



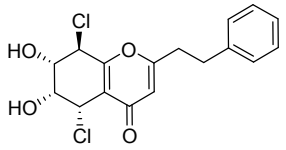
AC1 R_1 = H, R_2 = H, R_3 = OH, R_4 = H
AC2 R_1 = CH_3, R_2 = H, R_3 = OH, R_4 = OCH_3
AC3 R_1 = CH_3, R_2 = OH, R_3 = H, R_4 = H
AC4 R_1 = CH_3, R_2 = OCH_3, R_3 = H, R_4 = H
AC5 R_1 = CH_3, R_2 = OCH_3, R_3 = OCH_3, R_4 = H



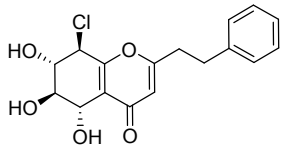
AC6



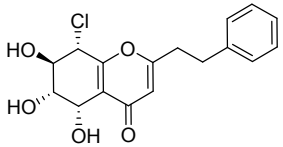
AC7



AC8



AC9



AC10

Fig. S5 2-(2-Phenylethyl)chromones identified from *Aquilaria* plants

Table S32 2-(2-Phenylethyl)chromones identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AC1	6-Hydroxy-2-[2-(4-hydroxyphenyl)ethyl]chromone	*A. sinensis*	fruit leaf petiole	$C_{17}H_{14}O_4$	282	180,190
AC2	6-Methoxy-2-[2-(3-methoxy-4-hydroxyphenyl)ethyl]chromone	*A. sinensis*	leaf petiole	$C_{19}H_{18}O_6$	326	190
AC3	7-Hydroxy-6-methoxy-2-(2-phenylethyl)chromone	*A. sinensis*	stem	$C_{18}H_{16}O_4$	296	174
AC4	6,7-Dimethoxy-2-(2-phenylethyl)chromone	*A. sinensis*	stem cell culture	$C_{19}H_{18}O_4$	310	174,199
AC5	6,7-Dimethoxy-2-[2-(4-methoxyphenyl)ethyl]chromone	*A. sinensis*	cell culture	$C_{20}H_{20}O_5$	340	199
AC6	5-Hydroxy-6-methoxy-2-(2-phenylethyl)chromone	*A. sinensis*	leaf petiole	$C_{18}H_{16}O_4$	296	190
AC7	Aquilarinoside C	*A. sinensis*	stem	$C_{25}H_{28}O_{11}$	504	201
AC8	(5*S*,6*R*,7*S*,8*R*)-5,8-Dichloro-6,7-dihydroxy-2-phenylethyl-5,6,7,8-tetrahydro-4*H*-chromen-4-one	*A. sinensis*	cell culture	$C_{17}H_{16}Cl_2O_4$	354	199
AC9	(5*S*,6*S*,7*S*,8*R*)-8-Chloro-5,6,7-trihydroxy-2-phenylethyl-5,6,7,8-tetrahydro-4*H*-chromen-4-one	*A. sinensis*	cell culture	$C_{17}H_{17}ClO_5$	336	199
AC10	(5*S*,6*R*,7*R*,8*S*)-8-Chloro-5,6,7-trihydroxy-2-phenylethyl-5,6,7,8-tetrahydro-4*H*-chromen-4-one	*A. sinensis*	cell culture	$C_{17}H_{17}ClO_5$	336	199

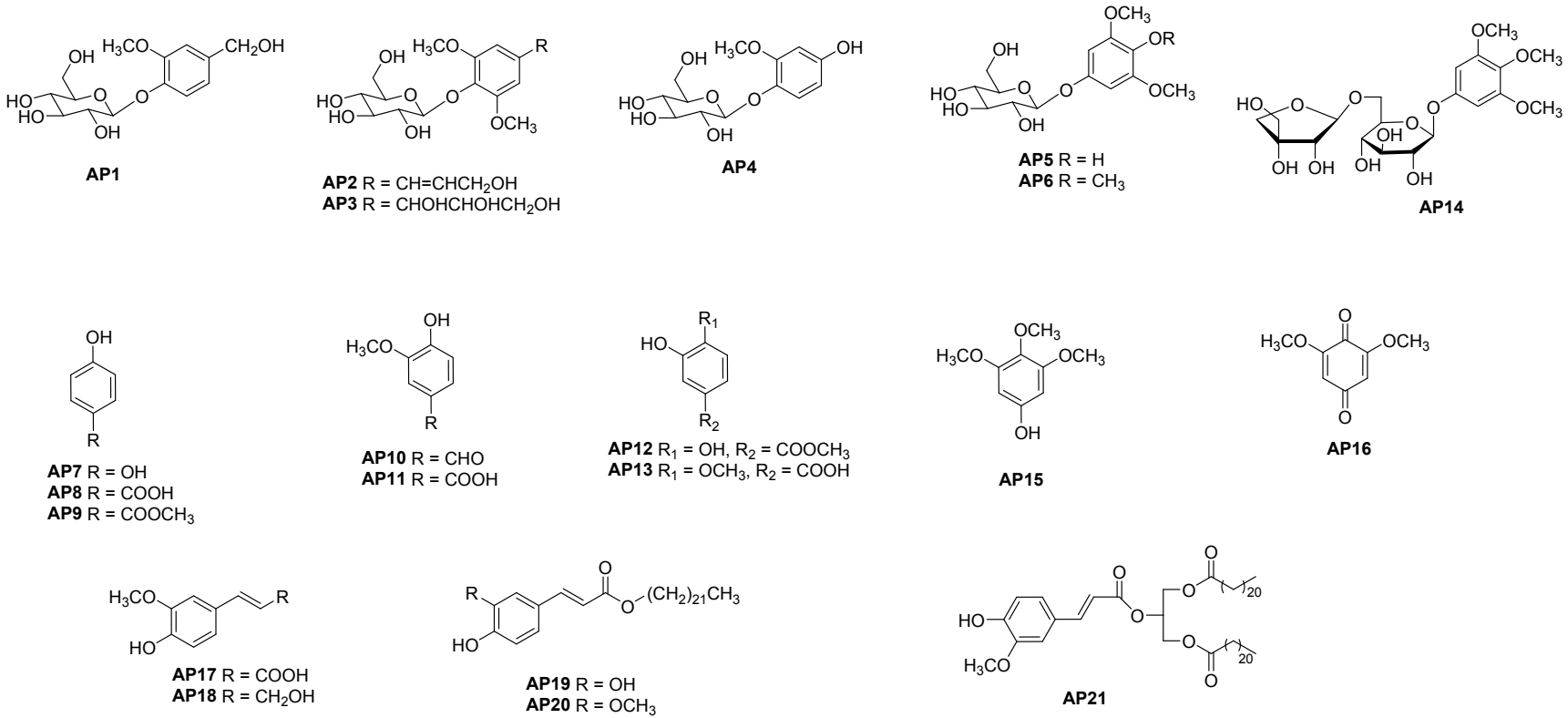


Fig. S6 Simple phenolic compounds identified from *Aquilaria* plants

Table S33 Simple phenolic compounds identified from *Aquilaria* plants

No.	compound	source	part	Formula	MW	Ref.
AP1	Vanilloloside	*A. sinensis*	stem	$C_{14}H_{20}O_8$	316	191
AP2	Syringin	*A. sinensis*	stem	$C_{17}H_{24}O_9$	372	191,196
AP3	4-(1,2,3-Trihydroxypropyl)-2,6-dimethoxyphenyl-1-*O*-β-D-glucopyranoside	*A. sinensis*	stem	$C_{17}H_{26}O_{11}$	406	164
AP4	Isotachioside	*A. sinensis*	stem	$C_{13}H_{18}O_8$	302	191
AP5	Koaburaside	*A. sinensis*	stem	$C_{14}H_{20}O_9$	332	196
AP6	3,4,5-Trimethoxyphenyl-1-*O*-β-D-glucopyranoside	*A. sinensis*	stem	$C_{15}H_{22}O_9$	346	196
AP7	Hydroquinone	*A. sinensis*	leaf	$C_6H_6O_2$	110	202
AP8	4-Hydroxybenzoic acid	*A. sinensis* *A. agallocha*	leaf bark	$C_7H_6O_3$	138	171,186,202
AP9	Methylparaben	*A. sinensis* *A. agallocha*	bark	$C_8H_8O_3$	152	169,186
AP10	Vanillin	*A. agallocha*	bark	$C_8H_8O_3$	152	186
AP11	Vanillic acid	*A. sinensis*	stem	$C_8H_8O_4$	168	174
AP12	Methyl 3,4-dihydroxybenzoate	*A. sinensis*	stem	$C_8H_8O_4$	168	174
AP13	Isovanillic acid	*A. agallocha*	bark	$C_8H_8O_4$	168	186
AP14	3,4,5-Trimethoxyphenyl-1-O-β-D-apiofuranosyl-(1"-6')glucopyranoside	*A. sinensis*	stem	$C_{20}H_{30}O_{13}$	478	196
AP15	3,4,5-Trimethoxyphenol	*A. sinensis*	stem	$C_9H_{12}O_4$	184	198
AP16	2,6-Dimethoxy-*p*-benzoquinone	*A. sinensis*	stem	$C_8H_8O_4$	168	174
AP17	Ferulic acid	*A. malaccensis* *A. agallocha*	stem bark	$C_{10}H_{10}O_4$	194	186,203
AP18	Coniferyl alcohol	*A. sinensis*	stem	$C_{10}H_{12}O_3$	180	198
AP19	Docosyl caffeate	*A. sinensis*	stem	$C_{31}H_{52}O_4$	488	174
AP20	Docosyl *trans*-ferulate	*A. sinensis*	stem	$C_{32}H_{54}O_4$	502	174
AP21	1,3-Dibehehyl-2-ferulyl glyceride	*A. malaccensis*	stem	$C_{57}H_{100}O_8$	912	203

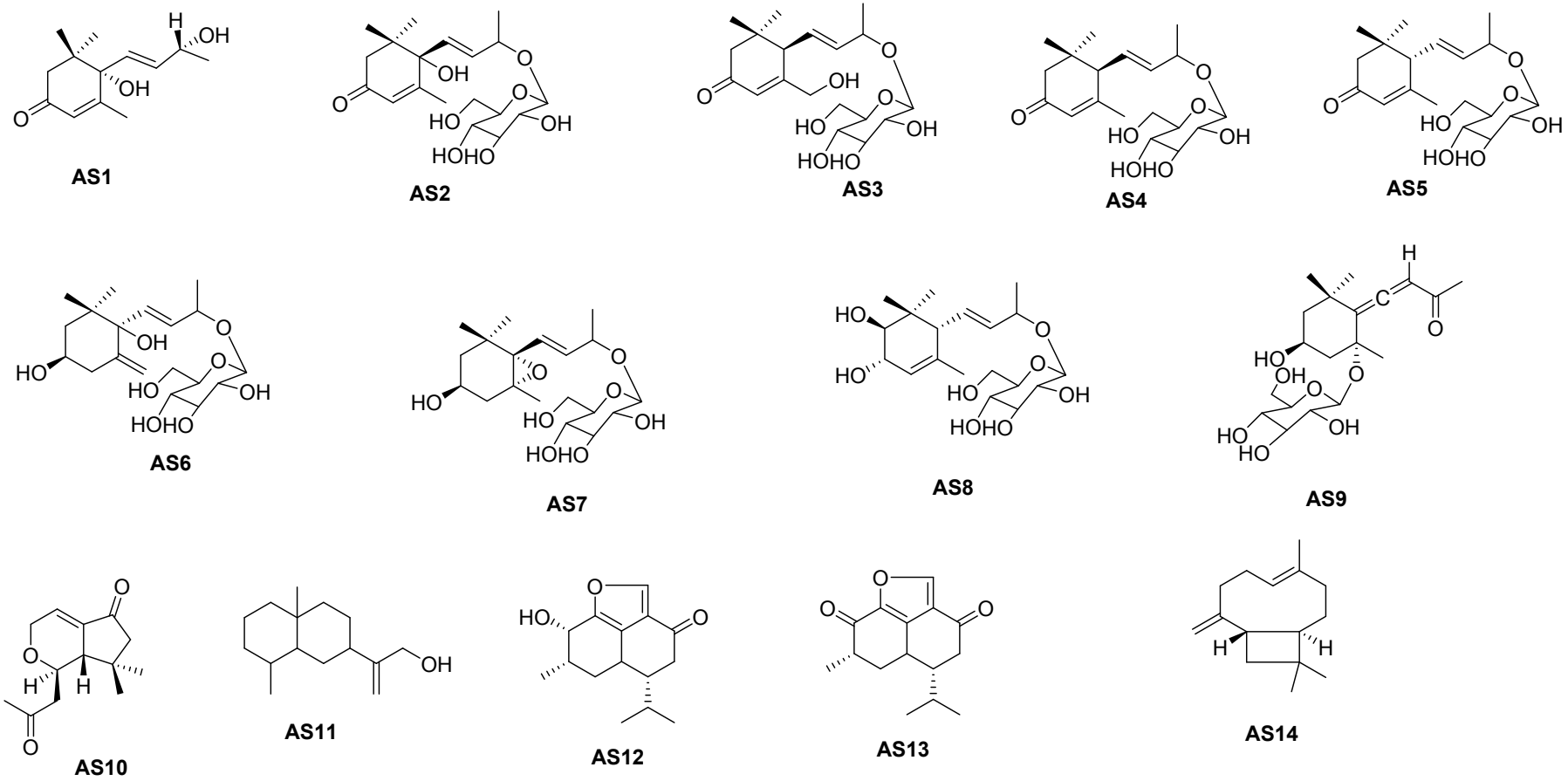


Fig. S7 Sesquiterpenes and degraded sesquiterpenes identified from *Aquilaria* plants

Table S34 Sesquiterpenes and degraded sesquiterpenes identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AS1	Blumenol A	*A. sinensis*	stem	$C_{13}H_{20}O_3$	224	174
AS2	Corchoionoside C	*A. sinensis*	leaf	$C_{19}H_{30}O_8$	386	206
AS3	Macarangloside D	*A. sinensis*	leaf	$C_{19}H_{30}O_8$	386	206
AS4	(+)-3-Oxo-α-ionol-β-D-glucopyranoside	*A. sinensis*	leaf	$C_{19}H_{30}O_7$	370	206
AS5	(–)-3-Oxo-α-ionol-β-D-glucopyranoside	*A. sinensis*	leaf	$C_{19}H_{30}O_7$	370	206
AS6	(9*S*)-Megastigma-4(13),7-diene-3,6,9-triol 9-*O*-β-D-glucopyranoside	*A. sinensis*	leaf	$C_{19}H_{32}O_8$	388	206
AS7	Staphylionoside H	*A. sinensis*	leaf	$C_{19}H_{32}O_8$	388	206
AS8	(9*S*)-Megastigma-4,7-diene-2,3,9-triol 9-*O*-β-D-glucopyranoside	*A. sinensis*	leaf	$C_{19}H_{32}O_8$	388	206
AS9	Citroside B	*A. sinensis*	leaf	$C_{19}H_{30}O_8$	386	206
AS10	Aquilarin B	*A. sinensis*	stem	$C_{13}H_{18}O_3$	222	207
AS11	Agarol	*A. malaccensis.*	stem	$C_{15}H_{26}O$	222	203
AS12	8β*H*-Dihydrogmelofuran	*A. malaccensis* *A. agallocha*	stem	$C_{15}H_{20}O_3$	248	203-204
AS13	Gmelofuran	*A. agallocha*	stem	$C_{15}H_{18}O_3$	246	204
AS14	β-Caryophyllene	*A. crassna*	stem	$C_{14}H_{22}O$	206	205

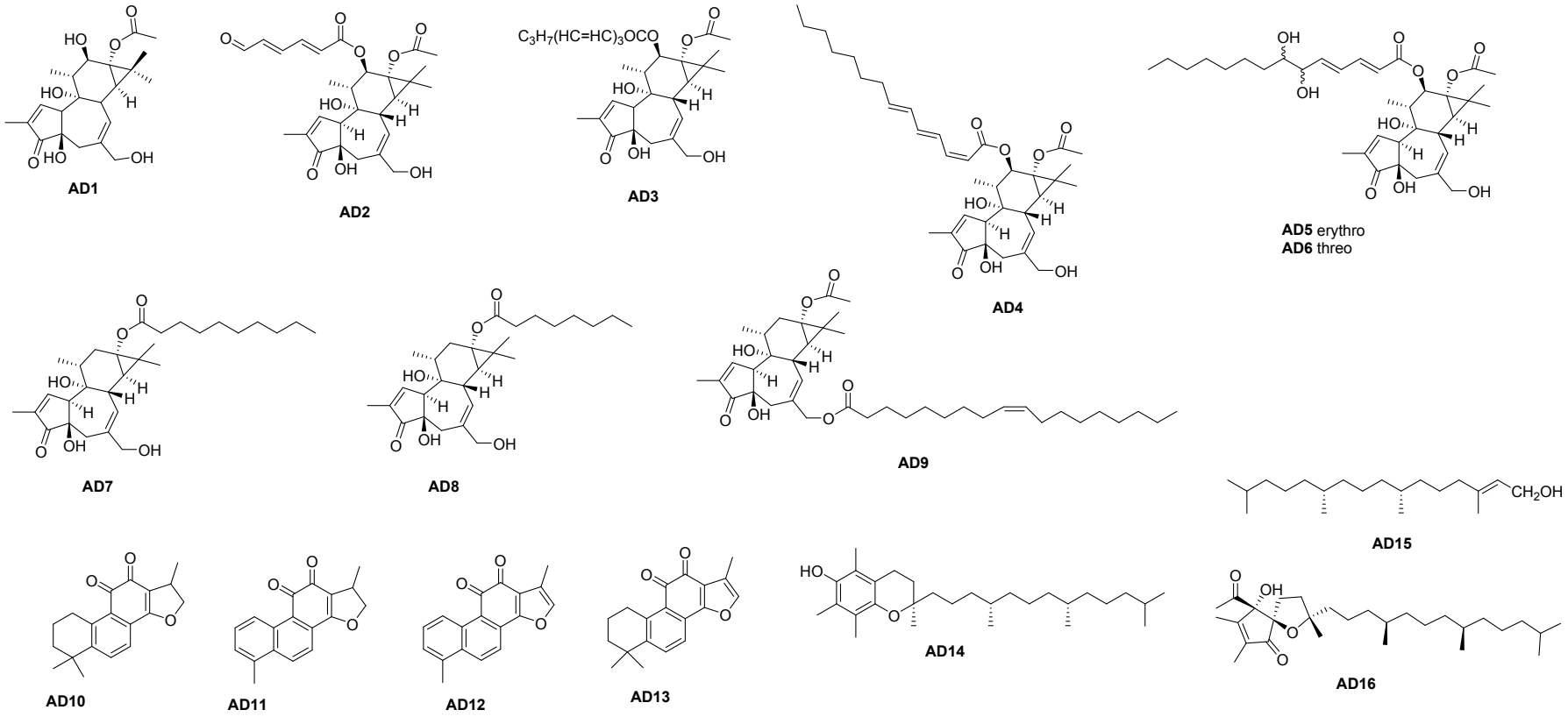


Fig. S8 Diterpenoids and diterpenoid derivatives identified from *Aquilaria* plants

Table S35 Diterpenoids and diterpenoid derivatives identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AD1	Phorbol 13-acetate	*A. sinensis*	stem	$C_{22}H_{30}O_7$	406	207
AD2	12-*O*-(2'*E*,4'*E*)-6-Oxohexa-2',4'-dienoylphorbol-13-acetate	*A. malaccensis*	seed	$C_{28}H_{34}O_9$	514	208
AD3	12-*O*-*n*-Deca-2,4,6-trienoylphorbol-13-acetate	*A. malaccensis*	stem	$C_{32}H_{42}O_8$	554	203
AD4	Aquimavitalin	*A. malaccensis*	seed	$C_{36}H_{50}O_8$	610	209
AD5	12-*O*-(2'*E*,4'*E*)6',7'-(*erythro*)-Dihydroxytetradeca-2',4'-dienoylphorbol-13-acetate	*A. malaccensis*	seed	$C_{36}H_{52}O_{10}$	644	208
AD6	12-*O*-(2'*E*,4'*E*)6',7'-(*threo*)-Dihydroxytetradeca-2',4'-dienoylphorbol-13-acetate	*A. malaccensis*	seed	$C_{36}H_{52}O_{10}$	644	208
AD7	12-*O*-Deoxyphorbol 13-decanoate	*A. malaccensis*	seed	$C_{30}H_{46}O_6$	502	208
AD8	Mellerin A	*A. malaccensis*	seed	$C_{28}H_{42}O_6$	474	208
AD9	12-Deoxy-13-*O*-acetylphorbol-20-(9'*Z*)-octadecenote	*A. malaccensis*	seed	$C_{40}H_{67}O_7$	654	208
AD10	Cryptotanshinone	*A. sinensis*	leaf	$C_{19}H_{20}O_3$	296	202
AD11	Dihydrotanshinone I	*A. sinensis*	leaf	$C_{18}H_{14}O_3$	278	202
AD12	Tanshinone I	*A. sinensis*	leaf	$C_{18}H_{12}O_3$	276	202
AD13	Tanshinone II_A	*A. sinensis*	leaf	$C_{19}H_{18}O_3$	294	202
AD14	α-Tocopherol	*A. sinensis*	stem	$C_{29}H_{50}O_2$	430	174
AD15	*trans*-Phytol	*A. sinensis*	stem	$C_{20}H_{40}O$	296	174
AD16	α-Tocospiro A	*A. sinensis*	stem	$C_{29}H_{50}O_4$	462	174

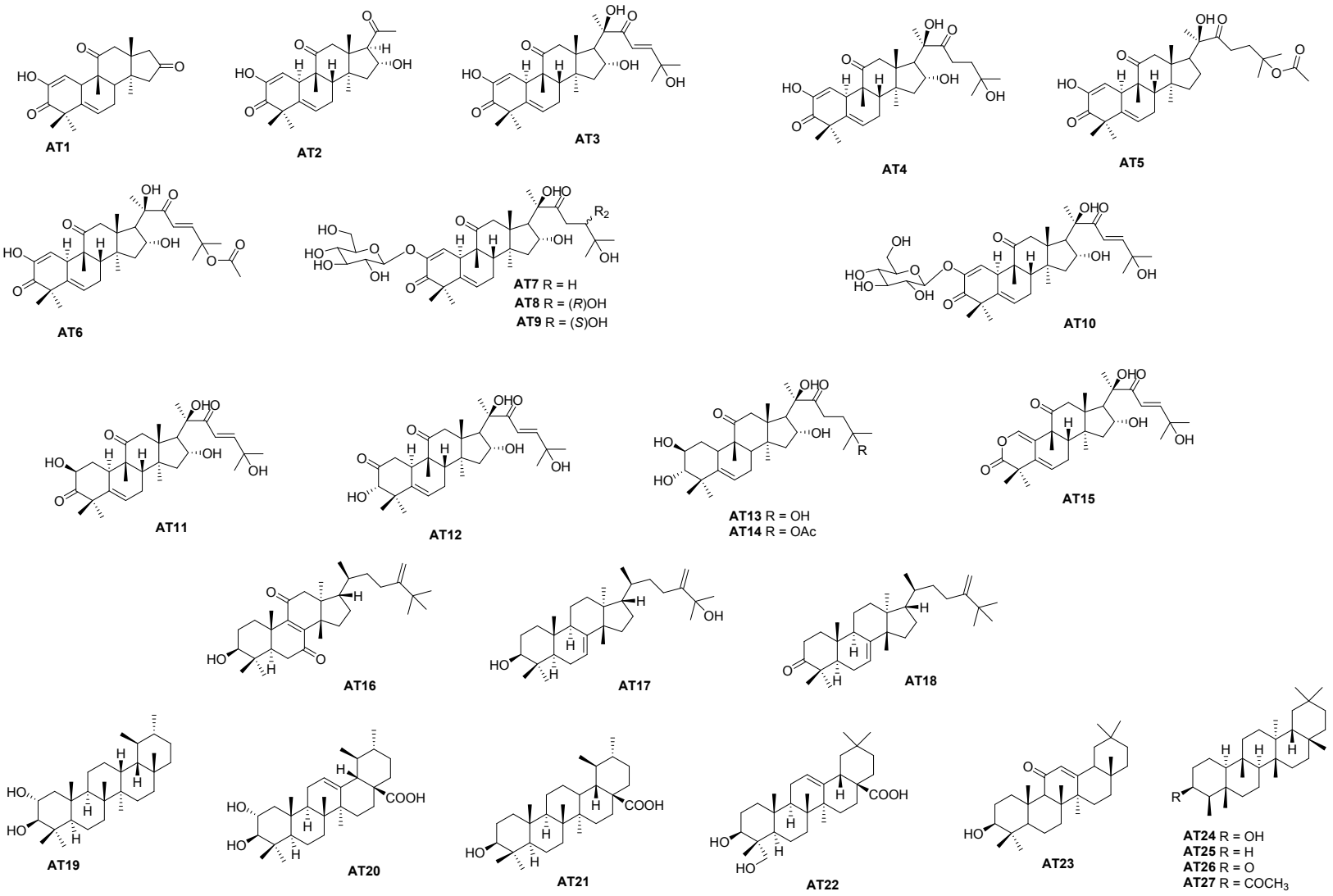


Fig. S9 Triterpenes identified from *Aquilaria* plants

Table S36 Triterpenes identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AT1	Endecaphyllacins B	*A. sinensis*	peel	$C_{22}H_{28}O_4$	356	211
AT2	Hexanorcucurbitacin I	*A. sinensis*	fruit	$C_{24}H_{32}O_5$	400	212
AT3	Cucurbitacin I	*A. sinensis*	fruit peel	$C_{30}H_{42}O_7$	514	211-212
AT4	Cucurbitacin L	*A. sinensis*	petiole leaf	$C_{30}H_{44}O_7$	516	190
AT5	Dihydrocucurbitacin E	*A. sinensis*	peel	$C_{32}H_{46}O_7$	542	211
AT6	Cucurbitacin E	*A. sinensis*	peel	$C_{32}H_{44}O_8$	556	211
AT7	Bryoamaride	*A. sinensis*	petiole leaf	$C_{36}H_{54}O_{12}$	678	190,206
AT8	2-*O*-β-D-Glucopyranosylcucurbitacin J	*A. sinensis*	petiole leaf	$C_{36}H_{54}O_{13}$	694	190
AT9	2-*O*-β-D-Glucopyranosylcucurbitacin K	*A. sinensis*	petiole leaf	$C_{36}H_{54}O_{13}$	694	190
AT10	2-*O*-β-D-Glucopyranosylcucurbitacin I	*A. sinensis*	petiole leaf peel	$C_{36}H_{56}O_{12}$	676	190,206,211
AT11	Cucurbitacin D	*A. sinensis*	fruit	$C_{30}H_{44}O_7$	516	212
AT12	Isocucurbitacin D	*A. sinensis*	fruit	$C_{30}H_{44}O_7$	516	212
AT13	Dihydrocucurbitacin F	*A. sinensis*	stem	$C_{30}H_{48}O_7$	520	207
AT14	Cucurbitacin	*A. sinensis*	stem	$C_{32}H_{50}O_8$	562	198
AT15	Neocucurbitacin B	*A. sinensis*	fruit	$C_{29}H_{40}O_7$	500	212
AT16	Aquilacallane B	*A. sinensis*	leaf petiole	$C_{32}H_{50}O_3$	482	165,190
AT17	Aquilacallane A	*A. sinensis*	leaf petiole	$C_{31}H_{52}O_2$	456	165,190

No.	Compound	Source	Part	Formula	MW	Ref.
AT18	24-Methylene-25-methyltirucall-7-en-3-one	*A. sinensis*	leaf	$C_{32}H_{52}O$	452	165
AT19	2α-Hydroxyursane	*A. sinensis*	leaf	$C_{30}H_{52}O_2$	444	202
AT20	2α-Hydroxyursolic acid	*A. sinensis*	leaf	$C_{30}H_{48}O_4$	472	202
AT21	Ursolic acid	*A. sinensis*	leaf	$C_{30}H_{50}O_3$	458	165
AT22	Hederagenin	*A. sinensis*	leaf	$C_{30}H_{48}O_4$	472	165
AT23	11-Oxo-β-amyrin	*A. sinensis*	leaf	$C_{30}H_{48}O_2$	440	165
AT24	Epifriedelanol	*A. sinensis* *A. crassna*	leaf	$C_{30}H_{52}O$	428	171,183
AT25	Friedelan	*A. sinensis*	leaf	$C_{30}H_{52}$	412	171
AT26	Friedelin	*A. sinensis*	leaf	$C_{30}H_{50}O$	426	171
AT27	3β-Acetoxyfriedelane	*A. sinensis*	leaf	$C_{32}H_{54}O$	454	165

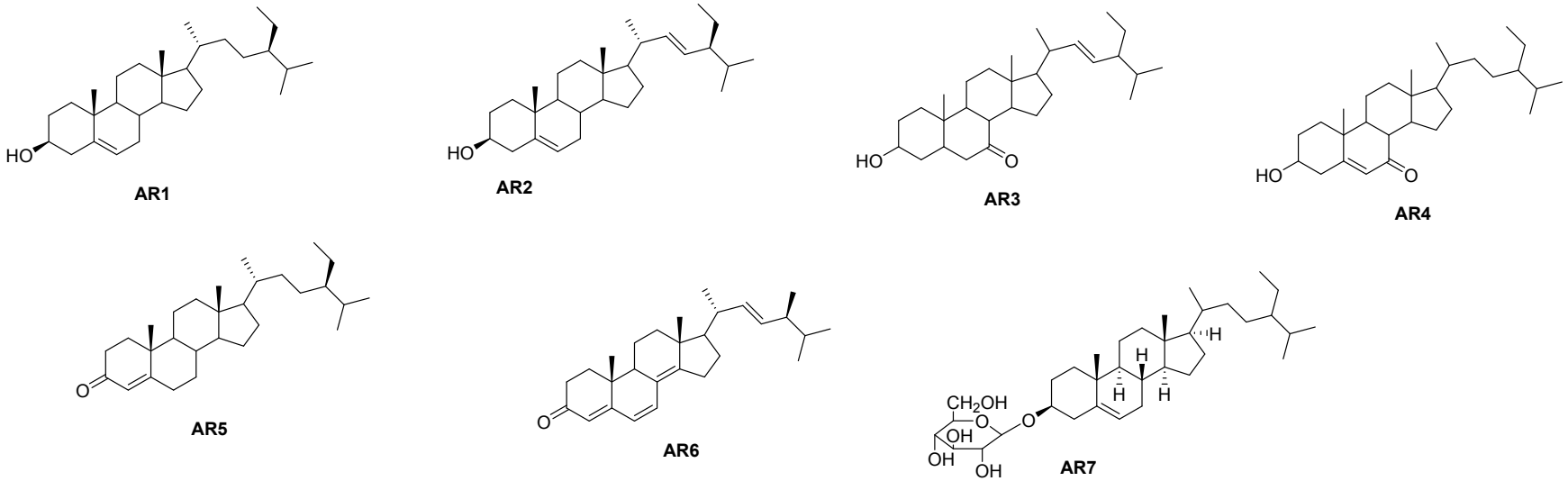


Fig. S10 Steroids identified from *Aquilaria* plants

Table S37 Steroids identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AR1	β-Sitosterol	*A. sinensis*	bark, fruit, leaf, stem	$C_{29}H_{50}O$	414	169,174,180,188,202
AR2	Stigmasterol	*A. sinensis*	leaf	$C_{29}H_{48}O$	412	188
AR3	7-Oxo-5,6-dihydrostigmasterol	*A. sinensis*	stem	$C_{29}H_{48}O_2$	428	196
AR4	7-Ketositosterol	*A. sinensis*	stem	$C_{29}H_{48}O_2$	428	196
AR5	β-Sitostenone	*A. sinensis*	stem	$C_{29}H_{48}O$	412	174,188
AR6	Ergosta-4,6,8(14),22-tetraen-3-one	*A. sinensis*	stem	$C_{28}H_{40}O$	392	174
AR7	Daucosterol	*A. sinensis*	fruit	$C_{35}H_{60}O_6$	576	180,202

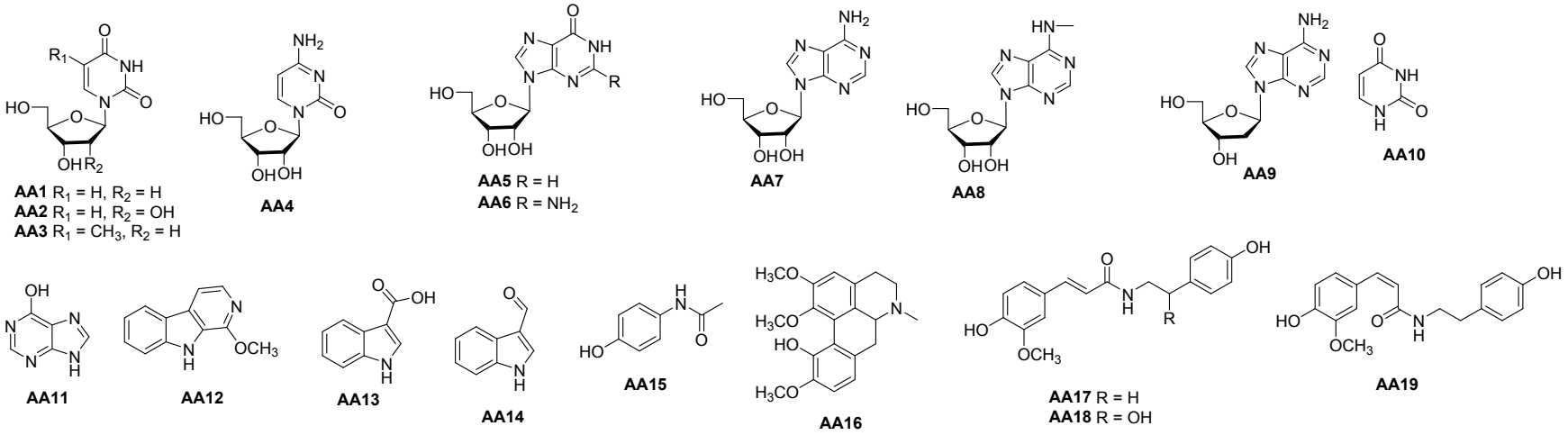


Fig. S11 Alkaloids identified from *Aquilaria* plants

Table S38 Alkaloids identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AA1	2'-Deoxyuridine	*A. sinensis*	cell culture	$C_9H_{12}N_2O_5$	228	199
AA2	Uridine	*A. sinensis*	petiole leaf cell culture	$C_9H_{12}N_2O_6$	244	190,199
AA3	Thymidine	*A. sinensis*	petiole leaf cell culture	$C_{10}H_{14}N_2O_5$	242	190,199
AA4	Cytidine	*A. sinensis*	petiole leaf	$C_9H_{13}N_3O_5$	243	190
AA5	Inosine	*A. sinensis*	petiole leaf	$C_{10}H_{12}N_4O_5$	268	190
AA6	Guanosine	*A. sinensis*	petiole leaf	$C_{10}H_{13}N_5O_5$	283	190
AA7	Adenosine	*A. sinensis*	leaf petiole cell culture	$C_{10}H_{13}N_5O_4$	267	164,190,199
AA8	N^6-Methyladenosine	*A. sinensis*	cell culture	$C_{11}H_{15}N_5O_4$	281	199
AA9	2'-Deoxy-D-adenosine	*A. sinensis*	cell culture	$C_{10}H_{13}N_5O_3$	251	199
AA10	Uracil	*A. sinensis*	leaf	$C_4H_4N_2O_2$	112	164
AA11	Hypoxanthine	*A. sinensis*	leaf	$C_5H_4N_5O$	136	164
AA12	Taraxacine A	*A. sinensis*	stem	$C_{12}H_{10}N_2O$	198	174
AA13	Indole-3-carboxylic acid	*A. sinensis*	fruit	$C_9H_7NO_2$	161	180
AA14	Indole-3-carboxaldehyde	*A. sinensis*	cell culture	C_9H_7NO	145	199
AA15	4'-Hydroxyacetanilide	*A. malaccensis*	leaf	$C_8H_9NO_2$	151	213
AA16	Isocorydine	*A. sinensis*	leaf	$C_{20}H_{23}NO_4$	341	171
AA17	*N-trans*-Feruloyltyramine	*A. sinensis*	cell culture	$C_{18}H_{19}NO_4$	313	199
AA18	*N-trans*-Feruloyloctopamine	*A. sinensis*	cell culture	$C_{18}H_{19}NO_5$	329	199
AA19	*N-cis*-Feruloyltyramine	*A. sinensis*	cell culture	$C_{18}H_{19}NO_4$	313	199

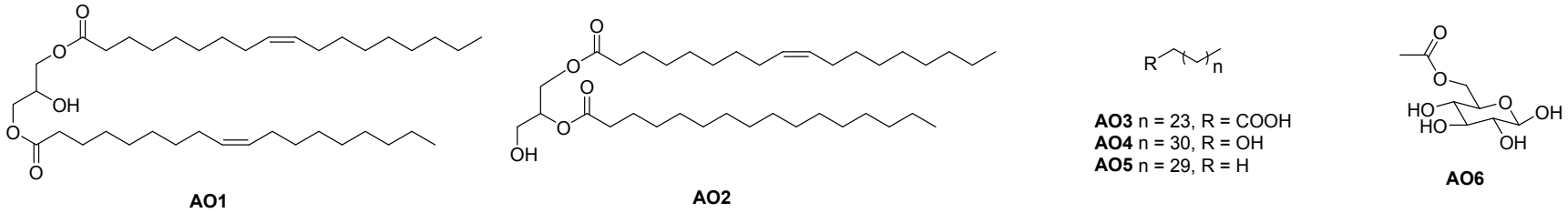


Fig. S12 Other compounds identified from *Aquilaria* plants

Table S39 Other compounds identified from *Aquilaria* plants

No.	Compound	Source	Part	Formula	MW	Ref.
AO1	1,3-Dioleoyl glyceride	*A. malaccensis*	seed	$C_{39}H_{72}O_5$	620	208
AO2	1-Oleoyl-2-palmitoyl glyceride	*A. malaccensis*	seed	$C_{37}H_{70}O_5$	594	208
AO3	Hexacosanic acid	*A. sinensis*	leaf	$C_{26}H_{52}O_2$	396	202
AO4	Triacontenoic	*A. sinensis*	leaf	$C_{32}H_{66}O$	466	171
AO5	Hentriacontane	*A. sinensis*	leaf	$C_{31}H_{64}$	436	171
AO6	6-*O*-Acetyl β-D-glucopyranose	*A. sinensis*	cell culture	$C_8H_{14}O_7$	222	199

Table S40 Genes related to the biosynthesis of sesquiterpenes in *Aquilaria* species

Species	Gene code	Accession No.	Encoded protein	Characterization	Ref.	Year
A. microcarpa	*Am-FaPS-1*	HM067872	putative farnesyl diphosphate synthase (FPPS, EC 2.5.1.10)	The expression level was increased in response to stimulation with MJ, YE or Ca^{2+}-ionophore, and in cells over-expressing of calmodulin gene *Am-rac2*.	223,240	2010
A. sinensis	*AsFPS1*	KC708224	farnesyl diphosphate synthase (FPPS, EC 2.5.1.10)	It was mainly expressed in root and stem, and was lower expressed in leaves.	224	2013
A. microcarpa	*FPS*	KU310684	farnesyl diphosphate synthase (FPPS, EC 2.5.1.10)	Co-expression of *FPS* and *GS* (KF800046) in *E. coli* or tobacco (*Nicotiana tabacum*) BY-2 cells efficiently enhanced the guaiene production.	232,234	2016
A. crassna	*AcC1*	GU083696	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	MJ treatment increases its expression. AcC1 expression did not have any TPS activity, while mutants M42 and M50 had δ-GS activity.	227-228	2010
A. crassna	*AcC2–AcC4*	GU083697–GU083699	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	MJ treatment increases their expression. The encoded proteins converted farnesyl pyrophosphate (FPP) to δ-guaiene (major), α-humulene, and δ-guaiene.	227-228	2010
A. crassna	*AcL154*	GU083700	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	MJ treatment increases its expression. AcL154 harbored an extra stop codon, which was substituted with that for Trp, so that the heterologously expressed protein converted FPP to δ-guaiene (major), α-humulene, and α-guaiene.	227-228	2010
A. sinensis	*ASS1*	JQ712682	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	The encoded enzyme ASS1 is capable of producing δ-guaiene and the minor products as β-elemene and α-guaiene from FPP. The expression of *ASS1* was upregulated significantly by mechanical wounding, MJ treatment, H_2O_2 treatment.	229,242	2013
A. sinensis	*ASS2–ASS3*	JQ712683 –JQ712684	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	The heterologous expression enzymes ASS2–ASS3 is capable of producing δ-guaiene and the minor products as β-elemene and α-guaiene from FPP.	229,242	2013
A. microcarpa	*GS-1*	KF800046	δ-guaiene synthase (δ-GS, EC 4.2.3.87)	Its expression was remarkably activated by the treatment with yeast extract (YE) or MJ, and induced in *cam1* and *rac2* mutants. Its translated protein catalyzed FPP to liberate δ-guaiene as the major product plus α-guaiene and germacrene A as the minor products.	230,232, 234,242	2014

Species	Gene code	Accession No.	Encoded protein	Characterization	Ref.	Year
A. microcarpa	*GS-2ΔNΔC*	KT283579	*δ*-guaiene synthase (*δ*-GS, EC 4.2.3.87)	Ten and nine amino acid residues of N- and C-terminal ends of the translated products of the clone remained undefined. The reaction products of recombinant enzyme with ligated N and C-terminal amino acid sequences were *α*-guaiene, *δ*-guaiene and *β*-elemene.	231	2015
A. microcarpa	*GS-3ΔNΔC*–*GS-4ΔNΔC*	KT283580–KT283581	*δ*-guaiene synthase (*δ*-GS, EC 4.2.3.87)	Ten and nine amino acid residues of N- and C-terminal ends of the translated products of these clones remained undefined. Its ligated recombinant enzymes produced *α*- and *δ*-guaiene, *β*-elemene plus *α*-humulene as a minor product.	231	2015
A. malaccensis	*AmGuaiS1*	KT380854	*δ*-guaiene synthase (*δ*-GS, EC 4.2.3.87)	The gene encoded protein is 99% similarity with *δ*-guaiene synthases, and was induced after just 2 h of wounding.	237	2016
A. crassna	*AcHS1*–*AcHS3*	KT893309–KT893311	*α*-humulene synthase (*α*-HS, EC:4.2.3.104)	MJ treatment increases their expression. The recombinant enzymes catalyzed FPP to generate *α*-humulene as the main product, as well as a trace amount of *β*-caryophyllene.	235	2016
A. sinensis	*As-SesTPS1*	KM881473	sesquiterpene synthase	The gene was highly expressed in the agarwood sample, and its encoded protein shared high similarity to multiple sesquiterpene synthase.	237	2015
A. malaccensis	*AmSesTPS1*	KT380853	sesquiterpene synthase	The gene was highly induced after 6 h post wounding, its encoded protein is 85% similar to the (–)-germacrene D synthases (GDS, EC 4.2.3.75).	238	2016
A. sinensis	*As-SesTPS*	KF135950	sesquiterpene synthase	The expression level in agarwood was much higher than that in whitewood. Its heterologous expression protein catalyzed the conversion of FPP to nerolidol 2 as a major product.	236	2017
A. sinensis	*AsVS*	MH378283	vetispiradiene synthase (VS, EC 4.2.3.21)	The relative expression of *AsVS* was continuously increased in the stem of *A. sinensis* during artificial induce agarwood formation.	239	2019

Table S41 Enzymes of the biosynthetic pathways of terpenes, steroids and aromatic polyketides

Abbreviation	Name	EC
MVA pathway		
AACT	Acetoacetyl-CoA thiolase	2.3.1.9
HMGS	3-Hydroxy-3-methylglutaryl-CoA synthase	2.3.3.10
HMGR	3-Hydroxy-3-methylglutaryl-CoA reductase	1.1.1.34
MK	Mevalonate kinase	2.7.1.36
MEP pathway		
DXS	1-Deoxy-D-xylulose 5-phosphate synthase	2.2.1.7
DXR	1-Deoxy-D-xylulose 5-phosphate reductoisomerase	1.1.1.267
MCT	2-*C*-methyl-D-erythritol 4-phosphate cytidylyl transferase	2.7.7.60
CMK	4-Diphosphocytidyl-2-*C*-methyl-D-erythritol kinase	2.7.1.148
MDS	2-*C*-methyl-D-erythritol 2,4-cyclodiphosphate synthase	4.6.1.12
HDS	4-Hydroxy-3-methylbut-2-en-1-yl diphosphate synthase	1.17.7.1
HDR	4-Hydroxy-3-methylbut-2-enyl diphosphate reductase	1.17.1.2
Terpenes and steriols		
IPPI	Isopentenyl-diphosphate delta-isomerase	5.3.3.2
FPPS	Farnesyl diphosphate synthase	2.5.1.10
GGPPS	Geranylgeranyl pyrophosphate synthase	2.5.1.29
SQS	Squalene synthase	2.5.1.21
NPPS	All-trans-nonaprenyl diphosphate synthase (geranyl-diphosphate specific)	2.5.1.84
GPPS	Geranyl diphosphate synthase	2.5.1.1
SQE	Squalene epoxidase	1.14.99.7
δ-GS	*δ*-Guaiene synthase	4.2.3.87
α-HS	*α*-humulene synthase	4.2.3.104
VS	Vetispiradiene synthase	4.2.3.21
Aromatic polyketides		
CHS	Chalcone synthase	2.3.1.74
CHI	Chalcone isomerase	5.5.1.6
FNS	Flavone synthase I	1.14.20.5
	Flavone synthase II	1.14.19.76
BPS	Benzophenone synthase	2.3.1.151
DCS	Diketide-CoA synthase	2.3.1.218
BAS	Benzalacetone synthase	2.3.1.212
OMT	*O*-methyltransferase	2.1.1