

1 611 **Supporting Information**
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3 612 *Balanophora dioica* ethanol extract ameliorates isoproterenol-induced
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5 613 myocardial injury by suppressing fibrosis, inflammation and apoptosis by
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7 614 regulating TLR4/MyD88/NF- κ B signaling pathway
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9 615 Ting Gao^a, Minjie Li^a, Meng Zhang^a, Yuxi Xiang^a, Zilong Huang^b, Weizhuo Tang^{*,b},
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11 616 Xiaoshu Zhang^{*,a}
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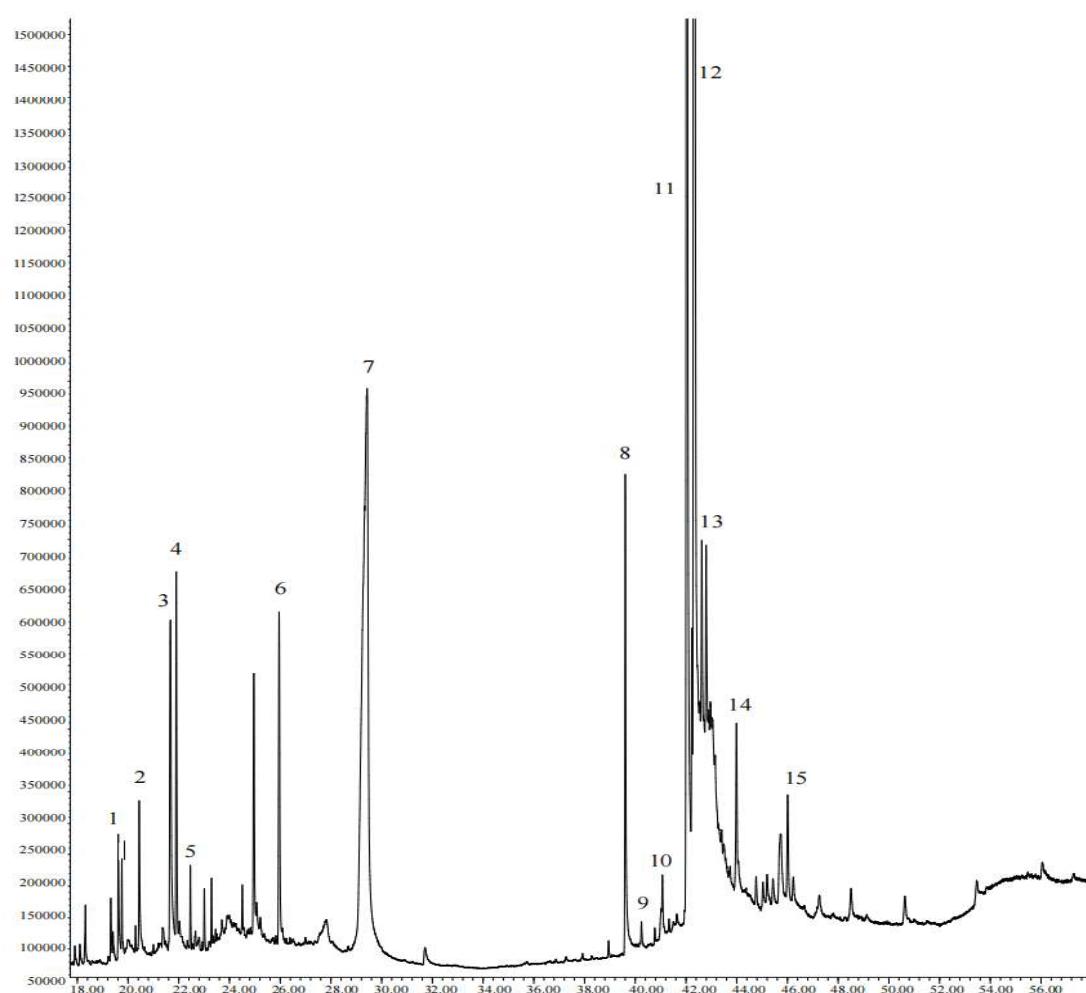
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Contents

- 2 619 **Figure S1. GC-MS spectrum of BDEE.**
- 3 620 **Table S1. Compounds in BDEE identified by GC-MS.**
- 4 621 **Figure S2. Liquid phase spectrogram of BDEE.**
- 5 622 **Figure S3. Positive ion mode mass spectrometry of BDEE.**
- 6 623 **Table S2. The compounds of BDEE detected in positive ion mode.**
- 7 624 **Figure S4. Negative ion mode mass spectrometry of BDEE.**
- 8 625 **Table S3. The compounds of BDEE detected in negative ion mode.**
- 9 626 **Reference**
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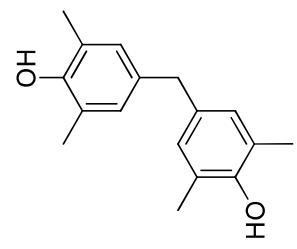
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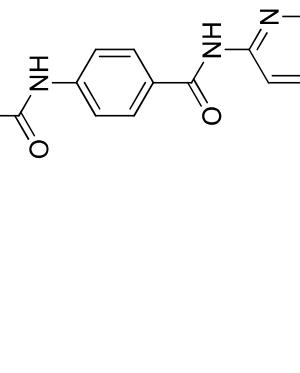
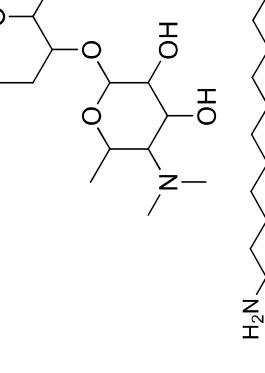
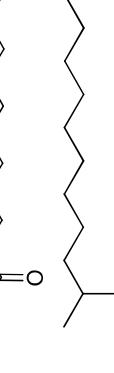
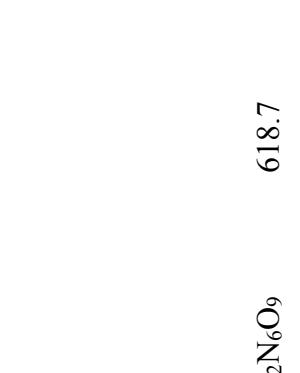
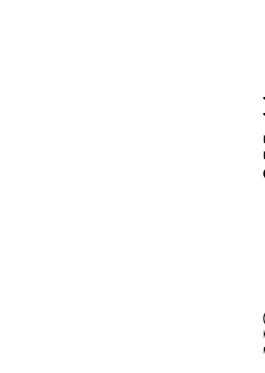
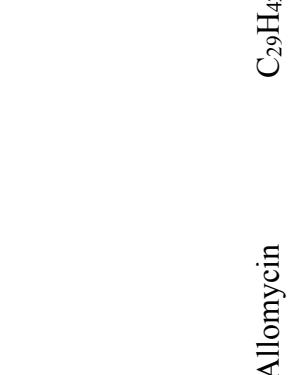
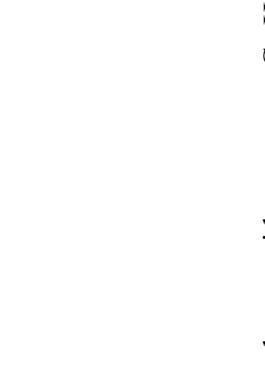
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630 Figure S1. GC-MS spectrum of BDEE.
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Table S1. Compounds in BDDE identified by GC-MS.

No.	t _R (min)	Compound	Formula	Molecular Weight	matching rate	Molecular Structure
1	19.757	Succinic Acid, 2-Methylpent-3-Yl Neopentyl Ester	C ₁₅ H ₂₈ O ₄	272.38	78	
2	20.444	Benzofuran, 2,3-dihydro-	C ₈ H ₈ O	120.15	83	
3	21.686	p-Isopropenylphenol	C ₉ H ₁₀ O	134.17	93	



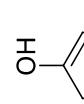
15	26	4	21.906	Phenol, 4,4'-methylenebis [2,6-dimethyl-]	C ₁₇ H ₂₀ O ₂	256.34	72
16	27	5	22.455	1-Acetyl-2-amino-3-cyano-7- isopropyl-4-methylazulene	C ₁₇ H ₁₈ N ₂ O	266.34	59
17	30	6	25.978	β -D-Glucopyranose, 1,6- anhydro-	C ₆ H ₁₀ O ₅	162.14	94
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7	29.392	Allomycin	$C_{29}H_{42}N_6O_9$	618.7	45			
8	39.605	Hexadecanamide	$C_{16}H_{33}NO$		255.44			
9	40.234	Pentadecane, 2-methyl-	$C_{16}H_{34}$		226.44			

15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65

10	41.084	2-(4'-Hydroxyphenyl)-2-(4'-methoxyphenyl) propane	C ₁₆ H ₁₈ O ₂	242.31	94
11	42.054	9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	281.5	99
12	42.326	4,4'-(1-methylethylidene) bis-Phenol	C ₁₅ H ₁₆ O ₂	228.29	98

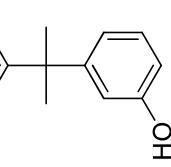
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42.793

3,4'-Isopropylidenediphenol

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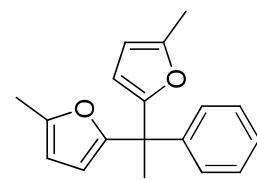


43.983

2,2'-(α -methylbenzylidene)
bis (5-methylfuran)

266.3

C₁₈H₁₈O₂

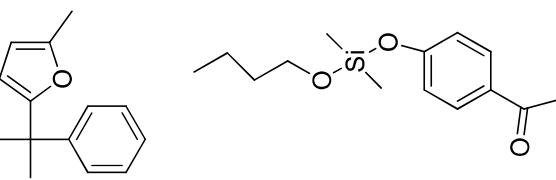


45.994

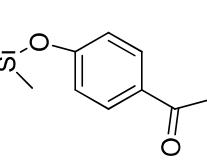
Silane, dimethyl(4-
acetylphenoxy) butoxy-

266.41

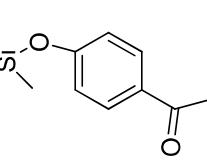
C₁₄H₂₂O₃Si



83



87



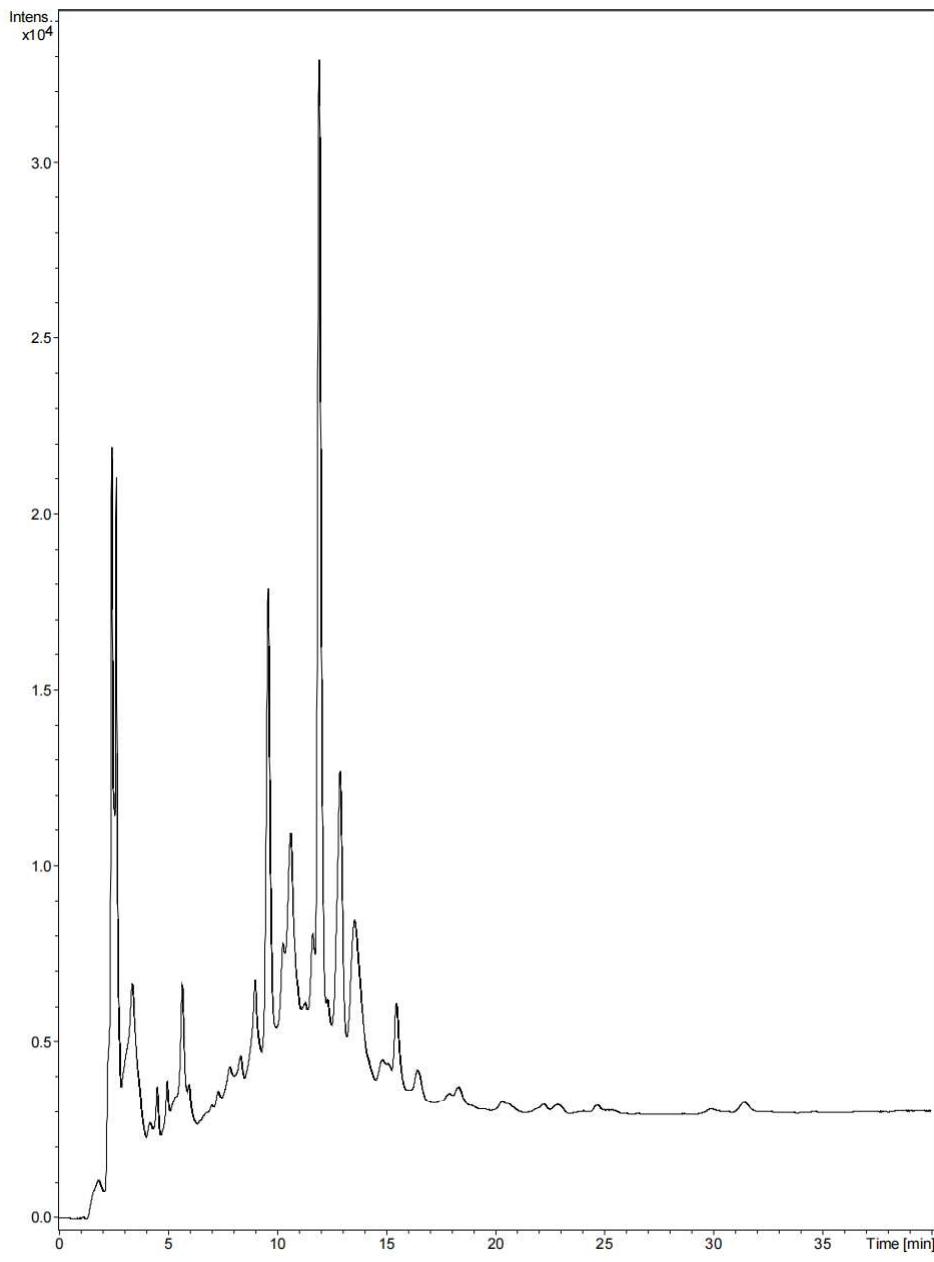


Figure S2. Liquid phase spectrogram of BDEE.

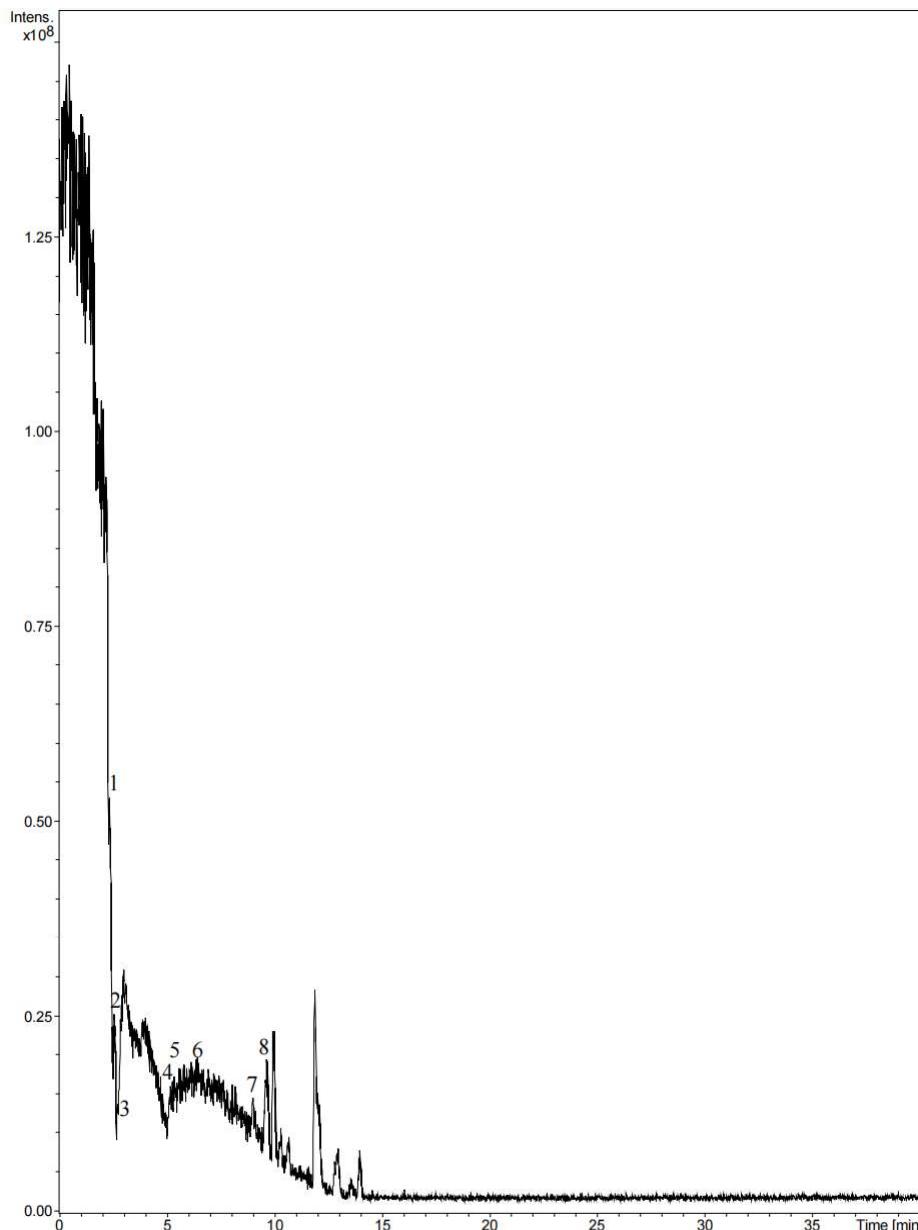
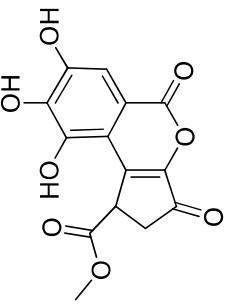
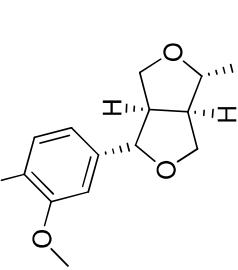
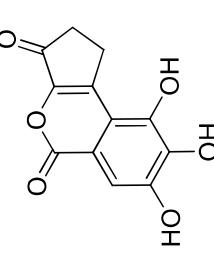
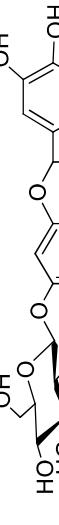
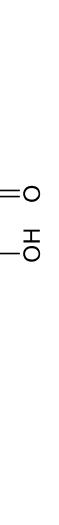


Figure S3. Positive ion mode mass spectrometry of BDEE.

Table S2. The compounds of BDEE detected in positive ion mode.

No.	t _R /min	m/z	Formula	Proposed compounds	Structure	References
1	2.29	329.0273 [M+Na] ⁺	C ₁₄ H ₁₀ O ₈	methyl brevifolinicarboxylate		[1] [4] [12]
2	2.66	359.1495 [M+H] ⁺	C ₂₀ H ₂₂ O ₆	pinoresinol		[2] [5] [6]
3	2.72	249.0393 [M+H] ⁺	C ₁₂ H ₈ O ₆	brevifolin		[1] [12]

26	4	5.08	365.1212 $[\text{M}+\text{Na}]^+$	$\text{C}_{16}\text{H}_{22}\text{O}_8$	coniferin	[2] [4] [6]
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7	9.21	473.1060 [M+Na] ⁺	 Naringenin-7-O- β -D-glucopyranoside
8	9.65	449.1700 [M+H] ⁺	 luteolin-7-O- β -D-glucoside

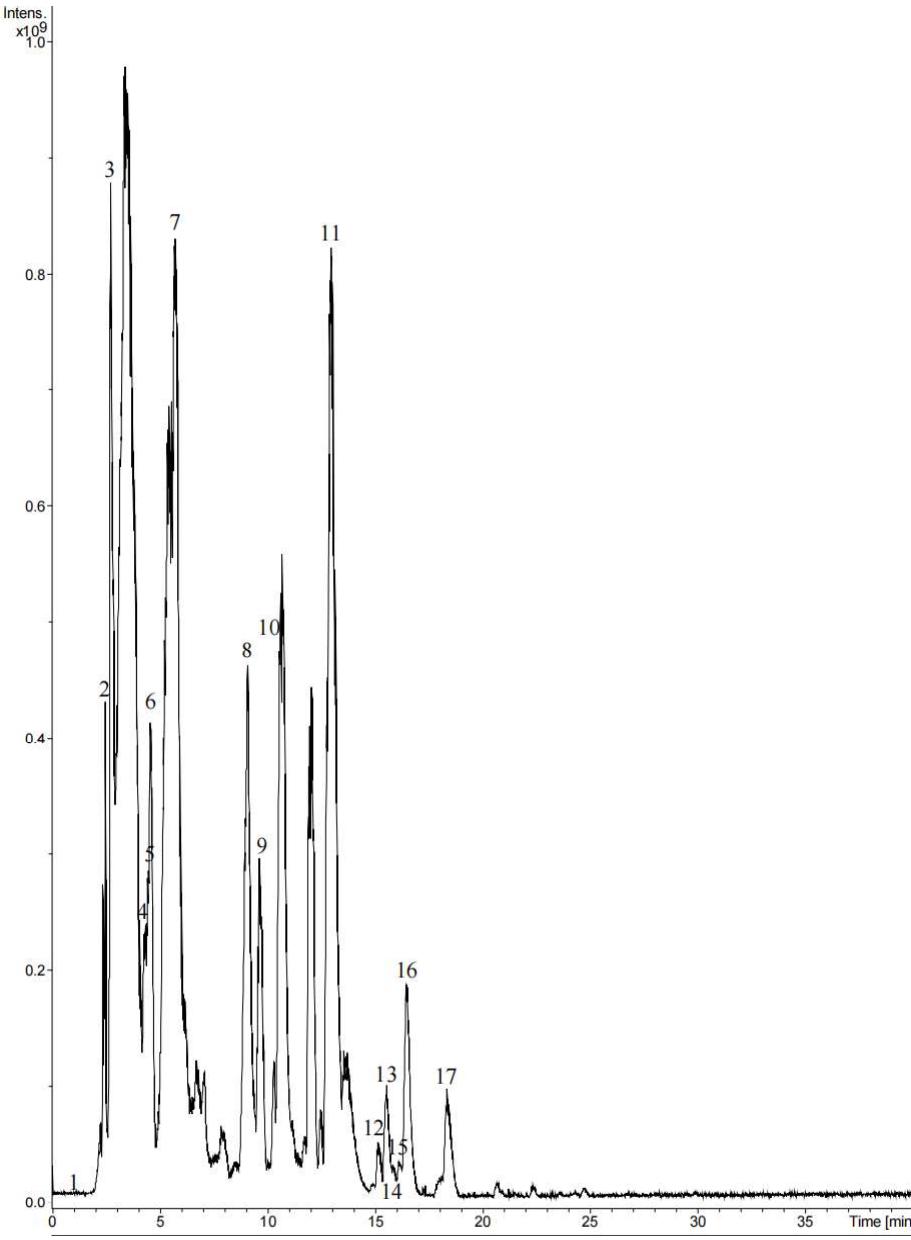
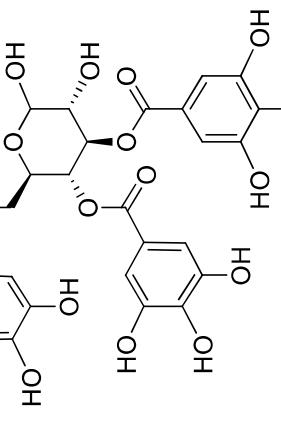
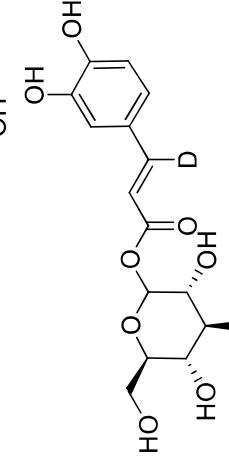
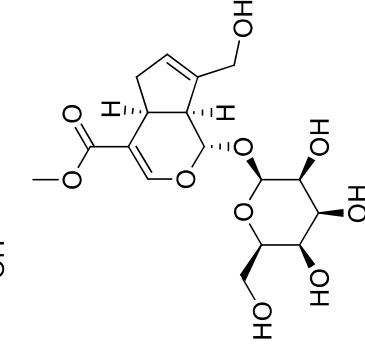


Figure S4. Negative ion mode mass spectrometry of BDEE.

4 Table S3. The compounds of BDEE detected in negative ion mode.

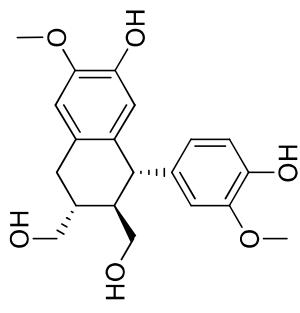
No.	tr/min	m/z	Formula	Proposed compounds	Structure	References
30						
31	1	0.81	283.2637 [M-H] ⁻	C ₁₈ H ₃₆ O ₂	stearic acid	
32						[13]
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38	2	2.61	355.1182 [M-H] ⁻	C ₂₀ H ₂₀ O ₆	balanophonin	
39						[12]
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49	3	2.90	483.0775 [M-H] ⁻	C ₂₀ H ₂₀ O ₁₄	2,6-di-O-galloyl-D-glucopyranose	[11] [12]
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4	4.56	635.0884 [M-H] ⁻	$C_{27}H_{24}O_{18}$	3,4,6-tri-O-galloyl-D-glucopyranose		[11] [12]
5	4.69	342.0934 [M-H] ⁻	$C_{15}H_{17}DO_9$	1-O-(E)-caffeooyl- β -D-glucopyranose		[8] [11] [12]
6	4.84	387.1291 [M-H] ⁻	$C_{17}H_{24}O_{10}$	geniposide		[12]

 1-O-(E)-caffeyl-3-O-galloyl-β-D-glucopyranose [9] [11] [12]	 eriodictyol [4]	 (-)lariciresinol [2][12]
7 5.56 493.0982 $[M-H]^-$	$C_{22}H_{22}O_{13}$	
8 9.68 287.0556 $[M-H]^-$	$C_{15}H_{12}O_6$	
9 9.97 359.1495 $[M-H]^-$	$C_{20}H_{24}O_6$	

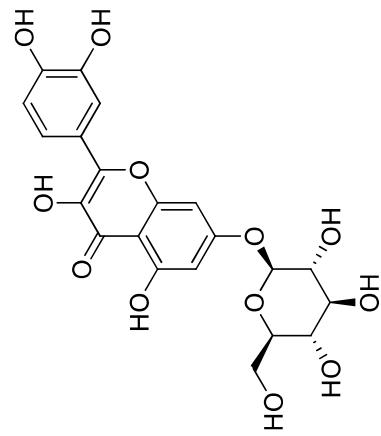
[1] [12]



isolariciresinol

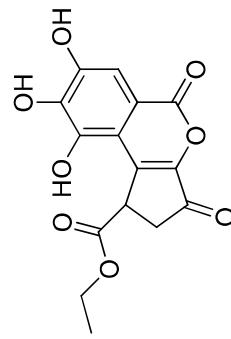
[12]

quercimeritrin

10 10.49 463.0877
[M-H]⁻ C₂₁H₂₀O₁₂

[1]

ethyl brevifolin carboxylate

11 13.25 319.0454
[M-H]⁻ C₁₅H₁₂O₈

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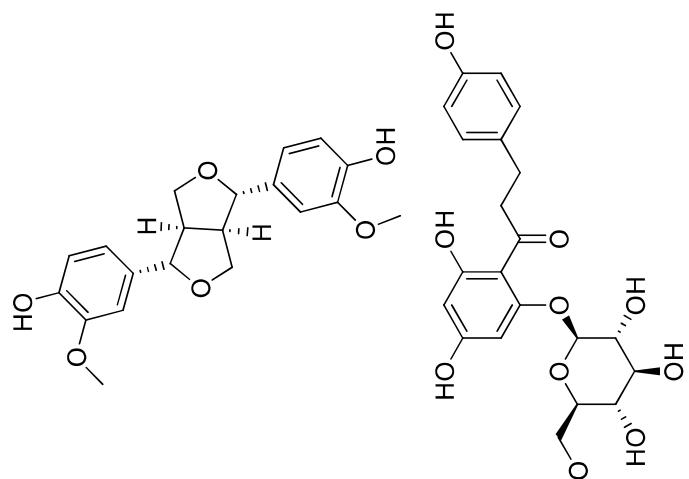
12	15.29	375.1338 [M-H] ⁻	C ₂₀ H ₂₂ O ₆
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13	15.57	435.1291 [M-H] ⁻	C ₂₁ H ₂₄ O ₁₀
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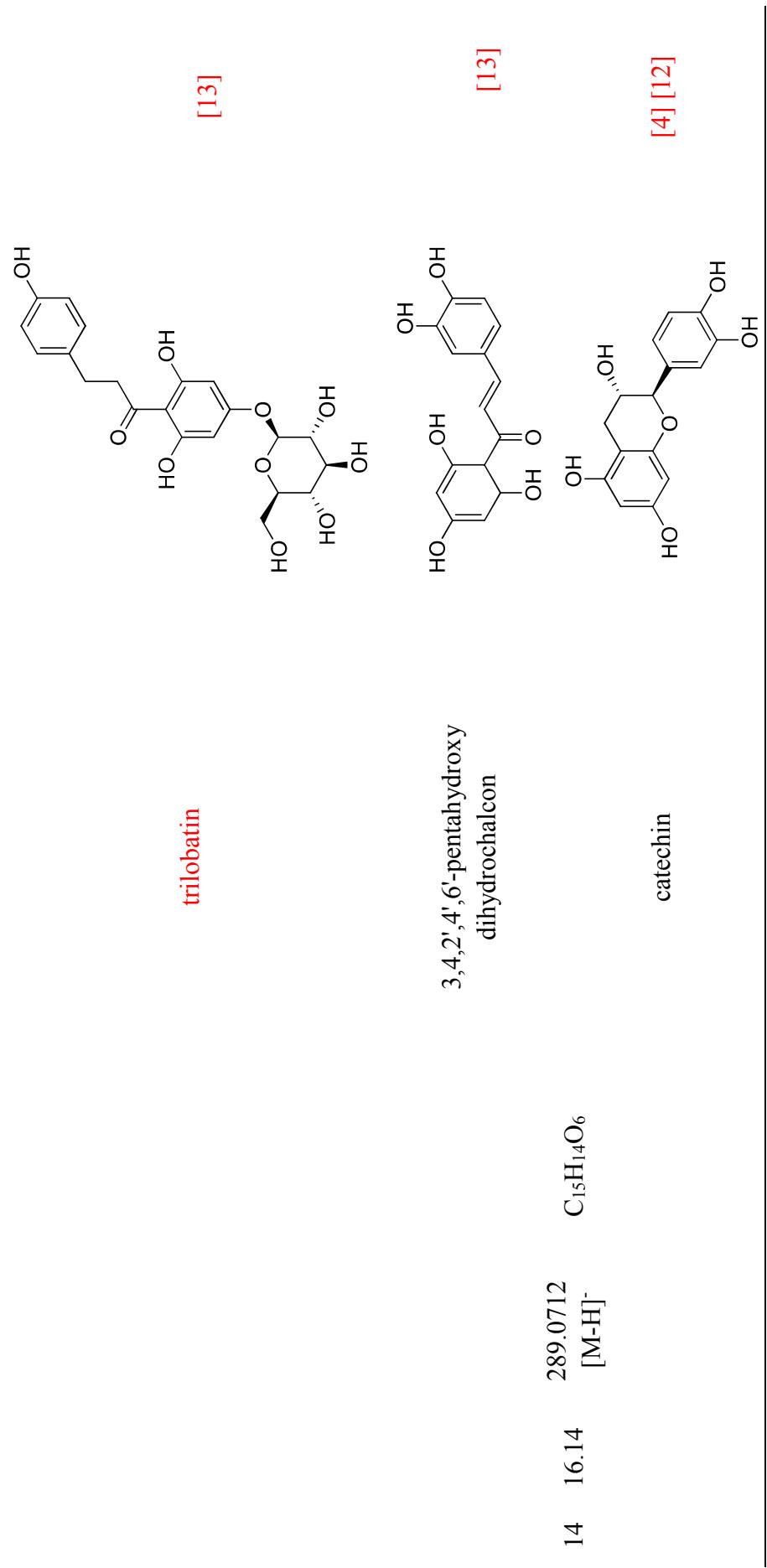
pinoresinol

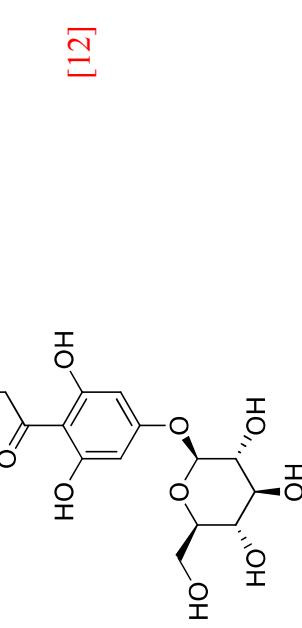
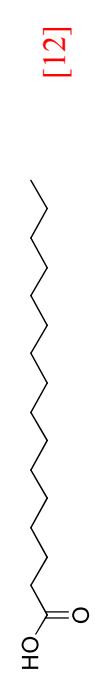
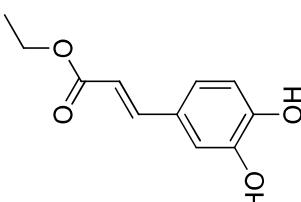
phloridzin

[2] [5] [6]



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21	16.23	465.1397 [M-H] ⁻	C ₂₂ H ₂₆ O ₁₁	hesperetin dihydrochalcone 4' <i>β</i> -D-glucoside 	[12]
15	16.73	255.2324 [M-H] ⁻	C ₁₆ H ₃₂ O ₂	palmitic acid 	[12]
49	18.47	207.0657 [M-H] ⁻	C ₁₁ H ₁₂ O ₄	balanophorin B 	[3][7][10] [12]

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