Electronic Supplementary Material (ESI) for Medical Chemistry Communications

Fast and effective identification of the bioactive compounds and their targets form the medicinal plants *via* computational chemical biology approach

Shoude Zhang[1,†], Weiqiang Lu[2,†], Xiaofeng Liu[2,†], Yanyan Diao[2], Fang Bai[2], Liyan Wang[2], Lei Shan[3,*], Jin Huang[2,*], Honglin Li[2,*], Weidong Zhang[1,3,*]

[1]School of Pharmacy, Shanghai Jiao Tong University, Shanghai 200240, China; [2]Shanghai Key Laboratory of Chemical Biology, School of Pharmacy, East China University of Science and Technology, Shanghai 200237, China; [3]Department of Phytochemistry, School of Pharmacy, Second Military Medical University, Shanghai 200433, China

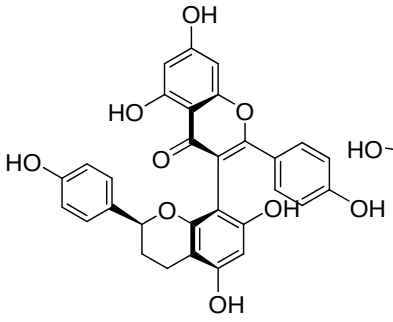
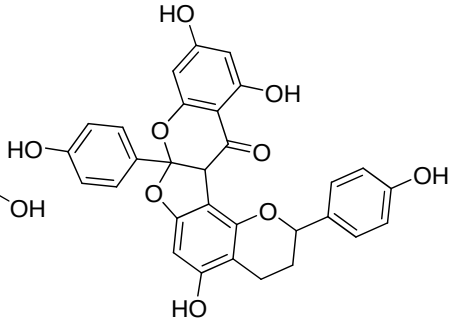
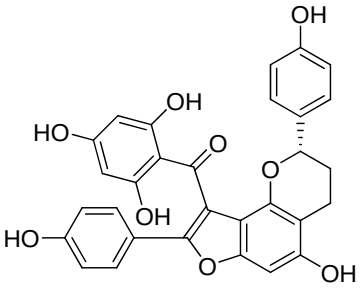
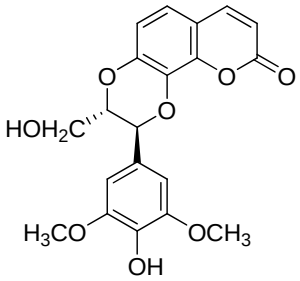
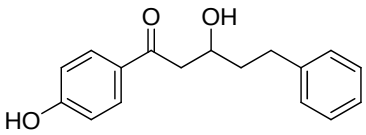
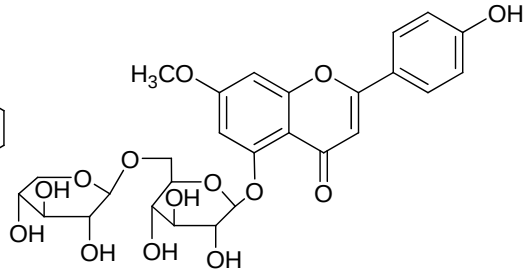
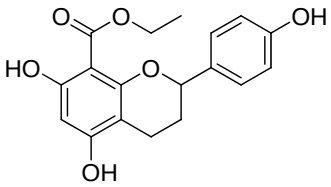
† These authors contributed equally to this work.

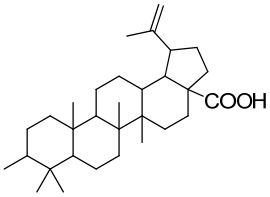
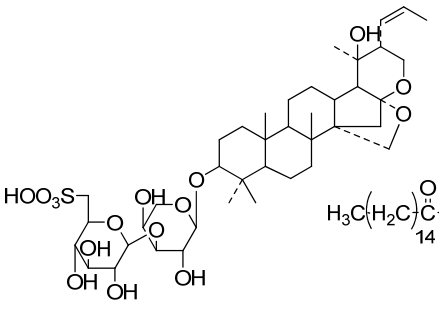
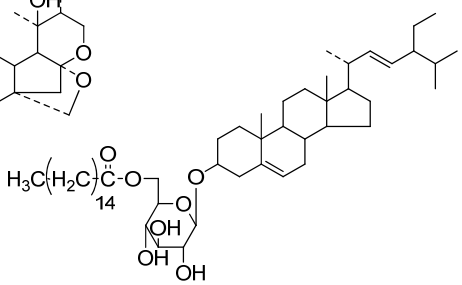
* To whom correspondence should be addressed.

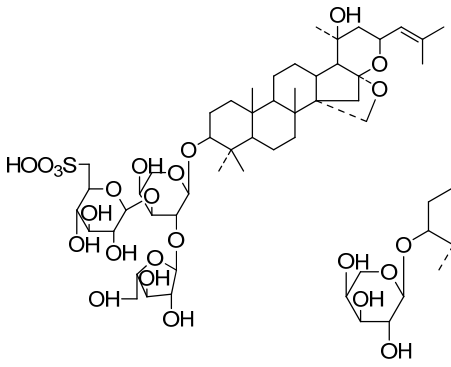
Tel: +86-21-64250213; Fax: +86-21-64250213;

Email: shanleish@yahoo.com.cn, huangjin@ecust.edu.cn, hlli@ecust.edu.cn, and wdzhangy@hotmail.com

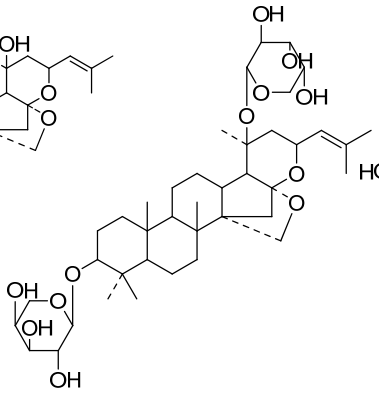
Table S2. Structures of all compounds

Bacopa monnieri(L.)Wettst	
	1
	2
	3
	4
	5
	6
	7

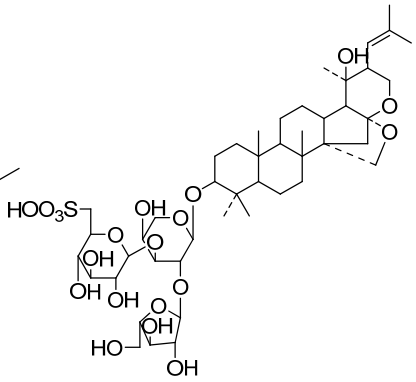
Daphne odora Thunb. var. *marginata*		
		
8	9	10



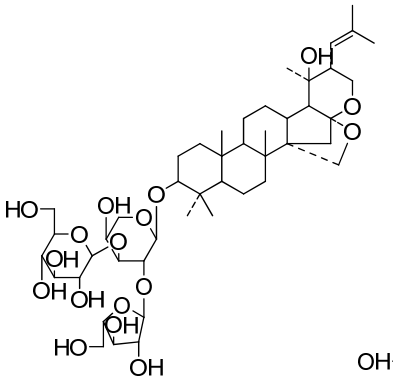
11



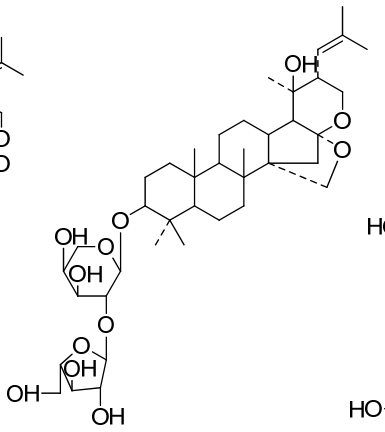
12



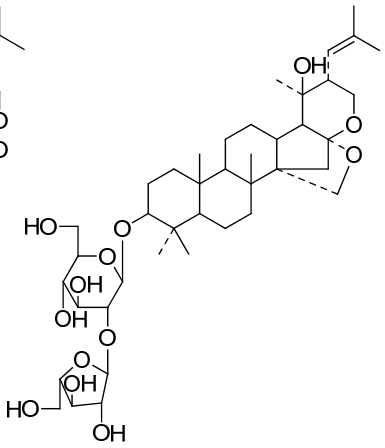
13



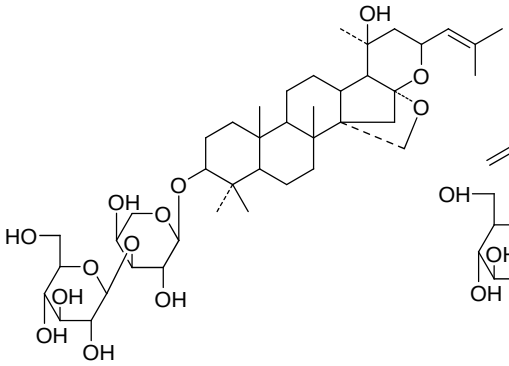
14



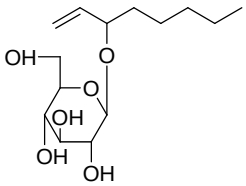
15



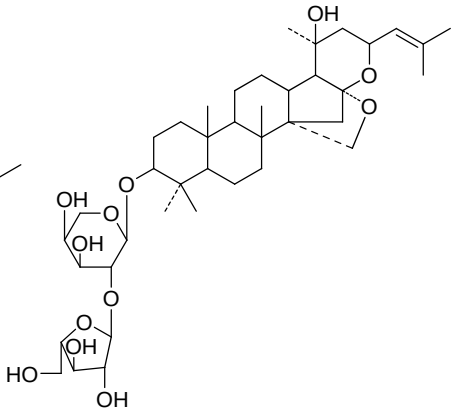
16



17

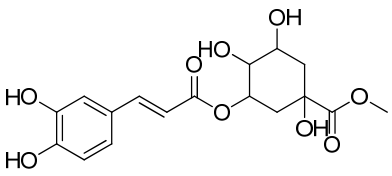


18

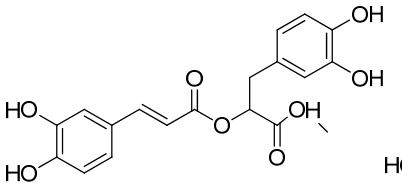


19

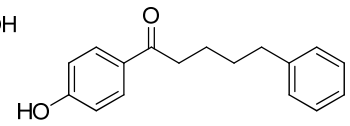
Analogues



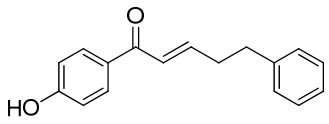
20



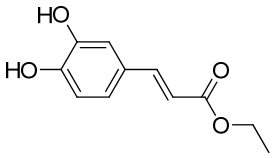
21



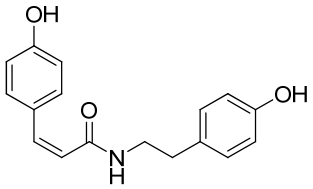
22



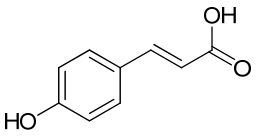
23



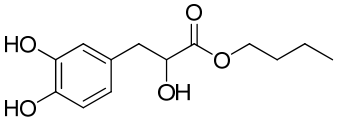
24



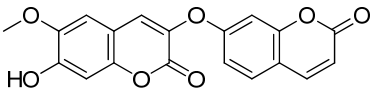
25



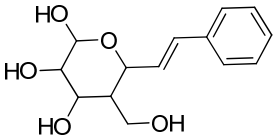
26



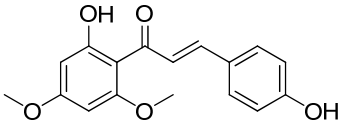
27



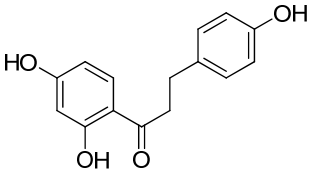
28



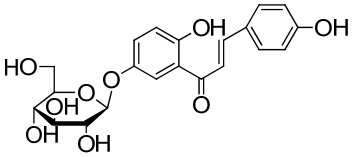
29



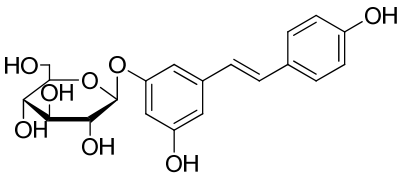
30



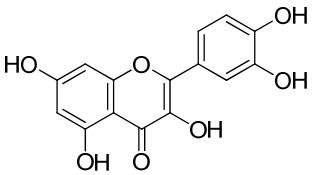
31



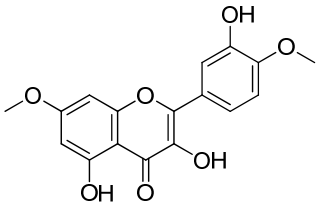
32



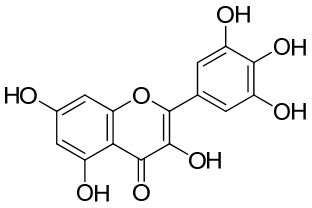
33



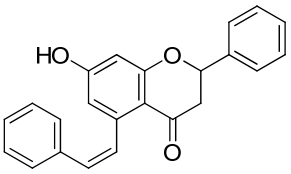
34



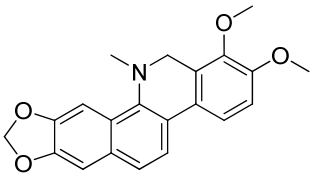
35



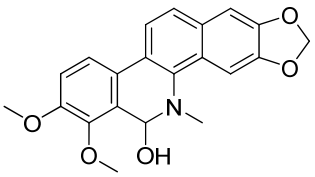
36



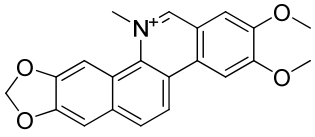
37



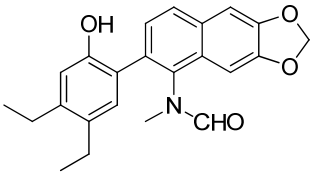
38



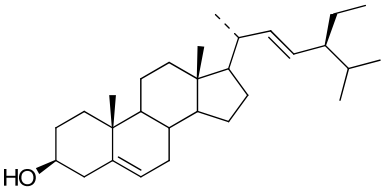
39



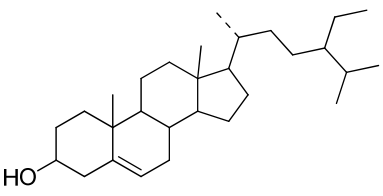
40



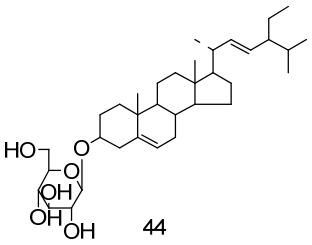
41



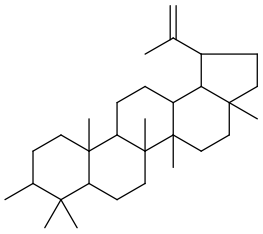
42



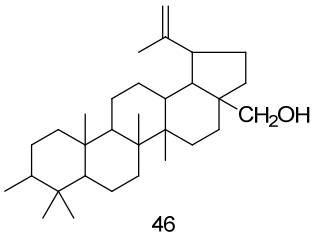
43



44



45



46

Chemistry

Compound 1: Daphnodorin D_2, isolated from *Daphne odora* Thunb. var. *marginata*; yellow powder; UV (MeOH) λ_{max} (log ε): 216, 268; ESI-MS: *m/z* 527 $[M+H]^+$; ^{1}H-NMR (500MHz, CD_3OD, δ): 1.64-2.03 (2H, m), 2.59 (2H, m), 4.84 (1H, dd, J = 10, 1 Hz), 6.06 (1H, s), 6.17 (1H, d, J = 2.0 Hz), 6.36 (1H, d, J = 2.0 Hz), 6.60 (2H, d, J = 8.0 Hz), 6.73 (2H, d, J = 9.0 Hz), 6.81 (2H, d, J = 8.0 Hz), 7.46 (2H, d, J = 9.0 Hz); ^{13}C-NMR (125MHz, CD_3OD, δ): 20.0, 30.5, 78.5, 94.6, 96.0, 99.8, 100.7, 103.0, 105.0, 114.2, 115.8, 115.8, 126.0, 128.1, 131.4, 134.4, 155.4, 155.9, 157.4, 157.7, 159.5, 160.9, 163.3, 164.6, 166.1, 183.7.

Compound 2: Daphnodorin C, isolated from *Daphne odora* Thunb. var. *marginata*; yellow powder; UV (MeOH) λ_{max} (log ε): 222, 283, 322 nm; ESI-MS: *m/z* 565 $[M+Na]^+$; ^{1}H-NMR (500MHz, DMSO-d_6, δ): 1.57 (1H, m), 2.27 (1H, m), 2.55 (2H, m), 4.80 (1H, d, J = 11.0 Hz), 5.46 (1H, s), 5.51 (1H, d, J = 2.0 Hz), 5.82 (1H, d, J = 2.0 Hz), 6.09 (1H, s), 6.59 (2H, d, J = 8.0 Hz), 6.68 (2H, d, J = 9.0 Hz), 6.85 (2H, d, J = 8.0 Hz), 7.03 (2H, d, J = 9.0 Hz); ^{13}C-NMR (125MHz, DMSO-d_6, δ): 19.1, 28.1, 75.7, 89.2, 89.3, 90.7, 93.7, 95.9, 102.4, 102.5, 102.6, 114.7, 123.3, 125.9, 128.7, 131.0, 152.2, 156.1, 157.5, 157.6, 158.9, 160.6, 167.9, 193.1.

Compound 3: Daphnodorin A, isolated from *Daphne odora* Thunb. var. *marginata*; yellow powder; UV (MeOH) λ_{max} (log ε): 209, 305 nm; ESI-MS: *m/z* 527 $[M+H]^+$; ^{1}H-NMR (500MHz, CD_3OD, δ): 1.69 (1H, m), 2.22 (1H, m), 2.62 (2H, m), 4.86 (1H, d, J = 11.0 Hz), 5.72 (1H, d, J = 2.0 Hz), 5.74 (1H, d, J = 2.0 Hz), 6.58 (1H, s), 6.60 (2H, d, J = 8.0 Hz), 6.78 (2H, d, J = 8.5 Hz), 6.85 (2H, d, J = 8.0 Hz), 7.39 (2H, d, J = 8.5 Hz); ^{13}C-NMR (125MHz, DMSO-d_6, δ): 19.6, 29.1, 76.1, 89.2, 94.5, 94.5,104.3, 105.8, 110.0,114.7, 115.6, 117.0, 121.2,125.9, 126.5, 131.4,146.3, 148.3, 152.2, 153.7,156.1, 157.4, 164.2, 165.1, 165.9, 194.6.

Compound 4: Isodaphneticin, isolated from *Daphne odora* Thunb. var. *marginata*; yellow powder; EI-MS: *m/z* 386 $[M]^+$; ^{1}H-NMR (500 MHz, DMSO-d_6, δ): 3.41 (1H, m), 3.67 (1H, m), 3.78 (6H, s), 4.32 (1H, m), 4.32 (1H, d, J = 8.0 Hz), 4.34 (1H, s), 6.33 (1H, d, J = 10.0 Hz), 6.76 (2H, s), 6.98 (1H, d, J = 9.0 Hz), 7.21 (1H, d, J = 9.0 Hz), 8.00 (1H, d, J = 10.0 Hz), 8.53 (1H, s); ^{13}C-NMR (125 MHz, DMSO-d_6, δ): 56.1,

59.8, 76.6, 78.0, 105.5, 112.7, 113.1, 113.3, 119.7, 125.8, 131.0, 136.2, 143.0, 144.8, 146.7, 147.9, 159.8.

Compound 5: Daphneolon, isolated from *Daphne odora* Thunb. var. *marginata*; white powder; EI-MS: *m/z* 270 $[M]^+$; ^{1}H-NMR (500MHz, CD_3OD, δ): 1.80 (2H, m); 2.72 (1H, m); 3.00 (1H, m); 3.08 (1H, m), 3.09 (1H, m), 4.14 (1H, m), 6.80 (2H, d, J = 7.0 Hz), 7.11 (1H, m), 7.15 (4H, m), 7.84 (2H, d, J = 7.0 Hz); ^{13}C-NMR (125MHz , CD_3OD, δ): 31.0, 38.3, 44.6, 66.9, 114.3, 124.8, 127.4, 127.5, 128.5, 130.1, 141.5, 161.9, 198.1.

Compound 6: Yuankanin, isolated from *Daphne odora* Thunb. var. *marginata*; white powder; UV (MeOH) λ_{max} (log ε): 262, 332; ESI-MS: *m/z* 601 $[M+Na]^+$, 285$[M+H\text{-glu-xyl}]^+$; ^{1}H-NMR (500MHz, DMSO-d_6, δ): 2.98-3.99 (m), 3.89 (3H, s), 4.19(1H, d, J = 7.0Hz), 4.77 (1H, d, J = 8.0Hz), 6.69 (1H, s), 6.87 (1H, d, J = 2.0Hz), 6.91 (2H, d, J = 8.0Hz), 7.02 (1H, d, J = 2.0Hz), 7.91 (2H, d, J = 8.0Hz); ^{13}C-NMR (125MHz , DMSO-d_6, δ): 56.1, 65.6, 68.6, 69.5, 69.8, 73.3, 73.4, 75.6, 75.9, 76.5, 96.6, 103.0, 103.8, 104.1, 105.8, 109.2, 115.9, 121.1, 128.1, 158.1, 158.4, 160.8, 161.3, 163.5, 176.8.

Compound 7: 5, 7, 4'-trihydroxy-8-ethoxycarbonyl flavan, isolated from *Daphne odora* Thunb. *var. actrocaulis* Rehd.; gray amorphous powder; UV (MeOH) λ_{max}(log ε): 226, 271, 308 nm; HRESIMS: *m/z* 330.1097 $[M]^+$; ^{13}H-NMR (500MHz, $CDCl_3$, δ): 5.17 (1H, d), 2.29 (1H, m), 2.03 (1H, m), 3.07 (1H, m), 2.88 (1H, m), 6.57 (1H, s), 7.63 (1H, d), 7.30 (2H, d), 7.63 (1H, d), 4.32 (2H, m), 1.22 (3H, t), 12.46 (br).

Compound 8: Betulinic acid, isolated from *Bacopa monnieri*(L.)Wettst; white powder; EI-MS: *m/z* 456 $[M]^+$; ^{1}H-NMR (500MHz, DMSO-d6, δ): 0.66 (3H, s), 0.78 (3H, s), 0.88 (3H, s), 0.89 (3H, s), 0.94 (3H, s), 1.65 (3H, s), 2.83 (1H, m), 3.00 (1H, m), 4.56 (1H, d, J = 0.52 Hz), 4.69 (1H, d, J = 1.62 Hz); ^{13}C-NMR (125MHz, DMSO-d6, δ): 38.1, 26.9, 76.6, 38.2, 54.8, 17.7, 36.7, 40.1, 49.8, 36.5, 20.3, 24.9, 37.5, 41.8, 28.9, 33.8, 55.2, 48.5, 46.4, 150.0, 29.9, 31.5, 27.8, 15.4, 15.6, 15.5, 14.1, 176.8, 109.1, 18.7.

Compound 9: Bacopaside VI, isolated from *Bacopa monnieri*(L.)Wettst; white powder; $[\alpha]_D$ -26.3° (MeOH, c 0.5); EI-MS: *m/z* 847 $[M + H]^+$; ^{1}H-NMR (500MHz,

DMSO-d_6, δ): 2.99 (1H, dd, J = 4.0 Hz, 12 Hz), 2.45 (1H, m), 0.95 (3H, s), 0.74 (3H, s), 1.02 (3H, s), 2.20 (1H, d, J = 11 Hz), 5.30 (1H, d, J = 10.0 Hz), 1.69 (3H, s), 1.61 (3H, s), 0.97 (3H, s), 0.78 (3H, s), 3-*O*-Ara: 4.16 (1H, d, J = 7.0 Hz), 3.50 (1H, m), 3.46 (1H, m), 3.82 (1H, m), 3.64 (1H, m), 3.43 (H, m), Glu: 4.40 (1H, d, J = 8.0 Hz,), 3.07 (1H, m), 3.17 (1H, m), 3.27 (1H, m), 3.07 (1H, m), 4.02 (1H, m), 3.77 (1H, m); ^{13}C-NMR (125MHz, DMSO-d6, δ): 38.0, 25.8, 87.7, 39.4, 55.2, 17.5, 35.8, 36.6, 52.0, 36.7, 21.0, 27.7, 35.8, 52.4, 35.2, 109.1, 50.0, 18.4, 15.9, 70.6, 25.9, 44.5, 64.9, 123.1, 132.1, 26.3, 18.3, 27.4, 16.2, 64.7, **3-*O*-Ara**: 05.5, 70.1, 82.9, 67.3, 65.7, **Glu**: 104.3, 73.8, 75.9, 69.8, 74.8, 65.7.

Compound 10: 3-*O*-stigmasterol-(6-*O*-palmitoyl)-*β*-*D*-glucopyranoside, isolated from *Bacopa monnieri*(L.)Wettst, white waxy solid; ES-MS: *m/z* 835 $[M + Na]^+$; ^{13}C-NMR (125MHz, CDCl3, δ): 37.5, 31.5, 79.9, 39.4, 140.8, 121.9, 31.9, 32.0, 50.4, 36.9, 21.5, 39.7, 42.2, 57.0, 24.6, 29.1, 56.2, 12.4, 19.8, 40.9, 21.5, 138.8, 129.5, 51.7, 31.9, 19.3, 12.3, 21.4, 18.7; **3-O-β-D-Glu**: 101.5, 73.9, 76.4, 70.6, 74.2, 63.6; **palmitoyl**: 174.8, 34.6, 32.3 23.0-30.0, 14.4.

Compound 11: Bacopaside IX, isolated from *Bacopa monnieri*(L.)Wettst; white powder; $[\alpha]_D$ -41.0 (MeOH, c 0.5); EI-MS: *m/z* 1023 $[M + 2Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.4, 26.4, 88.4, 39.5, 55.8, 18.0, 35.7, 37.2, 52.7, 36.9, 21.4, 28.3, 36.7, 53.2, 36.5, 110.0, 51.0, 18.5, 16.0, 71.5, 26.8, 45.1, 68.3, 126.7, 133.8, 25.7, 18.1, 27.5, 16.2, 65.5, **3-*O*-Ara**: 105.1, 75.9, 83.3, 66.9, 65.4, **Ara(f)**: 109.7, 83.3, 77.3, 84.4, 61.5, **Glu**: 104.7, 74.4, 77.0, 70.4, 76.0, 66.9.

Compound 12: Bacopasaponin A, isolated from *Bacopa monnieri*(L.)Wettst; white powder; EI-MS: *m/z* 759 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.3, 26.6, 88.5, 39.4, 55.8, 18.0, 35.9, 37.2, 52.7, 37.1, 21.4, 28.1, 35.6, 53.5, 37.1, 109.8, 52.5, 18.4, 15.9, 75.5, 24.9, 41.5, 68.5, 127.3, 133.6, 25.4, 18.0, 27.9, 16.4, 65.6, **3-*O*-Ara(p)**: 105.9, 71.0, 72.7, 67.4, 64.7, **20-*O*-Ara(p)**: 98.5, 72.7, 74.8, 69.0, 66.4.

Compound 13: Bacopaside I, isolated from *Bacopa monnieri*(L.)Wettst; white powder; $[\alpha]_D$ -44.2 (MeOH, c 0.5); EI-MS: *m/z* 977 $[M - H]^-$ 1023 $[M + 2Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.5, 26.5, 88.5, 39.6, 55.9, 18.1, 35.8, 37.3, 52.8, 37.0, 21.5, 28.4, 36.8, 53.3, 36.6, 110.1, 51.0, 18.6, 16.1, 71.6, 26.9, 45.9, 65.9, 123.8,

132.7, 25.8, 18.2, 27.6, 16.3, 65.6.

Compound 14: Bacopasaponin C, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: *m/z* 921 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.5, 26.4, 88.3, 39.5, 56.0, 18.0, 35.8, 37.2, 52.8, 37.0, 21.4, 28.3, 36.8, 53.2, 36.6, 109.9, 51.0, 18.5, 16.0, 71.5, 26.8, 46.0, 65.8, 123.8, 132.5, 25.6, 18.1, 27.6, 16.2, 65.5, **3-*O*-Ara**: 105.3, 76.6, 83.1, 68.1, 65.3, **Ara(f)**: 110.1, 83.4, 77.8, 84.8, 61.9, **Glu:** 104.6, 74.9, 77.8, 71.3, 78.1, 62.4.

Compound 15: Bacopasaponin B, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: *m/z* 759 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.5, 26.6, 88.8, 39.5, 55.9, 17.9, 35.8, 37.4, 52.9, 37.0, 21.6, 28.4, 36.9, 53.4, 36.9, 110.1, 51.2, 18.6, 16.1, 71.6, 26.9, 45.9, 65.9, 123.8, 132.6, 26.5, 18.3, 27.7, 16.5, 65.7. **3-*O*-Ara:** 105.5, 76.3, 73.5, 68.4, 65.7.

Compound 16: Bacopasaponin D, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: *m/z* 789 $[M+Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.4, 26.4, 88.7, 39.3, 55.7, 17.9, 35.7, 37.2, 52.6, 36.8, 21.4, 28.3, 36.8, 53.2, 36.6, 110.0, 50.9, 18.4, 15.9, 71.4, 26.9, 45.9, 65.8, 123.8, 132.6, 26.8, 18.2, 27.7, 16.5, 65.5, **3-*O*-Glu:** 105.5, 77.9, 88.7, 71.5, 77.8, 62.5, **Ara(f):** 109.2, 80.5, 78.3, 88.1, 62.6.

Compound 17: Bacopaside IV, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: *m/z* 789 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.3, 26.4, 88.1, 39.4, 55.7, 17.9, 35.7, 37.2, 52.6, 36.9, 21.4, 28.2, 36.7, 53.4, 36.5, 110.2, 53.6, 18.5, 15.9, 68.1, 29.7, 45.1, 68.2, 126.7, 133.7, 25.2, 17.9, 27.6, 16.4, 65.4. **3-*O*-Ara(p):** 107.0, 71.6, 83.8, 69.0, 66.6. **Glu:** 106.0, 75.4, 78.0, 71.2, 78.3, 62.3.

Compound 18: 1-octan-3-*O*-*β*-*D*-glucopyranoside, isolated from *Bacopa monnieri*(L.)Wettst; white amorphous powder; EI-MS: *m/z* 313.14 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 114.65, 140.43, 80.51, 34.68, 24.40, 31.77, 22.46, 13.83, **3-*O*-*β*-*D*-Glu:** 103.12, 75.11, 78.33, 71.40, 77.96, 62.51.

Compound 19: Bacopaside G, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: *m/z* 759 $[M + Na]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 38.4, 26.4, 88.7, 39.3, 55.7, 17.9, 35.7, 37.2, 52.6, 36.8, 21.4, 28.3, 36.8, 53.2, 36.6, 110.0, 53.6, 18.4, 15.9, 68.2, 29.7, 45.1, 68.3, 126.8, 133.8, 25.2, 18.2, 27.7, 16.5, 65.5,

3-*O*-Ara(p): 106.1, 76.2, 73.5, 68.7, 66.0, **Ara(f):** 109.9, 81.1, 78.5, 88.2, 62.7.

Compound 20: Methy-3-O-caffeoylquinate, isolated from *Ainsliaea rubrifolia* Franch.; white powder; ESI-MS: *m/z* 367 $[M - H]^-$; ^{1}H-NMR (CD3OD, 300MHz, δ): 7.53 (1H, d, *J* = 15.9 Hz), 7.04 (1H, d, *J* = 2.1 Hz), 6.96 (1H, dd, *J* = 8.1, 2.1 Hz), 6.88 (1H, d, *J* = 8.1 Hz), 6.22 (1H, d, *J* = 15.9 Hz), 5.27 (1H, m), 4.12 (1H, m), 3.75 (1H, m), 3.70 (3H, s), 2.02~2.25(4H, m); ^{13}C-NMR (CD3OD, 75 MHz, δ): 75.8 37.8, 72.5, 70.3, 71.8, 37.8, 175.4, 127.7, 115.7, 149.7, 146.9, 115.7, 122.8, 146.2, 118.6, 168.3, 52.8 (OCH3).

Compound 21: Methyl rosmarinate, isolated from *Dracocephalum forrestii*; yellow powder; ESI-MS: *m/z* 397 $[M + Na]^+$; ^{13}C-NMR (CD3OD, 150 MHz, δ): 128.8, 116.3, 147.9, 145.4, 117.5, 121.8, 37.9, 74.7, 172.2, 127.6, 114.2, 146.2, 149.8, 116.5, 123.2, 146.8, 115.3, 168.3, 52.7.

Compound 22: 1-(4-hydroxyphenyl)-5-phenyl-1-pentaone, isolated from Daphne odora Thunb. var. marginata; white powder; UV (MeOH) λmax (log ε): 276 nm; ESI-MS: *m/z* 255 $[M + H]^+$; ^{1}H-NMR (500MHz, DMSO-d6, δ): 2.92 (2H, t, *J* = 6.0Hz), 1.61 (2H, t, *J* = 3.0Hz), 1.61 (2H, t, *J* = 3.0Hz), 2.60 (2H, t, *J* = 6.0Hz), 7.84 (2H, d, *J* = 9.0Hz), 6.85 (2H, d, *J* = 9.0Hz), 6.85 (2H, d, *J* = 9.0Hz), 7.84 (2H, d, *J* = 9.0Hz), 7.18 (m), 7.27 (m), 7.18 (m), 7.27 (m), 7.18 (m), 10.28 (s); ^{13}C-NMR (125MHz, DMSO-d6, *δ*): 23.7, 30.5, 34.9, 37.1, 115.1, 115.1,128.3, 128.2, 128.1, 125.5, 128.1, 128.2, 130.3, 130.3, 142.0, 161.8,198.1.

Compound 23: 1-(4-hydroxyphenyl)-5-phenyl-2-penten-1-one), isolated from *Daphne tangutica* Maxim; white powder; EI-MS: *m/z* 252 $[M]^+$; ^{13}C-NMR (125MHz, DMSO-d6, *δ*): 187.3, 125.9, 146.7, 33.5, 33.7, 128.7, 130.9, 115.3, 162.0, 115.3, 130.9, 141.0, 128.3, 128.3, 125.8, 128.3, 128.3.

Compound 24: Caffeic acid ethyl ester, isolated from *Incarvillea mairei* var. *grandiflora* (Wehrhahn) Grierson; yellow amorpuous powder; ESI-MS: *m/z* 208; ^{1}H NMR (600MHz ,CD_3OD, *δ*): 7.02 (1H, d, 1.8 Hz), 6.76 (1H, d, 8.1 Hz), 6.91 (1H, dd, 8.1, 1.8 Hz), 7.52 (1H, d, 15.9 Hz), 6.23 (1H, d, 15.9 Hz), 4.18 (2H, q, 7.2 Hz), 1.28 (3H, t, 7.2 Hz); ^{13}C-NMR(150MHz, CD_3OD, *δ*): 128.2 (s), 115.6 (d), 147.3 (s), 150.0 (s), 117.0 (d), 123.4 (d), 147.2 (d), 115.8 (d), 169.8 (s), 61.9 (t), 15.1 (q).

Compound 25: N-p-cis-coumaroyltyramine, isolated from *Crinum asiaticum* L.; white amorphous powder; ESI-MS: *m/z* 282 $[M - H]^-$; ^{13}C-NMR (125MHz, DMSO-d6, δ): 34.4, 40.6, 115.1, 116.7 (C-6, 8, C-5′, 7′), 118.7, 125.9, 129.1, 129.5 (C-5, 9, C-4′, 8′), 138.5, 155.6, 158.7 , 165.2.

Compound 26: p-coumaric acid, isolated from *Incarvillea mairei* var. *grandiflora* (Wehrhahn) Grierson; white amorpuous powder; ESI-MS: *m/z* 164 $[M]^+$; ^{1}H NMR (600MHz ,CD_3OD, δ): 6.32 (1H, d, J = 16.0 Hz), 7.37 (1H, d, J = 16.0 Hz), 7.35 (2H, d, J = 8.5 Hz), 6.77 (2H, d, J = 8.5 Hz), 5.0 (4-OH), 6.41 (2'-H), 6.77 (3-H,5-H), 7.35 (2-H,6-H), 7.37 (7-H), 11.0 (3'-H); ^{13}C-NMR (150MHz ,CD_3OD, δ): 128.7 (s), 130.1 (d), 116.6 (d), 159.8 (s), 116.6 (d), 130.1 (d), 141.5 (d), 122.6 (d), 171.5 (s).

Compound 27: α-Trihydroxy-butyl phenylpropionate, isolated from*Dracocephalum forrestii*; yellow powder; ESI-MS: *m/z* 397 $[M + Na]^+$; ^{13}C-NMR (CD3OD, 150 MHz, δ): 129.8, 117.6, 146.1, 145.1, 116.2, 121.8, 41.2, 73.4, 175.6, 65.7, 31.7, 20.1, 14.0.

Compound 28: Daphnoretin, isolated from *Daphne odora* Thunb. *var. actrocaulis* Rehd.; white feathery crystals; UV (MeOH) λ_{max} (log ε): 222, 265, 324, 345 nm; ESI-MS: *m/z* 352$[M]^+$; ^{1}H-NMR (500MHz, DMSO-d_6, δ): 3.83 (3H, s, -OCH_3), 6.37 (1H, d, J = 9.5Hz), 6.87 (1H, s), 7.11 (1H, dd, J = 9.0Hz, 2.5Hz), 7.16 (1H, d, J = 2.5Hz), 7.21 (1H, s), 7.70 (1H, d, J = 9.0Hz), 7.86 (1H, s), 8.03 (1H, d, J = 9.5Hz), 10.22 (1H, s); ^{13}C-NMR (125MHz, DMSO-d_6, δ): 56.0, 102.7, 103.9, 109.4, 110.1, 113.4, 113.8, 114.3, 129.8, 130.7, 135.7, 143.9, 145.6, 147.3, 150.3, 154.9, 156.8, 159.6, 159.8.

Compound 29: Cinnamyl D-glucopyranoside, isolated from *Crinum latifalium* L; white amorpuous powder; ESI-MS: *m/z* 297 $[M + 1]^+$; ^{13}C-NMR (150MHz ,CD_3OD, δ): 138.3, 127.5, 129.6, 128.7, 129.6, 127.5, 133.8, 126.7, 70.7, **Glu**: 103.4, 75.2, 71.7, 78.1, 78.0, 62.8.

Compound 30: 2',4-Dihydroxy-4',6'-dimethoxychalcone, isolated from *Abies georgei* Orr; amorphous powder; EI-MS: *m/z* 315 $[M]^+$; HRESIMS(negative) $[M - H]^-$ *m/z* 313.1077; ^{13}C-NMR (150MHz, CD_3OD, δ): 143.2, 126.4, 193.9, 166.5, 168.6, 92.4d, 164.7, 106.6, 129.5, 131.1, 115.5, 163.0, 115.5, 131.1, 56.4, 55.9.

Compound 31: Davidigenin, isolated from *Blumea balsamifera* DC.; white powder; ESI-MS: *m/z* 257.4 $[M - H]^-$; ^{13}C-NMR (125 MHz, DMSO-d6, δ): 203.8, 164.4, 164.2, 155.5, 133.0, 131.0, 129.1, 115.0, 112.5, 102.4 , 39.3, 29.3.

Compound 32: Isoliquiritin, isolated from *Incarvillea sinensis* LAM; yellow amorphous powder; ESI-MS**:** *m/z* 487 $[M + Na]^+$, 463 $[M - H]^-$: ^{1}H-NMR (600 MHz, CD_3OD, δ): 7.69 (1H, d, J = 15.6 Hz), 7.79 (1H, d, J = 15.6 Hz), 7.70 (2H, d, J = 1.8 Hz), 6.86 (1H, d, J = 8.4 Hz), 7.57 (1H, dd, J = 8.4, 1.8Hz), Glc:5.21 (1H, d, J = 8.4 Hz), 7.14 (2H, d, J = 8.4 Hz), 7.97 (1H, d, J = 9 Hz), 6.41 (1H, dd, J = 9.0, 2.4Hz), 6.27 (1H, d, J = 2.4 Hz), 5.0 (1H, d, J = 7.8.Hz), 3.29-3.89 (6H, m); ^{13}C-NMR (150 MHz, CD_3OD, δ): 193.3(C=O), 120.1, 144.7, 130.6, 131.4, 118.0, 161.1, 114.5, 167.6, 103.9, 168.3, 109.5, 133.5; **Glc**: 101.8, 74.8, 78.0, 71.3, 78.3, 62.5.

Compound 33: Piceid, isolated from *Abies georgei* Orr; amorphous powder; ESI-MS**:** *m/z* 413 $[M + Na]^+$ 803 $[2M + Na]^+$; ^{13}C-NMR (150 MHz, CD_3OD, δ): 141.4, 107.0, 160.3, 104.0, 159.4, 108.3, 126.6, 129.9, 130.2, 128.9, 116.5, 158.3, 116.5, 128.9, 102.3, 74.9, 77.9, 71.4, 78.1, 62.5.

Compound 34: Quercetin, isolated from *Hypericum japonicum* Thunb.ex Murray; yellow needle crystal; EI-MS: m/z 302 $[M]^+$; ^{1}H-NMR (500 MHz, DMSO-d_6, δ) 7.69 (d, 1H, J = 2 Hz), 6.92 (dd, 1H, J = 8, 2 Hz), 6.89 (d, 1H, J = 9 Hz), 6.42 (d, 1H, J = 2 Hz), 6.20 (d, 1H, J=2 Hz), 12.49 (-OH), 10.80 (-OH), 9.60 (-OH), 9.35 (-OH), 9.35 (-OH); ^{13}C-NMR (125MHz, DMSO-d6, δ): 175.8, 163.8, 160.7, 156.1, 147.7, 146.8, 145.0, 135.7, 121.9, 119.9, 115.6, 115.0, 102.9, 98.1, 93.3.

Compound 35: 3,5,3′-trihydroxy-7,4′-dimethoxyflavone, isolated from *Blumea balsamifera* DC.; yellow powder; ESI-MS: *m/z* 353.2 $[M + Na]^+$; ^{1}H NMR (500 MHz, DMSO-d_6, δ): 3.79 (3H, s, OCH_3), 3.94 (3H, s, OCH_3), 6.20 (1H, d, J = 2.0 Hz), 6.40 (1H, d, J = 2.0 Hz), 7.07 (1H, d, J = 9.0 Hz), 7.60 (1H, dd, J = 9.0, 2.0 Hz), 7.61 (1H, d, J = 2.0 Hz); ^{13}C NMR (125 MHz, DMSO-d_6), δ): 56.3 (OCH_3), 60.5 (OCH_3), 94.7, 99.7, 105.9, 112.3, 116.1, 122.1, 124.2, 139.8, 147.6, 151.7, 157.6, 158.4, 163.1, 166.0, 180.0.

Compound 36: myricetin, isolated from *R. spinuliferum* Franch.; ESI-MS: *m/z* 319

$[M + H]^+$; ^{1}H-NMR (500 MHz, CD_3OD,δ): 6.17 (1H, d, J = 2.0 Hz), 6.37 (1H, d, J = 2.0 Hz), 7.41 (2H, s); ^{13}C-NMR (125 MHz, CD_3OD, δ): 94.4, 99.2, 104.4, 108.5, 123.1, 136.9, 137.3, 146.7, 147.97, 158.1, 162.4, 165.5, 177.2.

Compound 37: Communin A, isolated from *Polytrichum commune* L.ex Hedw.; Colorless needles ($CHCl_3$/MeOH), $[\alpha]_D$: −52 (*c* 0.1, MeOH); UV (EtOH) λ_{max} (log ε) 212 (4.83), 267 (3.68), 295 (2.65), 316 (2.59) nm; CD (MeOH); Δε = 350 (+5.0), 305 (-8.1); HRESIMS *m/z* 341.1176 ($[M - H]^-$ calcd for $C_{23}H_{17}O_3$, 341.1177); ^{13}C-NMR (CD_3OD, 150 MHz, δ): 78.5, 44.5, 191.5, 141.8, 112.2, 164.2, 101.9, 163.0, 111.7, 138.4, 125.4, 128.0, 126.0, 128.0, 125.4, 136.2, 128.4, 127.2, 127.8, 127.1, 128.2, 128.1, 130.8..

Compound 38: Dihydrochelerythrine, isolated from *Zanthoxylum nitidum* (Roxb.) DC.; white needle crystal; EI-MS: *m/z* 349 $[M]^+$; ^{1}H-NMR (500 MHz, CD_3OD, δ): 7.69 (s), 7.11 (s), 7.48 (d, J = 9.0 Hz), 7.70 (d, J = 9.0 Hz), 4.30 (s), 6.94 (d, J = 8.0 Hz), 7.50 (d, J = 8.0 Hz), 6.04 (s), 2.60 (s), 3.92 (s), 3.88 (s); ^{13}C-NMR (125 MHz, CD_3OD,δ): 100.7, 123.8, 147.5, 148.1, 104.3, 124.3, 130.8, 120.1, 48.8, 126.3, 146.2, 152.3, 111.1, 118.7, 126.3, 125.4, 143.9, 101.0, 41.3, 55.8, 61.1.

Compound 39: 8-hydroxydihydrochelerythrine, isolated from *Zanthoxylum nitidum* (Roxb.) DC.; white flake crystal; ESI-MS: *m/z* 366.4 $[M + H]^+$; ^{1}H-NMR (500 MHz, CD_3OD, δ): 7.92 (s), 7.16 (s), 7.45 (d, J = 8.0 Hz), 7.69 (d, J = 8.0 Hz), 6.60 (s), 6.85 (d, J = 8.0 Hz), 7.48 (d, J = 8.0 Hz), 6.11 (s), 3.05 (s), 2.42(s), 3.72(s); ^{13}C-NMR (125 MHz, CD_3OD, δ): 100.9, 123.1, 147.5, 148.1, 104.5, 123.3, 131.2, 119.9, 77.5, 126.2, 146.4, 152.2, 112.4, 118.7, 127.0, 125.6, 138.5, 101.1, 40.9, 60.4, 55.7.

Compound 40: Nitidine, isolated from *Zanthoxylum nitidum* (Roxb.) DC.; white needle crystal; EI-MS: m/z 348 $[M]^+$; ^{13}C-NMR (125 MHz, CD_3OD,δ): 105.4, 121.7, 150.6, 151.1, 107.1, 131.8, 134.6, 119.8, 152.0, 121.5, 109.6, 154.0, 160.8, 103.9, 134.4, 126.1, 146.2, 104.3, 52.1, 57.1, 57.8.

Compound 41: Isoarnottianamide, isolated from *Zanthoxylum nitidum* (Roxb.) DC.; white powder; EI-MS: m/z 381 $[M]^+$; ^{13}C-NMR (125 MHz, CD_3OD, δ): 100.7, 128.8, 149.6, 148.3, 104.7, 128.1, 131.4, 127.2, 150.0, 99.0, 147.4, 142.8, 113.7, 115.9, 131.7, 136.0, 101.6, 33.1, 164.9, 55.9, 56.7.

Compound 42: Stigmast-5,22-dien-3β-ol, isolated from *Gottschelia schizopleura*; Colorless needle crystal; EI-MS: m/z 412 $[M]^+$; ^{1}H-NMR (300 MHz, CDCl3, δ): 5.36 (1H, m), 5.16 (1H, dd, J = 15, 8.4 Hz), 5.02 (1H, dd, J = 15, 8.4 Hz), 3.53 (1H, m), 1.01 (3H, d, J = 7 Hz, H-21), 1.00 (3H, s), 0.88 (3H, d, J = 6 Hz), 0.84 (3H, d, J = 6 Hz), 0.82 (3H, t, J = 6.2 Hz), 0.70 (3H, s).

Compound 43: β-sitosterol, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: m/z 414 $[M]^+$; ^{1}H-NMR (500 MHz, CDCl3, δ): 0.72 (3H,s), 0.81 (3H, d, J = 7.0 Hz), 0.85 (3H, t, J = 8.0 Hz), 0.89 (3H, d, J = 6.0 Hz), 1.11 (3H, s), 1.08 (3H, d, J = 7.0 Hz), 3.60 (1H, m), 5.41 (1H, t, 2.3 Hz); ^{13}C-NMR (125 MHz, CDCl3, δ): 37.5, 31.8, 72.0, 42.3, 141.1, 121.9, 32.1, 31.0, 50.5, 36.8, 21.7, 40.2, 42.5, 56.8, 24.7, 29.3, 56.1, 12.3, 19.6, 40.7, 21.5, 138.6, 129.7, 51.4, 32.0, 19.4, 12.7, 21.3, 19.5.

Compound 44: Stigmasterol-3-O-β-D-glucopyranoside, isolated from *Bacopa monnieri*(L.)Wettst; white powder; ESI-MS: *m/z* 574 $[M]^+$; ^{13}C-NMR (125MHz, Py-d_5, δ): 37.5, 31.5, 79.3, 39.4, 140.8, 121.9, 31.9, 32.0, 50.4, 36.9, 21.5, 39.7, 42.2, 57.0, 24.6, 29.1, 56.2, 12.4, 19.8, 40.9, 21.5, 138.8, 129.5, 51.7, 31.9, 19.3, 12.3, 21.4, 18.7.

Compound 45: Lupeol, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; ^{13}C-NMR (125MHz, DMSO-d_6, δ): 39.0, 26.9, 77.8, 39.2, 55.5, 17.7, 34.4, 40.8, 50.4, 37.2, 20.3, 24.9, 38.0, 42.7, 28.9, 35.5, 42.9, 48.3, 47.9, 150.7, 29.8, 39.9, 28.3, 15.9, 16.1, 16.0, 14.4, 17.8, 109.6, 19.1.

Compound 46: 28-hydroxyllupeol, isolated from *Bacopa monnieri*(L.)Wettst; white needle crystal; EI-MS: m/z 442 $[M]^+$; ^{13}C-NMR (125MHz, $CDCl_3$, δ): 39.2, 27.6, 79.4, 37.6, 55.8, 18.7, 34.8, 39.3, 50.9, 37.5, 21.3, 25.8, 37.8, 41.7, 29.8, 34.4, 43.2, 49.3, 48.2, 150.8, 29.9, 29.7, 28.4, 16.4, 15.7, 16.4, 15.2, 61.0, 109.9, 19.5.