**Table S1**

*In vivo* constituents of VB.

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| NO. | Chemical name | Chemical structure | Reference |
| P1 | Resibufogenin  (C24H32O4) |  | Xia et al. 2010 |
| P2 | Bufalin  (C24H34O4) |  | Xia et al. 2010 |
| P3 | 19-oxo-bufalin  (C24H32O5) |  | Xia et al. 2010 |
| P4 | Desacetylcinobufagin  (C24H32O5) |  | Ning et al. 2010 |
| P5 | Marinobufagin  (C24H32O5) |  | Xia et al. 2010 |
| P6 | Resibufaginol  (C24H32O5) |  | Xia et al. 2010 |
| P7 | 19-hydroxybufalin  (C24H34O5) |  | Xia et al. 2010 |
| P8 | Desacetylbufotalin  (C24H34O5) |  | Xia et al. 2010 |
| P9 | Gamabufotalin  (C24H34O5) |  | Xia et al. 2010 |
| P10 | Telocinobufagin  (C24H34O5) |  | Xia et al. 2010 |
| P11 | 19-oxo-desacetylcinobufagin  (C24H30O6) |  | Xia et al. 2010 |
| P12 | Arenobufagin  (C24H32O6) |  | Xia et al. 2010 |
| P13 | Hellebrigenin  (C24H32O6) |  | Xia et al. 2010 |
| P14 | Cinobufagin  (C26H34O6) |  | Tao et al. 2017 |
| P15 | Bufotalin  (C26H36O6) |  | Tao et al. 2017 |
| P16 | Cinobufaginol  (C26H34O7) |  | Xia et al. 2010 |
| P17 | Cinobufotalin  (C26H34O7) |  | Liang et al. 2008 |
| M1 | 3-oxo-resibufogenin  (C24H30O4) |  | Zhu et al. 2013 |
| M2 | 3-epi-bufalin  (C24H32O4) |  | Xia et al. 2010 |
| M3 | 3-oxo-desacetylcinobufagin  (C24H30O5) |  | Ning et al. 2010; He et al. 2012 |
| M4 | 5β-hydroxyresibufogenin  (C24H32O5) |  | Zhu et al. 2013 |
| M5 | 3,14,15-trihydroxy-bufa-20,22-dienolide  (C24H34O5) |  | Zhu et al. 2013 |
| M6 | 6α-hydroxybufalin  (C24H34O5) |  | Xin et al. 2016 |
| M7 | 5β-hydroxybufalin  (C24H34O5) |  | Xin et al. 2016 |
| M8 | 1,5-dihydroxyresibufogenin  (C24H32O6) |  | Zhu et al. 2013 |
| M9 | 1-hydroxyldesacetylcinobufagin  (C24H32O6) |  | Ning et al. 2010 |
| M10 | 5,16-dihydroxy-resibufogenin  (C24H32O6) |  | Zhu et al. 2013 |
| M11 | 5-hydroxyldesacetylcinobufagin  (C24H32O6) |  | He et al. 2012 |
| M12 | 12,16-dihydroxy-resibufogenin  (C24H32O6) |  | Zhu et al. 2013 |
| M13 | 12-hydroxyldesacetylcinobufagin  (C24H32O6) |  | He et al. 2012 |
| M14 | 1α,5β-dihydroxybufalin  (C24H34O6) |  | Xin et al. 2016 |
| M15 | 3,5,14,15-tetrahydroxyl-bufa-20,22-dienolide  (C24H34O6) |  | Zhu et al. 2013 |
| M16 | 5β, 6α-dihydroxybufalin  (C24H34O6) |  | Xin et al. 2016 |
| M17 | 1,5-dihydroxyldesacetylcinobufagin  (C24H32O7) |  | Ning et al. 2010 |
| M18 | 1,12β-dihydroxydesacetylcinobufagin  (C24H32O7) |  | He et al. 2012 |
| M19 | 2,5-dihydroxyldesacetylcinobufagin  (C24H32O7) |  | Ning et al. 2010 |
| M20 | 3-oxo-cinobufagin  (C26H32O6) |  | He et al. 2012 |
| M21 | 5-hydroxyl-cinobufagin  (C26H34O7) |  | He et al. 2012 |
| M22 | 12-hydroxyl-cinobufagin  (C26H34O7) |  | He et al. 2012 |
| M23 | 3-sulfate-bufalin  (C24H34O7S) |  | Miyashiro et al. 2008 |
| M24 | 1,12β-dihydroxycinobufagin  (C26H34O8) |  | He et al. 2012 |
| M25 | 3-sulfate-marinobufagin  (C24H32O8S) |  | Miyashiro et al. 2008 |