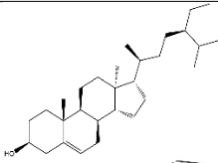
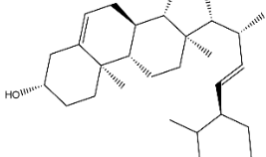
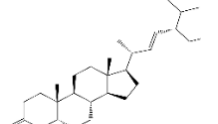
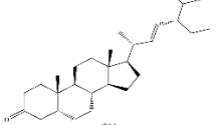
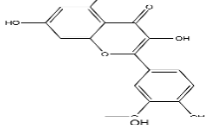
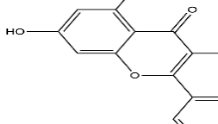
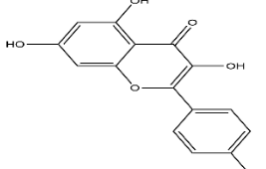
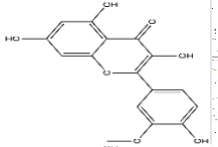
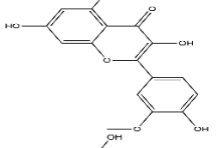
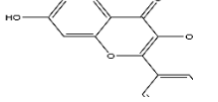
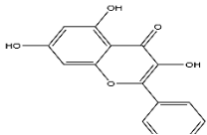
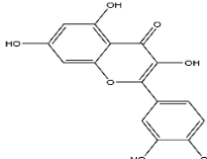
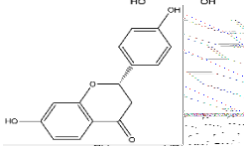
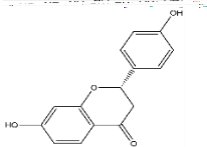
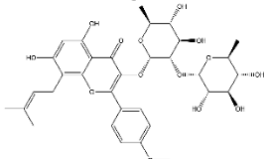
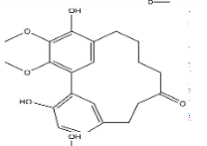
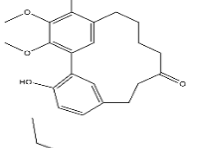
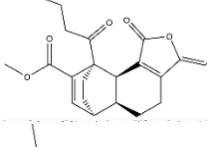
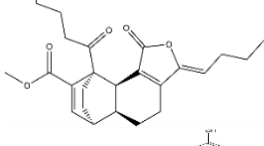
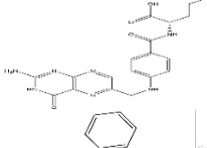
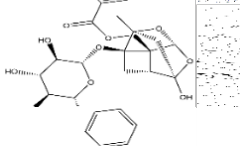
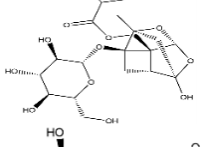
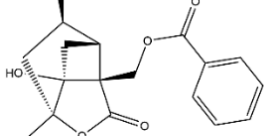


**Supplementary Table 1.** Test drug composition and dosage of BSHXF.

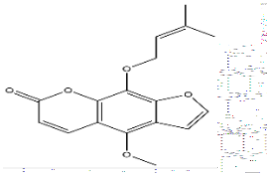
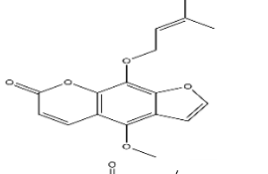
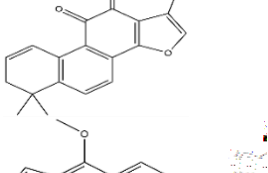
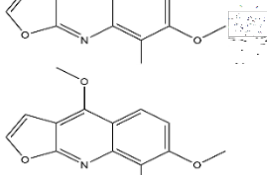
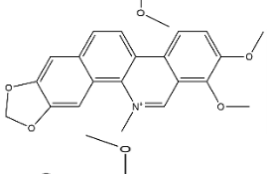
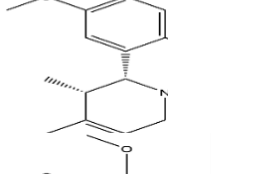
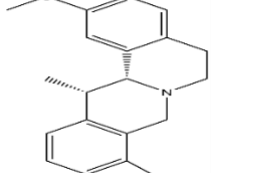
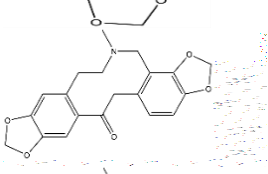
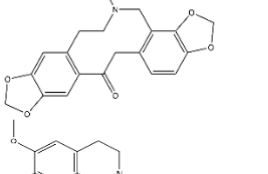
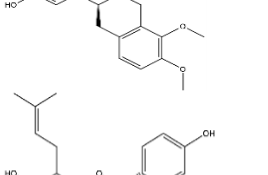
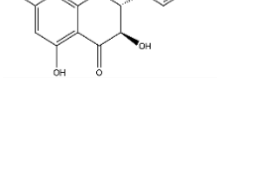
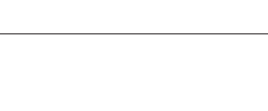
| Chinese name | Latin name                          | Dosage |
|--------------|-------------------------------------|--------|
| Shudihuang   | Rehmanniae Radix Praeparata (RRP)   | 10 g   |
| Tusizi       | Cuscutae Semen (CS)                 | 10 g   |
| Xianlingpi   | Epimrdii Herba (EH)                 | 10 g   |
| Danggui      | Angelicae Sinensis Radix (ASR)      | 10 g   |
| Chuanxiong   | Chuanxiong Rhizoma (CR)             | 10 g   |
| Baishao      | Paeoniae Radix Alba (PRA)           | 10 g   |
| Chaihu       | Radix Bupleuri (RB)                 | 6 g    |
| Zhimu        | Anemarrhenae Rhizoma (AR)           | 10 g   |
| Huangbai     | Phellodendri Chinrnsis Cortex (PCC) | 10 g   |

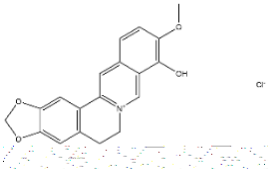
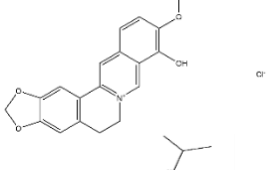
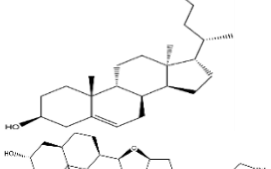
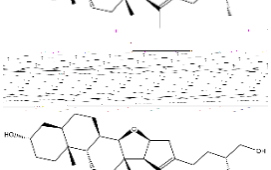

**Supplementary Table 2.** The detailed information of 52 predicted active monomers of BSHXF.

| No | Molecule ID | Componds              | Herb   | target number | Structure   |
|----|-------------|-----------------------|--|---------------|---|
| 1  | MOL000359   | sitosterol            | Shudihuang<br>Chuanxiong<br>Danggui<br>baishao       | 2             |    |
| 2  | MOL000449   | Stigmasterol          | Shudihuang<br>Danggui<br>Chaihu<br>Zhimu<br>Huangbai | 10            |    |
| 3  | MOL001558   | sesamin               | tusizi   | 14            |  |
| 4  | MOL000184   | Stigmastenone         | tusizi   | 1             |  |
| 5  | MOL000354   | isorhamnetin          | tusizi<br>chaihu                                     | 23            |  |
| 6  | MOL000358   | beta-sitosterol       | Tusizi<br>Danggui<br>Baishao<br>Huangbai             | 18            |  |
| 7  | MOL000422   | kaempferol            | Tusizi<br>Yinyanghuo<br>Baishao<br>Chaihu<br>zhimu   | 42            |  |
| 8  | MOL005043   | campest-5-en-3beta-ol | tusizi   | 1             |  |
| 9  | MOL005440   | Isofucosterol         | tusizi   | 2             |  |
| 10 | MOL005944   | matrine               | tusizi   | 8             |  |

| No  | Molecule ID | Compounds                | Herb                                       | target number | Structure   |
|-----|-------------|--------------------------|--|---------------|---|
| 11  | MOL000953   | Cholesterol              | tusizi                                     | 2             |    |
| 12  | MOL000098   | quercetin                | Tusizi<br>Yinyanghuo<br>Chaihu<br>Huangbai | 105           |    |
| 13  | MOL001771   | poriferast-5-en-3beta-ol | Yinyanghuo<br>Huangbai                     | 1             |    |
| 14  | MOL001792   | Liquiritigenin           | Yinyanghuo                                 |               |    |
| 15  | MOL004373   | Anhydroicaritin          | Yinyanghuo<br>zhimu                        | 23            |    |
| 16  | MOL001494   | Mandenol                 | Chuanxiong                                 | 2             |   |
| 17  | MOL002135   | Myricanone               | Chuanxiong                                 | 19            |  |
| 18. | MOL002140   | Perlolyrine              | Chuanxiong                                 | 3             |  |
| 19  | MOL002157   | wallichilide             | Chuanxiong                                 | 3             |  |
| 20  | MOL000433   | Folic acid               | Chuanxiong                                 | 2             |  |
| 21  | MOL001919   | Palbinone                | Danggui<br>Baishao<br>Huangbai             | 2             |  |
| 22  | MOL001924   | paeoniflorin             | Danggui<br>baishao                         | 4             |  |
| 23  | MOL001928   | albiflorin_qt            | Danggui                                    | 4             |  |

| No | Molecule ID | Componds               | Herb            | target number | Structure |
|----|-------------|------------------------|-----------------|---------------|-----------|
| 24 | MOL000211   | Mairin(Betulinic acid) | Danggui baishao | 1             |           |
| 25 | MOL000492   | Cianidanol             | baishao         | 5             |           |
| 26 | MOL001677   | asperglaucide          | Zhimu           | 5             |           |
| 27 | MOL004489   | Anemarsaponin F qt     | Zhimu           | 23            |           |
| 28 | MOL004514   | Timosaponin B III qt   | Zhimu           | 2             |           |
| 29 | MOL004528   | Icariin I              | Zhimu           | 1             |           |
| 30 | MOL000483   | n-cis-Feruloyltyramine | Zhimu           | 4             |           |
| 31 | MOL000546   | diosgenin              | Zhimu           | 12            |           |
| 32 | MOL000631   | coumaroyltyramine      | Zhimu           | 6             |           |
| 33 | MOL001454   | berberine              | Huangbai        | 12            |           |
| 34 | MOL001458   | coptisine              | Huangbai        | 8             |           |
| 35 | MOL002641   | Phellavin qt           | Huangbai        | 3             |           |

| No | Molecule ID | Componds               | Herb     | target number | Structure   |
|----|-------------|------------------------|----------|---------------|---|
| 36 | MOL002643   | delta 7-stigmastenol   | Huangbai | 1             |    |
| 37 | MOL002644   | Phellopterin           | Huangbai | 6             |    |
| 38 | MOL002651   | Dehydrotanshinone II A | Huangbai | 9             |    |
| 39 | MOL002662   | rutaecarpine           | Huangbai | 13            |    |
| 40 | MOL002663   | Skimmianin             | Huangbai | 2             |   |
| 41 | MOL001478   | Chelerythrine          | Huangbai | 4             |  |
| 42 | MOL002668   | Worenine               | Huangbai | 6             |  |
| 43 | MOL002670   | Cavidine               | Huangbai | 13            |  |
| 44 | MOL002672   | Hericenone H           | Huangbai | 1             |  |
| 45 | MOL000787   | Fumarine               | Huangbai | 15            |  |
| 46 | MOL000790   | Isocorypalmine         | Huangbai | 13            |  |
| 47 | MOL001130   | phellamurin_qt         | Huangbai | 7             |  |

| No | Molecule ID | Componds              | Herb     | target number | Structure  |
|----|-------------|-----------------------|----------|---------------|--|
| 48 | MOL001455   | (S)-Canadine          | Huangbai | 13            |   |
| 49 | MOL002894   | berberrubine          | Huangbai | 9             |   |
| 50 | MOL005438   | campesterol           | Huangbai | 1             |   |
| 51 | MOL006422   | thalifendine          | Huangbai | 10            |   |
| 52 | MOL004540   | Anemarsaponin<br>C_qt | Zhimu    | 3             |  |