**Supplementary Table S3. Basic information of the identified 31 compounds of Shugan Xiaozhi decoction (SX01~SX31)**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| NO. | Compounds name | CAS | PubChem\_CID | SMILES |
| SX01 | Gallic acid | 149-91-7 | 370 | C1=C(C=C(C(=C1O)O)O)C(=O)O |
| SX02 | Naringin | 10236-47-2 | 442428 | CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC=C(C=C5)O)O)CO)O)O)O)O)O |
| SX03 | Neohesperidin | 13241-33-3 | 442439 | CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C=C5)OC)O)O)CO)O)O)O)O)O |
| SX04 | Poncirin | 14941-08-3 | 442456 | CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC=C(C=C5)OC)O)CO)O)O)O)O)O |
| SX05 | Gardenoside | 24512-62-7 | 24721095 | COC(=O)C1=CO[C@@H]([C@@H]2[C@H]1C=C[C@]2(CO)O)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O |
| SX06 | Genipin-1-β-gentiobioside | 29307-60-6 | 3082301 | COC(=O)C1=COC(C2C1CC=C2CO)OC3C(C(C(C(O3)COC4C(C(C(C(O4)CO)O)O)O)O)O)O |
| SX07 | Chlorogenic acid | 327-97-9 | 1794427 | C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O |
| SX08 | Geniposide | 27745-20-6 | 107848 | COC(=O)C1=COC(C2C1CC=C2CO)OC3C(C(C(C(O3)CO)O)O)O |
| SX09 | Albiflorin | 39011-90-0 | 24868421 | CC12CC(C3CC1(C3(C(=O)O2)COC(=O)C4=CC=CC=C4)OC5C(C(C(C(O5)CO)O)O)O)O |
| SX10 | Liquiritin-apioside or isomer | 74639-14-8 | 10076238 | C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)OC4C(C(C(C(O4)CO)O)O)OC5C(C(CO5)(CO)O)O |
| SX11 | Liquiritin | 551-15-5 | 503737 | C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)OC4C(C(C(C(O4)CO)O)O)O |
| SX12 | Pentagalloylglucose | 14937-32-7 | 65238 | C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O)OC(=O)C6=CC(=C(C(=C6)O)O)O |
| SX13 | Isochlorogenic acid A | 89919-62-0 | 6474310 | C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O |
| SX14 | Paeoniflorin | 23180-57-6 | 442534 | CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)C5=CC=CC=C5)OC6C(C(C(C(O6)CO)O)O)O)O |
| SX15 | 6``-O-trans-p-cinnamoyl genipingentiobioside | N/A | N/A | O=C(OC)C1=CO[C@@H](O[C@@H]2O[C@H](CO[C@@H]3O[C@H](COC(C=CC4=CC=CC=C4)=O)[C@@H](O)C(O)[C@H]3O)[C@@H](O)C(O)[C@H]2O)[C@@]5([H])[C@@]1(CC=C5CO)[H] |
| SX16 | 22β-Acetoxyglycyrrhizin acid | N/A | N/A | C[C@@]1(C(O)=O)CC(C([C@@]2(C)CC3)=CC(C([C@](CC[C@H](O[C@@H]4O[C@H](C(O)=O)[C@@H](O)C(O)[C@H]4O[C@@H]5O[C@H](C(O)=O)[C@@H](O)C(O)[C@H]5O)C6(C)C)(C)C6CC7)[C@]27C)=O)[C@]3(C)C(OC(C)=O)C1 |
| SX17 | cis-Crocin2/trans-crocin2/  cis-crocin2`/trans-crocin2` | N/A | N/A | OC[C@H]1O[C@@H](OC[C@@H]2[C@@H](O)[C@H](O)[C@@H](O)[C@H](OC(/C(C)=C/C=C/C(C)=C/C=C/C=C(/C=C/C=C(C(O)=O)\C)C)=O)O2)[C@H](O)[C@@H](O)[C@@H]1O |
| SX18 | 16-Oxoalisol A | 124515-98-6 | 9983614 | CC(CC(C(C(C)(C)O)O)O)C1=C2CC(C3C4(CCC(=O)C(C4CCC3(C2(CC1=O)C)C)(C)C)C)O |
| SX19 | Glycyrrhizic acid | 1405-86-3 | 14982 | CC1(C2CCC3(C(C2(CCC1OC4C(C(C(C(O4)C(=O)O)O)O)OC5C(C(C(C(O5)C(=O)O)O)O)O)C)C(=O)C=C6C3(CCC7(C6CC(CC7)(C)C(=O)O)C)C)C)C |
| SX20 | O-Acetyl-saikosaponin or isomer (a) | N/A | N/A | O[C@H]([C@@H](O)[C@H](O[C@H]1[C@@H](O)[C@@H](C)O[C@@H](O[C@@H]2[C@@](C(CC[C@]3(C)C4C=CC5(OC6)[C@@]3(C)C[C@H](O)C76C5CC(C)(C)CC7)[C@]4(C)CC2)(C)CO)[C@@H]1O)O8)[C@H](O)[C@H]8COC(C)=O |
| SX21 | 16-Oxo-alisol A 24 acetate | N/A | N/A | O=C1CC[C@@]2(C)C(CC[C@@]([C@](C3)(C)C(C[C@@H]4O)=C([C@H](C)C[C@@H]([C@@H](OC(C)=O)C(C)(O)C)O)C3=O)(C)[C@]24[H])C1(C)C |
| SX22 | 16-Oxo-alisol A 23 acetate | N/A | N/A | O[C@@H](C(C)(O)C)[C@@H](OC(C)=O)C[C@@H](C)C1=C(C[C@@H]2O)[C@@](CC1=O)(C)[C@@]([C@]32[H])(C)CCC4C(C)(C)C(CC[C@@]43C)=O |
| SX23 | Aurantio-obtusin | 67979-25-3 | 155011 | CC1=CC2=C(C(=C1O)OC)C(=O)C3=C(C(=C(C=C3C2=O)O)OC)O |
| SX24 | Saikosaponin a | 20736-09-8 | 167928 | CC1C(C(C(C(O1)OC2CCC3(C(C2(C)CO)CCC4(C3C=CC56C4(CC(C7(C5CC(CC7)(C)C)CO6)O)C)C)C)O)OC8C(C(C(C(O8)CO)O)O)O)O |
| SX25 | Saikosaponin d | 20874-52-6 | 51346137 | CC1C(C(C(C(O1)OC2C(C(OC(C2O)OC3CCC4(C(C3(C)CO)CCC5(C4C=CC67C5(CC(C8(C6CC(CC8)(C)C)CO7)O)C)C)C)CO)O)O)O)O |
| SX26 | O-Acetyl-saikosaponin or isomer (d) | N/A | N/A | O[C@H]1[C@H](O)[C@@H](COC(C)=O)O[C@@H](O[C@H]2[C@@H](O)[C@@H](C)O[C@@H](O[C@@H]3[C@@](C)(CO)C(CC[C@]4(C)C5C=CC6(OC7)[C@@]4(C)C[C@@H](O)C87C6CC(C)(C)CC8)[C@]5(C)CC3)[C@@H]2O)[C@@H]1O |
| SX27 | Kaempferol-3-O-galactoside | 23627-87-4 | 5282149 | C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O |
| SX28 | Tumulosic acid | 508-24-7 | 12314446 | CC(C)C(=C)CCC(C1C(CC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C)C)C)O)C(=O)O |
| SX29 | Alisol F | 155521-45-2 | 101661882 | CC1CC(OC2C1=C3CC(C4C5(CCC(=O)C(C5CCC4(C3(C2)C)C)(C)C)C)O)C(C(C)(C)O)O |
| SX30 | Obtusifolin | 477-85-0 | 3083575 | CC1=CC2=C(C(=C1O)OC)C(=O)C3=C(C2=O)C=CC=C3O |
| SX31 | Licoricone | 51847-92-8 | 5319013 | CC(=CCC1=C(C=C(C(=C1OC)C2=COC3=C(C2=O)C=CC(=C3)O)O)OC)C |