**Supplementary material**

**Exploring the mechanism of anti-chronic heart failure effect of Qiweiqiangxin І granules based on metabolomics**

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Table S1 Information on 33 characteristic compounds designated by QWQX І granules

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | RT/min | name | molecular formula | source |
| 123456789101112131415161718192021222324252627282930313233 | 0.580.6591.0321.1081.5381.8182.0732.7763.5833.9844.4335.3285.55.7676.4976.6427.8548.668.9839.73611.58111.65411.72311.79611.95812.19612.75712.86913.04113.39714.10714.24914.56 | *β*-(3,4-Dihydroxyphenyl)-D-lactic acidGamma-aminobutyric acidL-AdenosineSalvioloneAlangisideThreoninDihydroisotanshinone IOnoninHydroxytanshinone IIA*β*-sitosterolGinsenoside La.qtTrifolirhizinEthyl methoxycinnamateMalyngamide JLithospermic acidBuntansin ASalvianolic acid GMelitric acid BPsuedohypericinDehydrouvaolAgnosteroneLupenone20-HexadecanoylingenolIlexoside A21-Isopropyl-28,29,30-trinor-17,19,21-gammaceratrieneIlexgenin A20S-ginsenoside Rs3TanshinaldehydePerrottetin DIsotanshinone IIMiltironeCryptotanshinoneApollinine | C9H10O5C4H9NO2C10H13N5O4C18H20O2C25H31NO10C4H9NO3C18H14O3C22H24O9C19H18O4C30H52OC30H50O3C22H22O10C12H14O3C33H53NO9C27H22O12C11H8O5C18H12O7C30H16O9C18H26O10C19H20O3C30H46OC36H58O4C30H48OC35H56O8C30H46C30H46O6C19H22O5C19H16O4C19H20O3C18H14O3C19H22O2C19H22O3C22H18O5 | Radix SalviaeHedysarum Multijugum Maxim.Panax Ginseng C. A. Mey.Radix SalviaeCinnamomum cassia PreslRadix SalviaeRadix SalviaeHedysarum Multijugum Maxim.Radix SalviaeLepidii Semen Descurainiae SemenPanax Ginseng C. A. Mey.Panax Ginseng C. A. Mey.Cinnamomi RamulusRadix SalviaeRadix SalviaeRadix SalviaeRadix SalviaePanax Ginseng C. A. MeyRadix Salviae MiltiorrhiaeRadix SalviaeRadix Ilicis PubescentisPanax Ginseng C. A. MeyAstragalus membranaceus BgeRadix Ilicis PubescentisAstragalus membranaceus BgeRadix Ilicis PubescentisHedysarum Multijugum Maxim.Radix SalviaeRadix SalviaeRadix SalviaeRadix SalviaeRadix SalviaeRadix Salviae |

Table S2 Mass spectrometry conditions

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| --- |
| 6540 Q-TOF MS conditions |
| Capillary voltage | 3500V |
| Gas temperature | 320℃ |
| Gas flow rate | 8 L/min |
| Nebulizer | 35 psig |
| Sheath gas temperature | 350℃ |
| Sheath gas flow rate | 1l L/min |
| Nozzle voltage | 1500V |
| Fragmentor | 175V |
| Skimmer | 65V |
| Scan rate | 4 spectra/s |

The instrument mode is Extended Mass Range (2 GHz), the acquisition mode is full scan, and the scan mass-to-charge ratio range is 50-1500, with positive mode reference ions of 121.0509 and 922.0098, and negative mode reference ions of 112.9855 and 1033.9881.

Table S3 Gradient elution conditions

|  |  |  |  |
| --- | --- | --- | --- |
| Time | Flow rate | Mobile phase A | Mobile phase B |
| (min) | (mL/min) | (%) | (%) |
| 0 | 0.4 | 98 | 2 |
| 1 | 0.4 | 98 | 2 |
| 15 | 0.4 | 0 | 100 |
| 18 | 0.4 | 0 | 100 |
| 18.01 | 0.4 | 98 | 2 |
| 20 | 0.4 | 98 | 2 |



**Figure S1 Chemical composition in QWQX І.** (A)The chromatogram of the QWQX І (B) Assigned structures of 33 characteristic compounds in QWQX І.



**Figure S2 Metabolic profile of rat plasma.** (A) Total ion flow chromatogram in negative mode; (B) Total ion flow chromatogram in positive mode; (C) Quality control samples PCA scores in negative mode; (D) Quality control samples PCA scores in positive mode.



**Figure S3 Metabolic profile of rat cardiac tissue.** (A) Total ion flow chromatogram in negative mode; (B) Total ion flow chromatogram in positive mode; (C) Quality control samples PCA scores in negative mode; (D) Quality control samples PCA scores in positive mode.