

Supporting Information:

**Integrated Multi-omics techniques and Network Pharmacology
Analysis to Explore the Material Basis and Mechanism of Simiao Pill
in the Treatment of Rheumatoid Arthritis**

**Yuming Wang[†], Fangfang Zhang[†], Xiaokai Li[†], Xue Li, Jiayi Wang, Junjie He,
Xiaoyan Wu, Siyu Chen, Yanjun Zhang^{*}, Yubo Li^{*}**

School of Chinese Materia Medica, Tianjin University of Traditional Chinese
Medicine, Tianjin, 301617, China

***Co-corresponding authors:**

Dr. Yubo Li, School of Chinese Materia Medica, Tianjin University of Traditional
Chinese Medicine, No. 10 Poyang Lake Road, West Zone, Tuanbo New City, Jinghai
District, Tianjin 301617, China. E-mail: yaowufenxi001@sina.com.

Dr. Yanjun Zhang, School of Chinese Materia Medica, Tianjin University of
Traditional Chinese Medicine, No. 10 Poyang Lake Road, West Zone, Tuanbo New
City, Jinghai District, Tianjin 301617, China. E-mail: Tianjin_tcm001@sina.com.

†Author contribution

Yuming Wang, Fangfang Zhang and Xiaokai Li contributed equally to this work.

Table S1. Information on blood-inlet components in Simiao pills

No.	Molecular Name	Herb	PubChem CID	Molecular Formula	MW
1	Berberine	Phellodendron chinense Schneid.	2353	C ₂₀ H ₁₈ NO ₄	336.4
2	Palmatine	Phellodendron chinense Schneid.	19009	C ₂₁ H ₂₂ NO ₄	352.4
3	Lotusine	Phellodendron chinense Schneid.	5274587	C ₁₉ H ₂₄ NO ₃ ⁺	314.4
4	Berberrubine	Phellodendron chinense Schneid.	72703	C ₁₉ H ₁₆ NO ₄	357.8
5	Dauricine	Phellodendron chinense Schneid.	73400	C ₃₈ H ₄₄ N ₂ O ₆	624.8
6	Beta-Eudesmol	Atractylodes lancea (Thunb.) DC.	91457	C ₁₅ H ₂₆ O	222.37
7	Atractylodin	Atractylodes lancea (Thunb.) DC.	5321047	C ₁₃ H ₁ O	182.2
8	Magnoflorine	Phellodendron chinense Schneid.	73337	C ₂₀ H ₂₄ NO ₄	342.4
9	Phellodendrine	Phellodendron chinense Schneid.	3081405	C ₂₀ H ₂₄ NO ₄	342.4

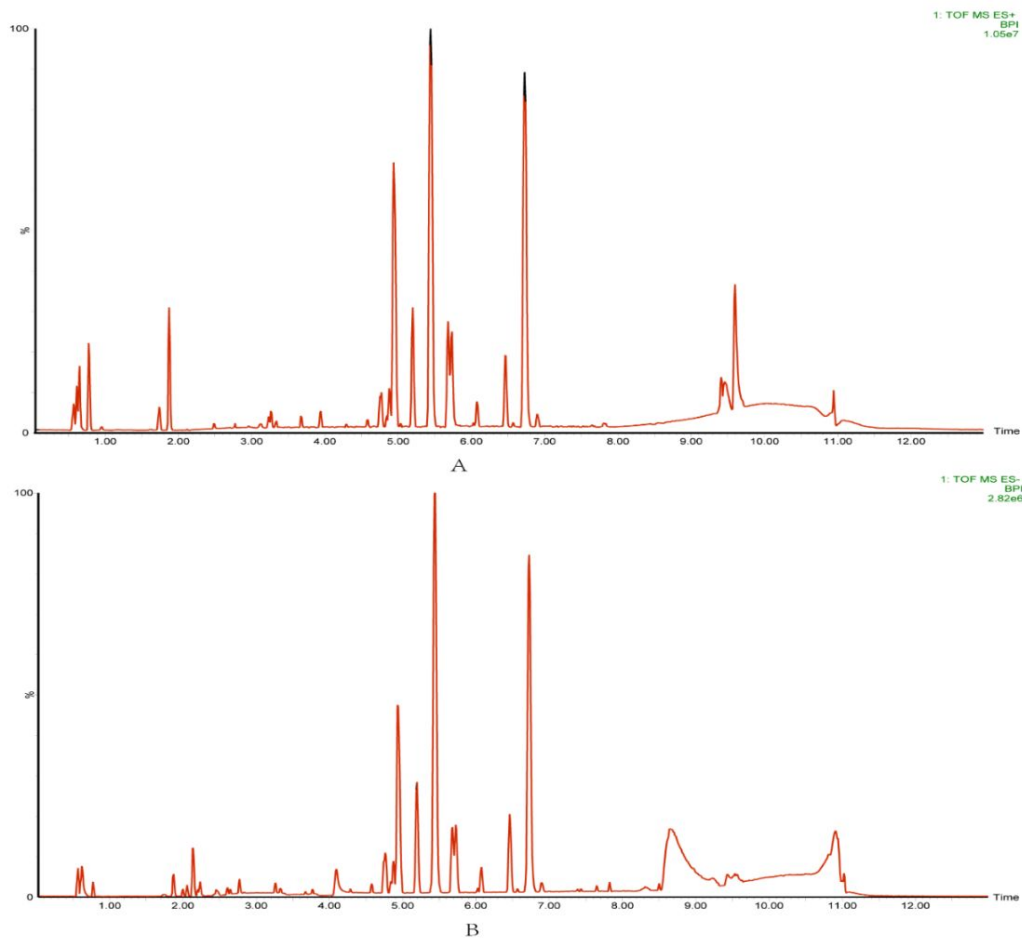


Figure S1. BPI diagram of plasma QC samples (A:Positive ion mode; B:Negative ion mode)

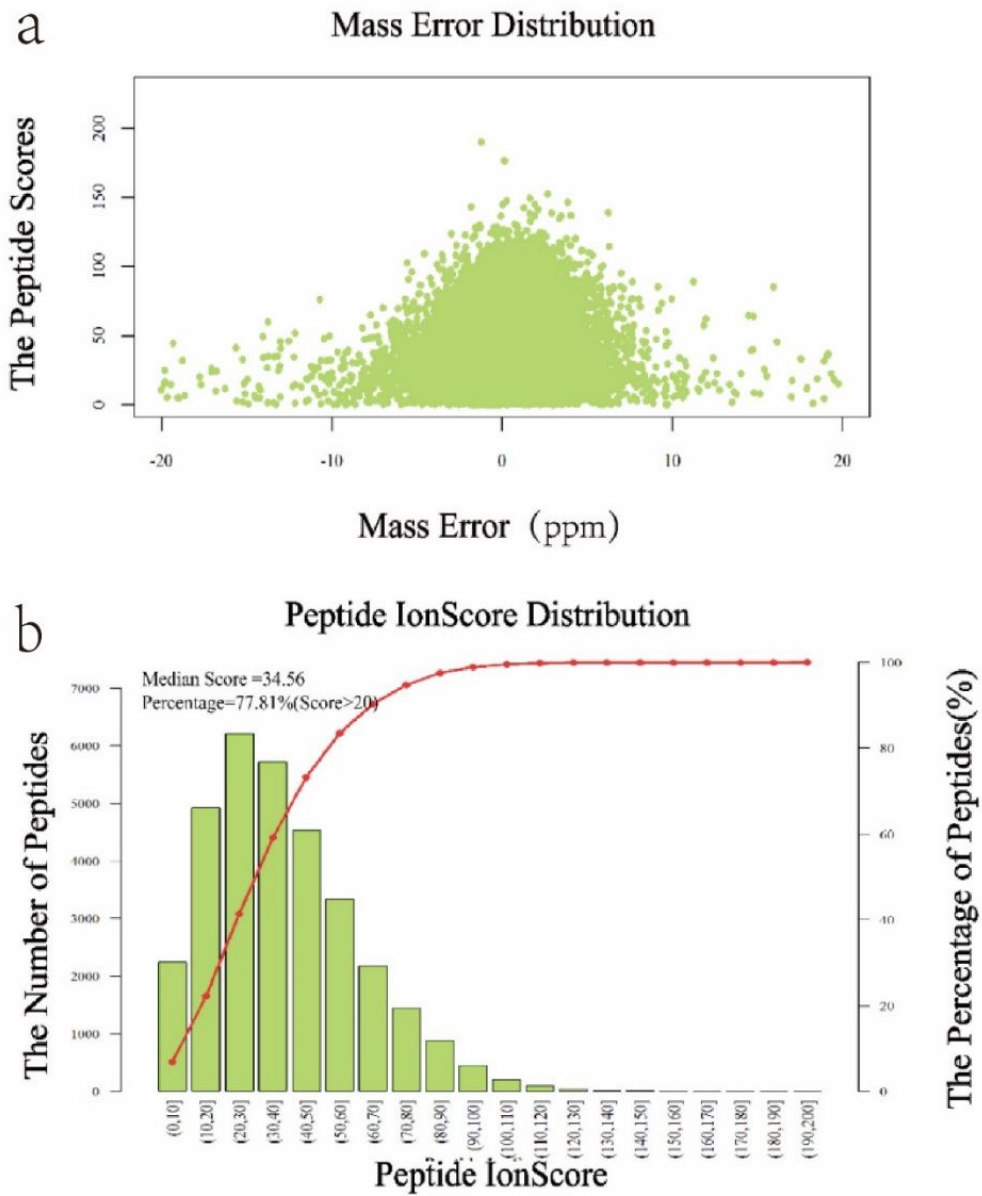


Figure S2. Proteomics analysis. a: Biased mass distribution of peptide ions; b: Peptide ion score profiles

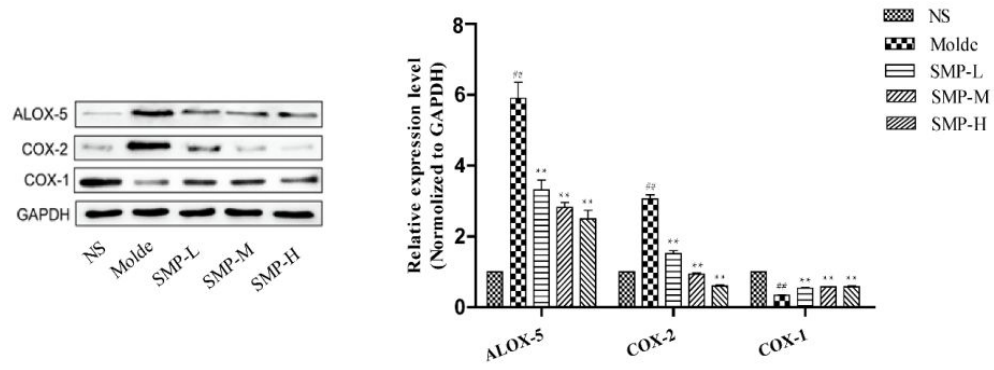


Figure S3. Protein expression levels of ALOX-5, COX-2 and COX-1 genes($n=3$)
 ($\#p<0.05$, $\#\#p<0.01$ compared with control group, $*p<0.05$, $**p<0.01$ compared with model)

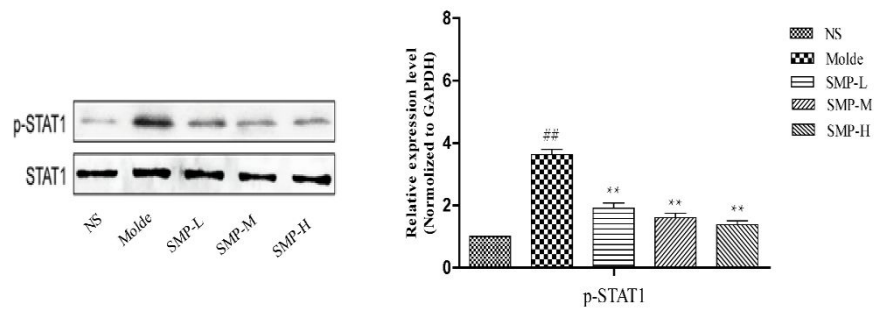


Figure S4. Protein expression levels of P-STAT1 genes($n=3$)
 ($\#p<0.05$, $\#\#p<0.01$ compared with control group, $*p<0.05$, $**p<0.01$ compared with model)

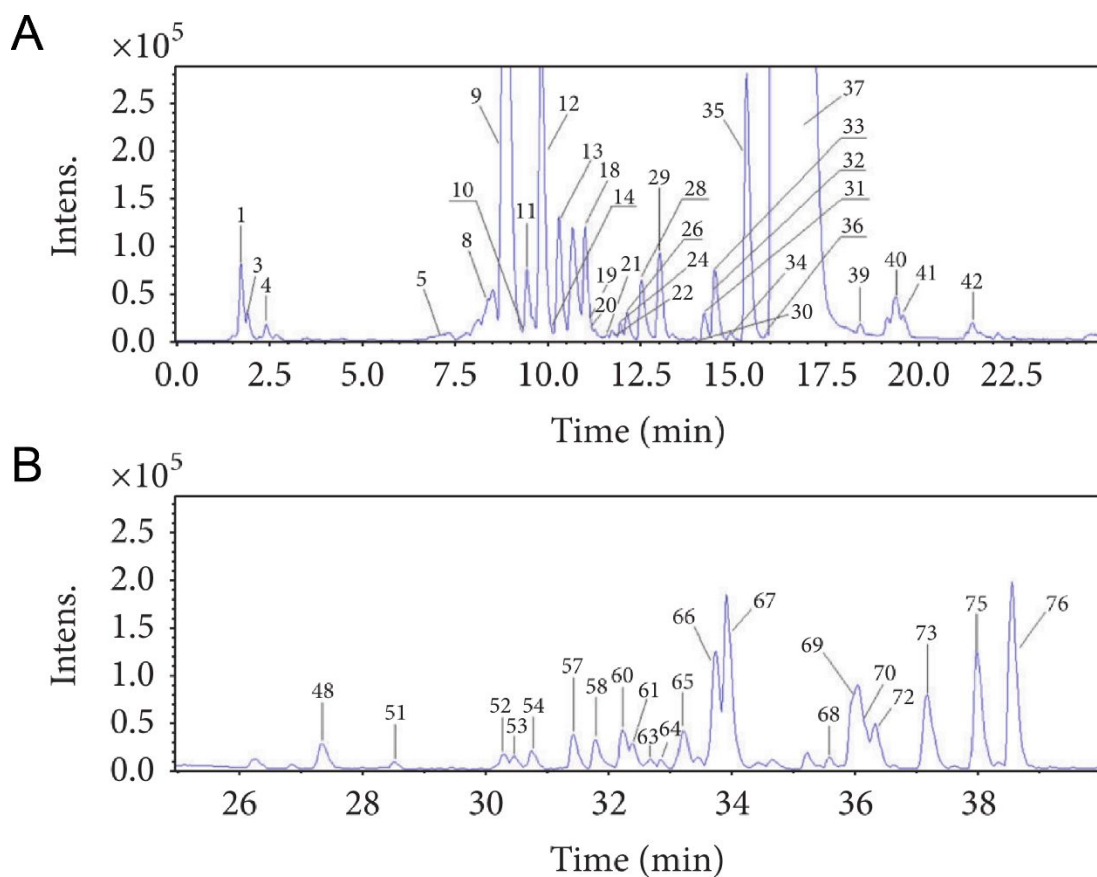


Figure S5. Base peak chromatograms obtained by HPLC/Q-TOF-MS in the positive mode of SMP. (Chromatograms at 0 to 25 min: (A); Chromatogram at 25–40 min: (B))

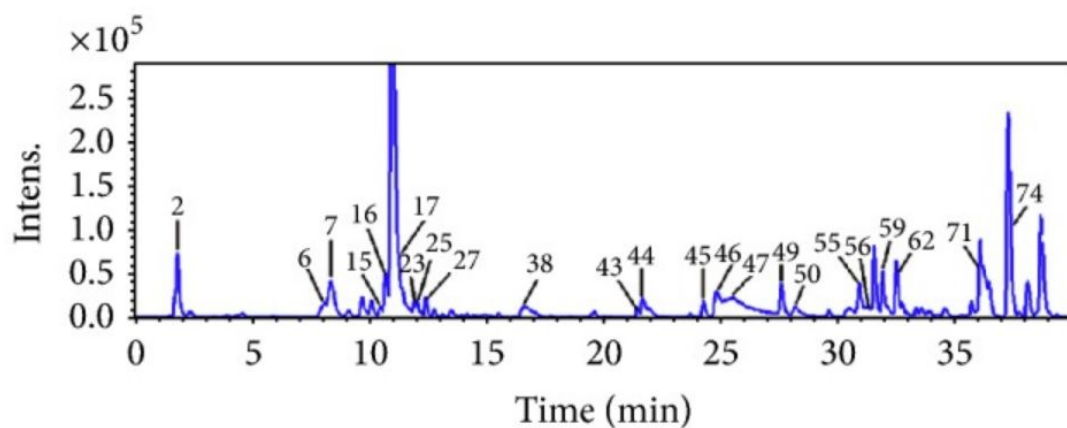


Figure S6. Base peak chromatograms obtained by HPLC/Q-TOF-MS in the negative mode of SMP