**Supporting Information**

**Identification and quantitation of NF-κB inhibitory components in Weichang'an pill based on UHPLC-QE-MS and spectrum-effect relationships**

Xiaoxia Caoa,b,1, Cunyu Hua,b,1, Fei Shanga,b, Yingshuang Lva,b, Ziyan Biana,b, Qing Yuana,b, Han Zhanga,b, Yi Wanga,b, Nan Lia,b, Lin Wangc, Yujing Wangc, Yingjie Sunc, Lin Miaoa,b, Yanxu Changa,b, Yuefei Wanga,b, Wenzhi Yanga,b, Lijuan Chaia,b,\*, Peng Zhanga,b,\*

a*State Key Laboratory of Component-based Chinese Medicine, Tianjin Key Laboratory of TCM Chemistry and Analysis, Tianjin University of Traditional Chinese Medicine, Tianjin 301617, China*

b*Haihe Laboratory of Modern Chinese Medicine, Tianjin 301617, China*

*cLerentang Pharmaceutical Factory, Tianjin Pharmaceutical Da Ren Tang Group Corporation Ltd*

*These authors contributed equally to this work.*

E-mail addresses: zhangpeng@tjutcm.edu.cn (Peng Zhang), cljuan1258@163.com(Lijuan Chai)

Table S1 Batch number and date of manufacture

Table S2 Precision test results (n = 6)

Table S3 Results of the repetitive tests ( n= 6)

Table S4 Stability test results (n = 6)

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Table S6 The fingerprints of chemical composition of WCAP has a common peak relative peak area

Table S7 The fingerprints of chemical composition of WCAP has a common relative retention time

Table S8 NF-κB inhibitory activity of the 10 compounds in WCAP

Fig S1 Bar chart of the sum of content in 16 batches of WCAP

**Table S1** Batch number and date of manufacture

|  |  |  |
| --- | --- | --- |
| Sample number | batch number | Production date |
| S605 | 1530605 | 2017-06-02 |
| S826 | 1530826 | 2019-02-18 |
| S932 | 1530932 | 2019-09-24 |
| S936 | 1530936 | 2019-09-24 |
| S938 | 1530938 | 2019-09-24 |
| S939 | 1530939 | 2019-09-24 |
| S940 | 1530940 | 2019-09-24 |
| S942 | 1530942 | 2019-10-25 |
| S944 | 1530944 | 2019-10-25 |
| S953 | 1530953 | 2019-11-03 |
| S954 | 1530954 | 2019-11-03 |
| S955 | 1530955 | 2019-11-03 |
| S956 | 1530956 | 2019-11-03 |
| S963 | 1530963 | 2019-12-06 |
| S964 | 1530964 | 2019-12-06 |
| S969 | 1530969 | 2019-12-06 |

**Table S2** Precision test results (n = 6)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak number | 1 | 2 | 3 | 4 | 5 | 6 | mean | RSD(%) |
| 1 | 67021 | 67035 | 67795 | 66763 | 67205 | 67663 | 67247 | 0.54 |
| 2 | 329019 | 307646 | 317879 | 321743 | 321623 | 320359 | 319712 | 1.99 |
| 3 | 308972 | 301614 | 309868 | 310911 | 312019 | 313318 | 309450 | 1.22 |
| 4 | 86099 | 86543 | 86663 | 86321 | 86761 | 87194 | 86597 | 0.40 |
| 5 | 154538 | 156011 | 157125 | 159528 | 161942 | 160982 | 158354 | 1.69 |
| 6 | 258788 | 255767 | 258436 | 260868 | 262329 | 263113 | 259884 | 0.96 |
| 7 | 121682 | 122311 | 123251 | 124880 | 125507 | 125708 | 123890 | 1.26 |
| 8 | 260854 | 260146 | 262720 | 266184 | 267521 | 268512 | 264323 | 1.23 |
| 9 | 2630811 | 2635617 | 2651027 | 2675440 | 2684302 | 2693531 | 2661788 | 0.90 |
| 10 | 77115 | 78844 | 79613 | 81497 | 81524 | 82704 | 80216 | 2.35 |
| 11 | 965761 | 976954 | 985197 | 995280 | 999236 | 1002514 | 987490 | 1.32 |
| 12 | 585932 | 588350 | 591267 | 596411 | 597773 | 599928 | 593277 | 0.86 |
| 13 | 94818 | 94608 | 94862 | 95455 | 94849 | 95251 | 94974 | 0.30 |

**Table S3** Results of the repetitive tests ( n= 6)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak number | 1 | 2 | 3 | 4 | 5 | 6 | mean | RSD(%) |
| 1 | 65086 | 65615 | 65639 | 68133 | 65704 | 65114 | 65882 | 1.57 |
| 2 | 300925 | 305420 | 315915 | 313734 | 310073 | 311365 | 309572 | 1.63 |
| 3 | 313883 | 317414 | 313658 | 308799 | 314482 | 318367 | 314434 | 0.98 |
| 4 | 72131 | 73396 | 73212 | 73810 | 75543 | 73695 | 73631 | 1.38 |
| 5 | 159250 | 160978 | 161758 | 160647 | 163247 | 163235 | 161519 | 0.88 |
| 6 | 276286 | 275233 | 276440 | 278978 | 282698 | 282254 | 278648 | 1.05 |
| 7 | 129448 | 122301 | 129778 | 130575 | 132795 | 131071 | 129328 | 2.57 |
| 8 | 272937 | 276865 | 274073 | 275805 | 279503 | 277820 | 276167 | 0.80 |
| 9 | 2650794 | 2685002 | 2600697 | 2678229 | 2659621 | 2687516 | 2660310 | 1.12 |
| 10 | 81747 | 83449 | 82631 | 83625 | 84724 | 84609 | 83464 | 1.25 |
| 11 | 986086 | 1000540 | 991886 | 998250 | 1013704 | 1003026 | 998915 | 0.87 |
| 12 | 589672 | 599871 | 593566 | 597251 | 607295 | 599148 | 597801 | 0.92 |
| 13 | 93172 | 94383 | 93080 | 93823 | 95063 | 94115 | 93939 | 0.73 |

**Table S4** Stability test results (n = 6)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak number | 0 h | 2 h | 6 h | 8 h | 12 h | 24 h | mean | RSD(%) |
| 1 | 65110 | 67804 | 65447 | 69322 | 69532 | 65177 | 67065 | 2.84 |
| 2 | 324103 | 325045 | 316928 | 333937 | 334076 | 335585 | 328279 | 2.07 |
| 3 | 309127 | 318107 | 313729 | 323540 | 324819 | 321718 | 318507 | 1.75 |
| 4 | 87171 | 87328 | 87706 | 88883 | 88979 | 87263 | 87888 | 0.86 |
| 5 | 161998 | 162540 | 163937 | 165956 | 166621 | 168089 | 164857 | 1.34 |
| 6 | 274152 | 269010 | 273068 | 275144 | 276591 | 278868 | 274472 | 1.11 |
| 7 | 127663 | 128333 | 127248 | 127841 | 127773 | 127973 | 127805 | 0.26 |
| 8 | 271151 | 272620 | 274924 | 277617 | 279117 | 281051 | 276080 | 1.27 |
| 9 | 2722388 | 2742322 | 2770003 | 2783681 | 2795853 | 2784786 | 2766506 | 0.94 |
| 10 | 84120 | 84331 | 84587 | 86056 | 85752 | 86716 | 85260 | 1.13 |
| 11 | 1013463 | 1021611 | 1030348 | 1036372 | 1039991 | 1047301 | 1031514 | 1.10 |
| 12 | 605608 | 608493 | 615696 | 619124 | 621355 | 625013 | 615882 | 1.12 |
| 13 | 96026 | 96728 | 97450 | 97585 | 97601 | 98150 | 97257 | 0.71 |

**Table S5** Sample recovery rate test results (n = 6)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| compound | The original quantity(μg/mL) | addition(μg/mL) | Measure the quantity(μg/mL) | recovery rate% | average recovery rate % | RSD (%) |
| Ferulic acid | 3.10 | 2.56 | 5.64 | 99.22 |  |  |
| 3.20 | 6.35 | 101.56 | 100.95 | 1.46 |
| 3.84 | 7.02 | 102.08 |  |  |
| Narirutin | 68.77 | 54.72 | 125.33 | 103.36 |  |  |
| 68.40 | 137.03 | 99.80 | 100.83 | 1.13 |
| 82.08 | 150.31 | 99.34 |  |  |
| Naringin | 74.30 | 59.73 | 135.36 | 102.23 |  |  |
| 74.66 | 148.92 | 99.95 | 99.43 | 0.85 |
| 89.56 | 160.39 | 96.12 |  |  |
| Hesperidin | 18.26 | 13.96 | 32.10 | 99.14 |  |  |
| 17.45 | 35.74 | 100.17 | 99.02 | 1.14 |
| 20.94 | 38.73 | 97.76 |  |  |
| Neohesperidin | 32.25 | 27.17 | 60.17 | 102.76 |  |  |
| 33.96 | 67.34 | 103.33 | 101.98 | 0.53 |
| 40.75 | 72.94 | 99.85 |  |  |
| Aloe emodin | 1.92 | 1.61 | 3.58 | 103.11 |  |  |
| 2.02 | 3.87 | 96.66 | 100.34 | 1.85 |
| 2.42 | 4.37 | 101.24 |  |  |
| Rhein | 4.00 | 1.54 | 5.51 | 98.05 |  |  |
| 1.92 | 5.91 | 99.48 | 99.47 | 1.21 |
| 2.30 | 6.32 | 100.87 |  |  |
| Emodin | 4.17 | 3.10 | 7.18 | 97.10 |  |  |
| 3.88 | 8.04 | 99.82 | 98.83 | 1.09 |
| 4.65 | 8.80 | 99.57 |  |  |
| Honokiol | 96.96 | 79.29 | 177.87 | 102.04 |  |  |
| 99.11 | 196.18 | 100.11 | 101.83 | 0.30 |
| 118.93 | 219.88 | 103.35 |  |  |
| Costunolide | 20.89 | 17.02 | 37.88 | 99.82 |  |  |
| 21.27 | 42.09 | 99.67 | 99.33 | 2.47 |
| 25.52 | 46.03 | 98.51 |  |  |
| Magnolol | 65.84 | 54.09 | 118.43 | 97.23 |  |  |
| 67.61 | 134.67 | 101.80 | 99.29 | 0.65 |
| 81.13 | 146.04 | 98.85 |  |  |
| Chrysophanol | 15.58 | 12.66 | 28.81 | 104.50 |  |  |
| 15.17 | 31.27 | 103.42 | 103.15 | 0.70 |
| 18.98 | 34.85 | 101.53 |  |  |
| Physcion | 2.65 | 2.05 | 4.67 | 98.54 |  |  |
| 2.56 | 5.18 | 98.83 | 99.23 | 2.18 |
| 3.07 | 5.73 | 100.33 |  |  |

**Table S6** The fingerprints of chemical composition of WCAP has a common peak relative peak area

|  |
| --- |
| common peak relative peak area |
| Peak number | Retention time | S605 | S826 | S932 | S936 | S938 | S939 | S940 | S942 | S944 | S953 | S954 | S955 | S956 | S963 | S964 | S969 | Mean | RSD(%) |
| 1 | 6.125 | 0.031 | 0.023 | 0.042 | 0.036 | 0.022 | 0.022 | 0.029 | 0.028 | 0.043 | 0.030 | 0.031 | 0.067 | 0.096 | 0.031 | 0.029 | 0.050 | 0.038 | 49.25 |
| 2 | 6.447 | 0.663 | 0.152 | 0.255 | 0.215 | 0.140 | 0.142 | 0.217 | 0.179 | 0.341 | 0.194 | 0.257 | 0.501 | 0.558 | 0.153 | 0.136 | 0.218 | 0.270 | 58.39 |
| 3 | 6.96 | 0.917 | 0.154 | 0.294 | 0.322 | 0.144 | 0.155 | 0.251 | 0.193 | 0.408 | 0.202 | 0.289 | 0.550 | 0.549 | 0.167 | 0.169 | 0.269 | 0.315 | 63.49 |
| 4 | 7.401 | 0.068 | 0.030 | 0.068 | 0.064 | 0.033 | 0.034 | 0.045 | 0.043 | 0.069 | 0.046 | 0.059 | 0.131 | 0.145 | 0.041 | 0.042 | 0.070 | 0.062 | 51.39 |
| 5 | 8.083 | 0.392 | 0.090 | 0.174 | 0.209 | 0.083 | 0.089 | 0.129 | 0.109 | 0.211 | 0.119 | 0.174 | 0.341 | 0.309 | 0.083 | 0.090 | 0.142 | 0.172 | 55.22 |
| 6 | 11.925 | 0.063 | 0.029 | 0.048 | 0.043 | 0.045 | 0.048 | 0.062 | 0.048 | 0.049 | 0.048 | 0.048 | 0.055 | 0.099 | 0.080 | 0.063 | 0.085 | 0.057 | 30.29 |
| 7 | 12.497 | 0.197 | 0.066 | 0.045 | 0.045 | 0.043 | 0.045 | 0.047 | 0.046 | 0.046 | 0.046 | 0.048 | 0.047 | 0.052 | 0.047 | 0.075 | 0.098 | 0.062 | 60.72 |
| 8 | 15.976 | 0.122 | 0.111 | 0.106 | 0.118 | 0.106 | 0.113 | 0.096 | 0.110 | 0.106 | 0.104 | 0.116 | 0.118 | 0.107 | 0.101 | 0.096 | 0.100 | 0.108 | 7.05 |
| **9(S)** | 16.26 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.00 |
| 10 | 16.514 | 0.050 | 0.040 | 0.030 | 0.030 | 0.035 | 0.036 | 0.017 | 0.035 | 0.033 | 0.033 | 0.037 | 0.041 | 0.045 | 0.038 | 0.037 | 0.037 | 0.036 | 19.37 |
| 11 | 16.783 | 0.036 | 0.051 | 0.028 | 0.024 | 0.054 | 0.033 | 0.025 | 0.035 | 0.034 | 0.049 | 0.052 | 0.035 | 0.048 | 0.053 | 0.026 | 0.056 | 0.040 | 27.97 |
| 12 | 17.318 | 0.405 | 0.341 | 0.352 | 0.372 | 0.361 | 0.372 | 0.357 | 0.351 | 0.355 | 0.344 | 0.378 | 0.369 | 0.364 | 0.361 | 0.385 | 0.339 | 0.363 | 4.60 |
| 13 | 18.043 | 0.153 | 0.177 | 0.148 | 0.147 | 0.118 | 0.159 | 0.138 | 0.129 | 0.129 | 0.124 | 0.139 | 0.147 | 0.237 | 0.204 | 0.180 | 0.180 | 0.157 | 19.65 |
| 14 | 19.573 | 0.035 | 0.027 | 0.028 | 0.029 | 0.022 | 0.031 | 0.027 | 0.026 | 0.025 | 0.023 | 0.028 | 0.030 | 0.038 | 0.033 | 0.030 | 0.028 | 0.029 | 13.87 |

**Table S7** The fingerprints of chemical composition of WCAP has a common relative retention time

|  |
| --- |
| common relative retention time |
| Peak number | S605 | S826 | S932 | S936 | S938 | S939 | S940 | S942 | S944 | S953 | S954 | S955 | S956 | S963 | S964 | S969 | Mean | RSD(%) |
| 1 | 0.380 | 0.378 | 0.379 | 0.383 | 0.377 | 0.378 | 0.376 | 0.376 | 0.376 | 0.376 | 0.376 | 0.375 | 0.376 | 0.373 | 0.371 | 0.371 | 0.376 | 0.79 |
| 2 | 0.393 | 0.398 | 0.398 | 0.401 | 0.397 | 0.398 | 0.397 | 0.396 | 0.396 | 0.396 | 0.396 | 0.395 | 0.396 | 0.394 | 0.392 | 0.392 | 0.396 | 0.58 |
| 3 | 0.421 | 0.431 | 0.432 | 0.438 | 0.430 | 0.430 | 0.429 | 0.428 | 0.428 | 0.428 | 0.427 | 0.426 | 0.427 | 0.424 | 0.420 | 0.420 | 0.427 | 1.06 |
| 4 | 0.444 | 0.460 | 0.460 | 0.468 | 0.458 | 0.458 | 0.456 | 0.455 | 0.455 | 0.456 | 0.455 | 0.453 | 0.455 | 0.449 | 0.444 | 0.444 | 0.454 | 1.39 |
| 5 | 0.489 | 0.501 | 0.502 | 0.508 | 0.500 | 0.500 | 0.498 | 0.497 | 0.497 | 0.497 | 0.496 | 0.495 | 0.496 | 0.491 | 0.485 | 0.486 | 0.496 | 1.17 |
| 6 | 0.731 | 0.734 | 0.735 | 0.736 | 0.734 | 0.734 | 0.734 | 0.734 | 0.733 | 0.734 | 0.733 | 0.733 | 0.734 | 0.732 | 0.731 | 0.731 | 0.733 | 0.19 |
| 7 | 0.772 | 0.769 | 0.769 | 0.770 | 0.769 | 0.769 | 0.769 | 0.769 | 0.769 | 0.768 | 0.768 | 0.768 | 0.769 | 0.767 | 0.766 | 0.766 | 0.769 | 0.18 |
| 8 | 0.982 | 0.982 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.982 | 0.982 | 0.982 | 0.982 | 0.982 | 0.982 | 0.983 | 0.05 |
| **9(S)** | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.00 |
| 10 | 1.015 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.015 | 1.016 | 1.016 | 1.015 | 1.015 | 1.015 | 1.015 | 1.015 | 1.016 | 0.05 |
| 11 | 1.033 | 1.031 | 1.033 | 1.033 | 1.031 | 1.032 | 1.032 | 1.032 | 1.033 | 1.032 | 1.032 | 1.033 | 1.033 | 1.031 | 1.032 | 1.032 | 1.032 | 0.07 |
| 12 | 1.066 | 1.066 | 1.066 | 1.066 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.064 | 1.065 | 0.05 |
| 13 | 1.109 | 1.112 | 1.111 | 1.112 | 1.110 | 1.110 | 1.110 | 1.109 | 1.110 | 1.109 | 1.109 | 1.109 | 1.109 | 1.108 | 1.108 | 1.107 | 1.110 | 0.12 |
| 14 | 1.205 | 1.207 | 1.207 | 1.208 | 1.205 | 1.204 | 1.204 | 1.203 | 1.204 | 1.203 | 1.204 | 1.203 | 1.202 | 1.201 | 1.202 | 1.199 | 1.204 | 0.19 |

**Table S8** NF-κB inhibitory activity of the 10 compounds in WCAP

|  |  |
| --- | --- |
| components | content（μg/g） |
| S939 | S953 | S956 |
| Ferulic acid | 144.67±0.0691 | 145.67±0.0023 | 231.00±0.0115 |
| Narirutin | 4478.33±0.0028 | 4587.33±0.0040 | 4347.67±0.0101 |
| Naringin | 4743.00±0.0081 | 4727.67±0.0002 | 4500.33±0.0032 |
| Hesperidin | 1232.33±0.0119 | 1167.33±0.0603 | 1323.33±0.0054 |
| Neohesperidin | 2498.00±0.037 | 2278.67±0.0193 | 2207.00±0.0214 |
| Aloe emodin | 69.67±0.0287 | 66.67±0.0100 | 100.67±0.0033 |
| Rhein | 119.00±0.0294 | 119.00±0.0224 | 104.00±0.0048 |
| Emodin | 270.00±0.0136 | 298.33±0.0190 | 188.67±0.0177 |
| Honokiol | 5865.67±0.0004 | 6049.33±0.0050 | 4725.67±0.0014 |
| Costunolide | 1189.67±0.0010 | 1233.67±0.0059 | 1001.33±0.026 |
| Magnolol | 4165.00±0.0804 | 4030.67±0.0017 | 3334.00±0.0062 |
| Chrysophanol | 485.33±0.0128 | 483.33±0.0006 | 584.00±0.0054 |
| Physcion | 114.33±0.0023 | 111.00±0.0345 | 115.67±0.0014 |

**Table S6** The fingerprint of chemical components of WCAP shared peak relative peak area

|  |
| --- |
| Common peak relative peak area |
| Peak number | Rt | S605 | S826 | S932 | S936 | S938 | S939 | S940 | S942 | S944 | S953 | S954 | S955 | S956 | S963 | S964 | S969 | Mean | RSD(%) |
| 1 | 6.125 | 0.031 | 0.023 | 0.042 | 0.036 | 0.022 | 0.022 | 0.029 | 0.028 | 0.043 | 0.030 | 0.031 | 0.067 | 0.096 | 0.031 | 0.029 | 0.050 | 0.038 | 49.25 |
| 2 | 6.447 | 0.663 | 0.152 | 0.255 | 0.215 | 0.140 | 0.142 | 0.217 | 0.179 | 0.341 | 0.194 | 0.257 | 0.501 | 0.558 | 0.153 | 0.136 | 0.218 | 0.270 | 58.39 |
| 3 | 6.96 | 0.917 | 0.154 | 0.294 | 0.322 | 0.144 | 0.155 | 0.251 | 0.193 | 0.408 | 0.202 | 0.289 | 0.550 | 0.549 | 0.167 | 0.169 | 0.269 | 0.315 | 63.49 |
| 4 | 7.401 | 0.068 | 0.030 | 0.068 | 0.064 | 0.033 | 0.034 | 0.045 | 0.043 | 0.069 | 0.046 | 0.059 | 0.131 | 0.145 | 0.041 | 0.042 | 0.070 | 0.062 | 51.39 |
| 5 | 8.083 | 0.392 | 0.090 | 0.174 | 0.209 | 0.083 | 0.089 | 0.129 | 0.109 | 0.211 | 0.119 | 0.174 | 0.341 | 0.309 | 0.083 | 0.090 | 0.142 | 0.172 | 55.22 |
| 6 | 11.925 | 0.063 | 0.029 | 0.048 | 0.043 | 0.045 | 0.048 | 0.062 | 0.048 | 0.049 | 0.048 | 0.048 | 0.055 | 0.099 | 0.080 | 0.063 | 0.085 | 0.057 | 30.29 |
| 7 | 12.497 | 0.197 | 0.066 | 0.045 | 0.045 | 0.043 | 0.045 | 0.047 | 0.046 | 0.046 | 0.046 | 0.048 | 0.047 | 0.052 | 0.047 | 0.075 | 0.098 | 0.062 | 60.72 |
| 8 | 15.976 | 0.122 | 0.111 | 0.106 | 0.118 | 0.106 | 0.113 | 0.096 | 0.110 | 0.106 | 0.104 | 0.116 | 0.118 | 0.107 | 0.101 | 0.096 | 0.100 | 0.108 | 7.05 |
| **9(S)** | 16.26 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.00 |
| 10 | 16.514 | 0.050 | 0.040 | 0.030 | 0.030 | 0.035 | 0.036 | 0.017 | 0.035 | 0.033 | 0.033 | 0.037 | 0.041 | 0.045 | 0.038 | 0.037 | 0.037 | 0.036 | 19.37 |
| 11 | 16.783 | 0.036 | 0.051 | 0.028 | 0.024 | 0.054 | 0.033 | 0.025 | 0.035 | 0.034 | 0.049 | 0.052 | 0.035 | 0.048 | 0.053 | 0.026 | 0.056 | 0.040 | 27.97 |
| 12 | 17.318 | 0.405 | 0.341 | 0.352 | 0.372 | 0.361 | 0.372 | 0.357 | 0.351 | 0.355 | 0.344 | 0.378 | 0.369 | 0.364 | 0.361 | 0.385 | 0.339 | 0.363 | 4.60 |
| 13 | 18.043 | 0.153 | 0.177 | 0.148 | 0.147 | 0.118 | 0.159 | 0.138 | 0.129 | 0.129 | 0.124 | 0.139 | 0.147 | 0.237 | 0.204 | 0.180 | 0.180 | 0.157 | 19.65 |
| 14 | 19.573 | 0.035 | 0.027 | 0.028 | 0.029 | 0.022 | 0.031 | 0.027 | 0.026 | 0.025 | 0.023 | 0.028 | 0.030 | 0.038 | 0.033 | 0.030 | 0.028 | 0.029 | 13.87 |

**Table S7** chemical component fingerprints of WCAP shared peak relative retention time

|  |
| --- |
| Common peak relative retention time |
| Peak number | S605 | S826 | S932 | S936 | S938 | S939 | S940 | S942 | S944 | S953 | S954 | S955 | S956 | S963 | S964 | S969 | Mean | RSD(%) |
| 1 | 0.380 | 0.378 | 0.379 | 0.383 | 0.377 | 0.378 | 0.376 | 0.376 | 0.376 | 0.376 | 0.376 | 0.375 | 0.376 | 0.373 | 0.371 | 0.371 | 0.376 | 0.79 |
| 2 | 0.393 | 0.398 | 0.398 | 0.401 | 0.397 | 0.398 | 0.397 | 0.396 | 0.396 | 0.396 | 0.396 | 0.395 | 0.396 | 0.394 | 0.392 | 0.392 | 0.396 | 0.58 |
| 3 | 0.421 | 0.431 | 0.432 | 0.438 | 0.430 | 0.430 | 0.429 | 0.428 | 0.428 | 0.428 | 0.427 | 0.426 | 0.427 | 0.424 | 0.420 | 0.420 | 0.427 | 1.06 |
| 4 | 0.444 | 0.460 | 0.460 | 0.468 | 0.458 | 0.458 | 0.456 | 0.455 | 0.455 | 0.456 | 0.455 | 0.453 | 0.455 | 0.449 | 0.444 | 0.444 | 0.454 | 1.39 |
| 5 | 0.489 | 0.501 | 0.502 | 0.508 | 0.500 | 0.500 | 0.498 | 0.497 | 0.497 | 0.497 | 0.496 | 0.495 | 0.496 | 0.491 | 0.485 | 0.486 | 0.496 | 1.17 |
| 6 | 0.731 | 0.734 | 0.735 | 0.736 | 0.734 | 0.734 | 0.734 | 0.734 | 0.733 | 0.734 | 0.733 | 0.733 | 0.734 | 0.732 | 0.731 | 0.731 | 0.733 | 0.19 |
| 7 | 0.772 | 0.769 | 0.769 | 0.770 | 0.769 | 0.769 | 0.769 | 0.769 | 0.769 | 0.768 | 0.768 | 0.768 | 0.769 | 0.767 | 0.766 | 0.766 | 0.769 | 0.18 |
| 8 | 0.982 | 0.982 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.983 | 0.982 | 0.982 | 0.982 | 0.982 | 0.982 | 0.982 | 0.983 | 0.05 |
| **9(S)** | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 0.00 |
| 10 | 1.015 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.016 | 1.015 | 1.016 | 1.016 | 1.015 | 1.015 | 1.015 | 1.015 | 1.015 | 1.016 | 0.05 |
| 11 | 1.033 | 1.031 | 1.033 | 1.033 | 1.031 | 1.032 | 1.032 | 1.032 | 1.033 | 1.032 | 1.032 | 1.033 | 1.033 | 1.031 | 1.032 | 1.032 | 1.032 | 0.07 |
| 12 | 1.066 | 1.066 | 1.066 | 1.066 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.065 | 1.064 | 1.065 | 0.05 |
| 13 | 1.109 | 1.112 | 1.111 | 1.112 | 1.110 | 1.110 | 1.110 | 1.109 | 1.110 | 1.109 | 1.109 | 1.109 | 1.109 | 1.108 | 1.108 | 1.107 | 1.110 | 0.12 |
| 14 | 1.205 | 1.207 | 1.207 | 1.208 | 1.205 | 1.204 | 1.204 | 1.203 | 1.204 | 1.203 | 1.204 | 1.203 | 1.202 | 1.201 | 1.202 | 1.199 | 1.204 | 0.19 |



**Fig S1** Bar chart of the sum of content in 16 batches of WCAP