**Supporting Information**

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

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Table S1 Batch number and date of manufacture

Table S2 Precision test results (n = 6)

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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](javascript:;) | 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](javascript:;) | 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](javascript:;) | 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](javascript:;) | 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 |

堆积柱状图

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