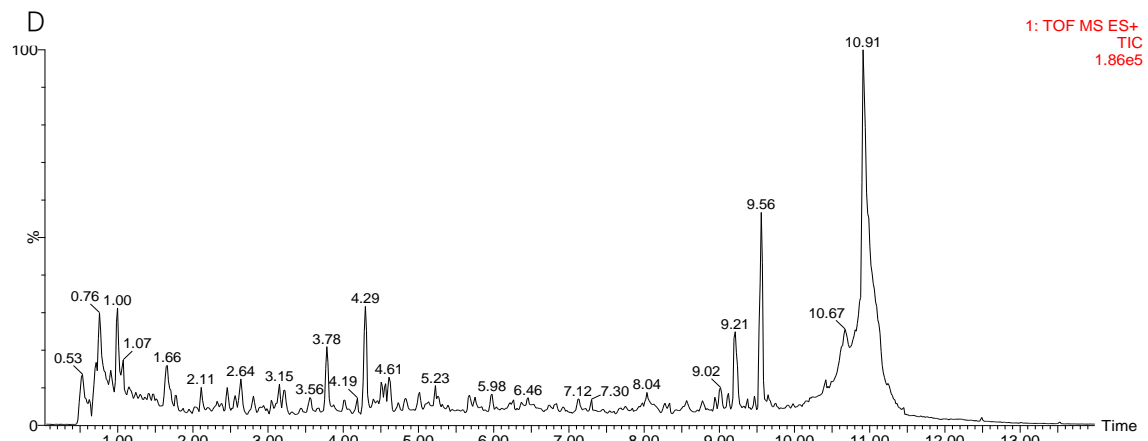
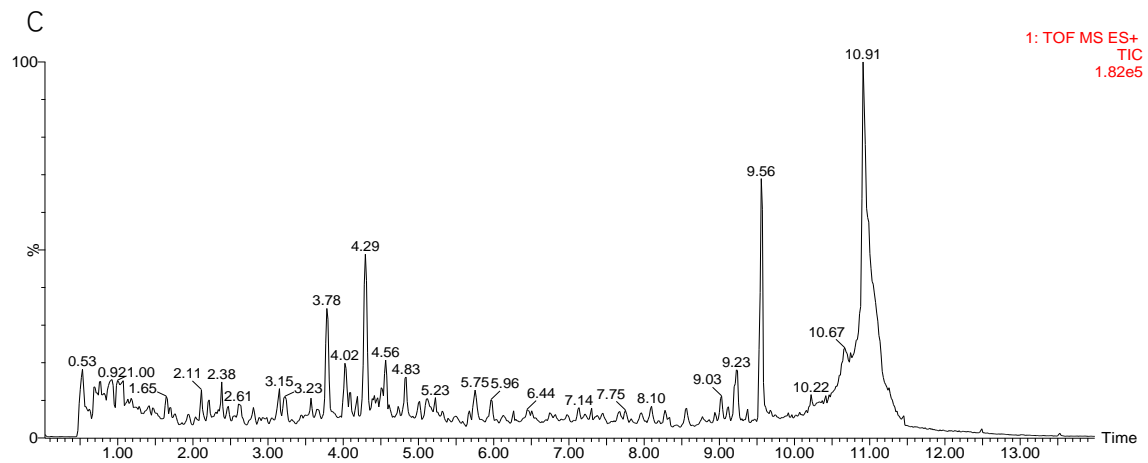
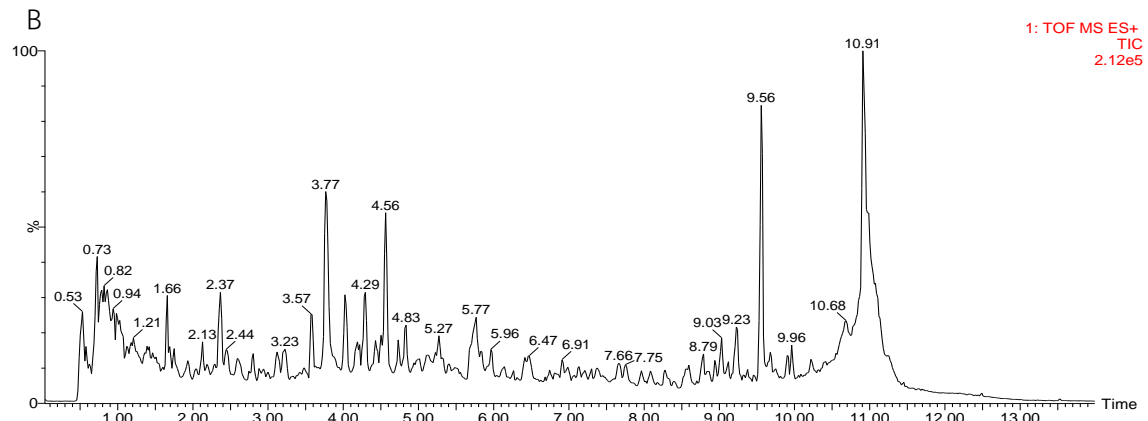
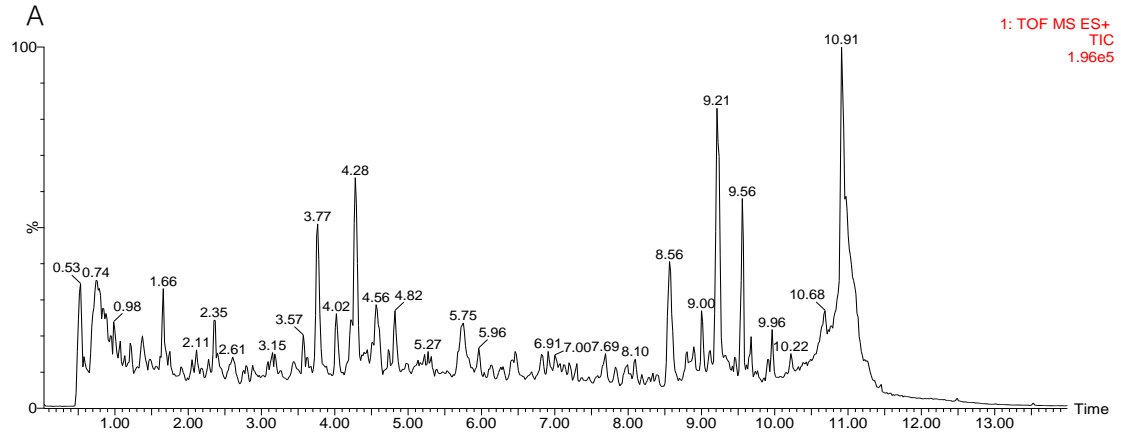


Figure S1 HPLC fingerprint of water decoction(a), supernatant(b) and essential oil(c) fractions of *T. patula*.

Notes: (1) patuletin, (2) quercetin-7-*O*- α -L-rhamnosepyranoside, (3) quercetin-3-*O*- α -L-arabinopyranoside, (4) kaempferol-3-*O*- β -D-glucopyranoside, (5) kaempferol-3-*O*- β -D-xylopyranoside, (6) kaempferol-3-*O*- α -L-rhamnosepyranoside, (7) kaempferol, (8) kaempferol-3-*O*- α -L-arabinopyranoside.



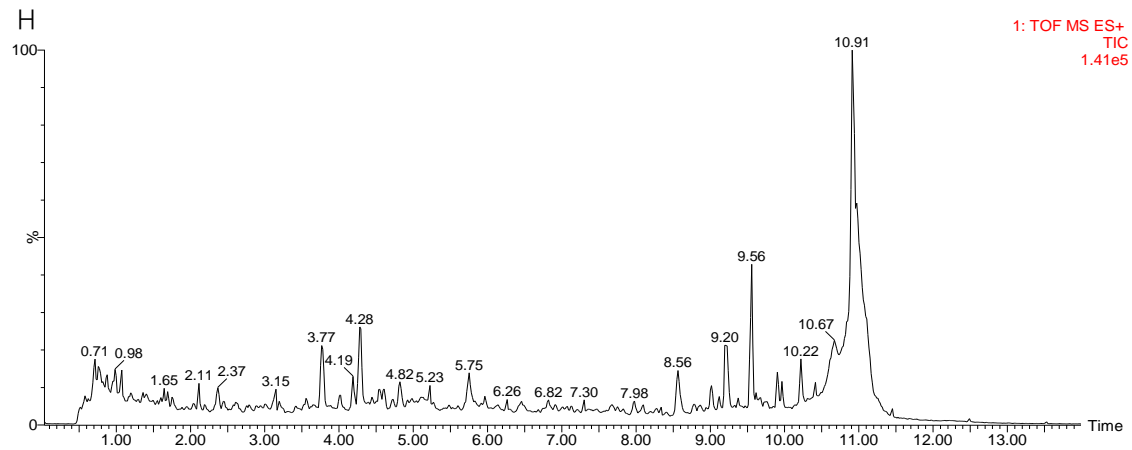
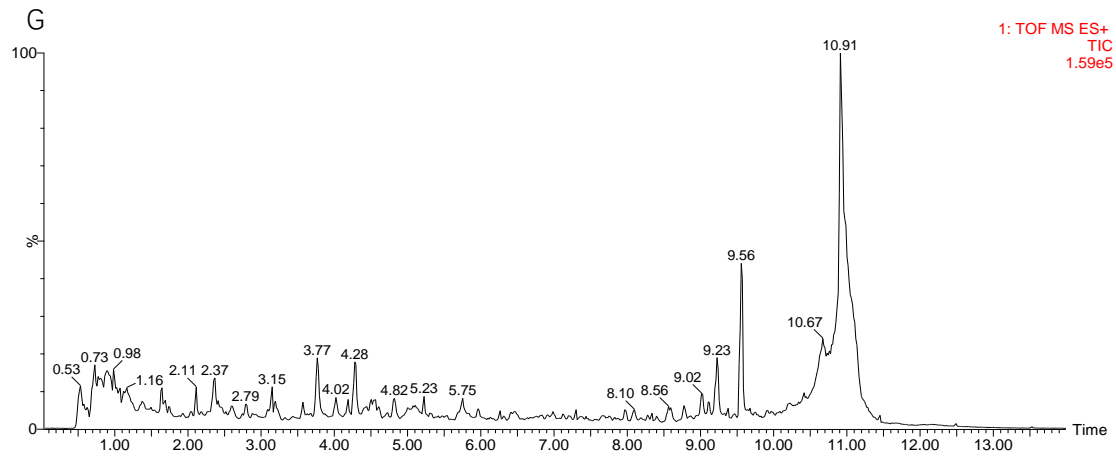
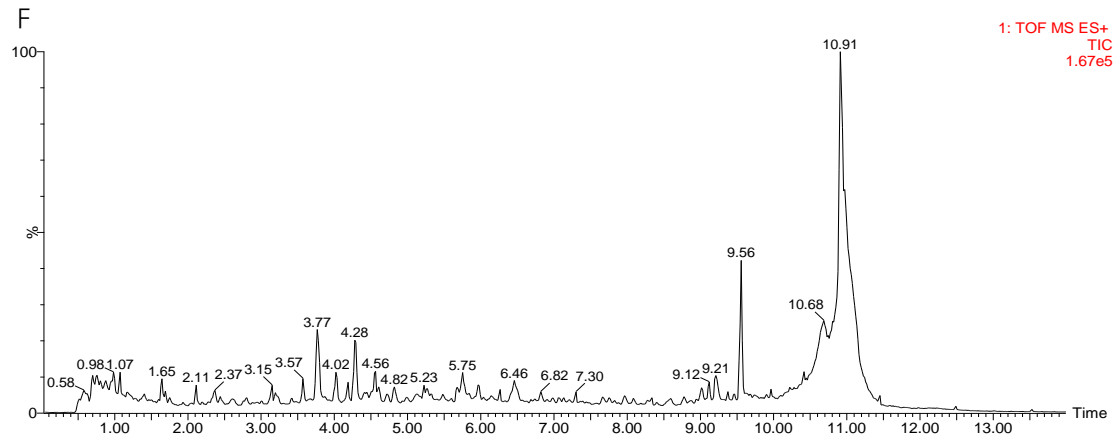
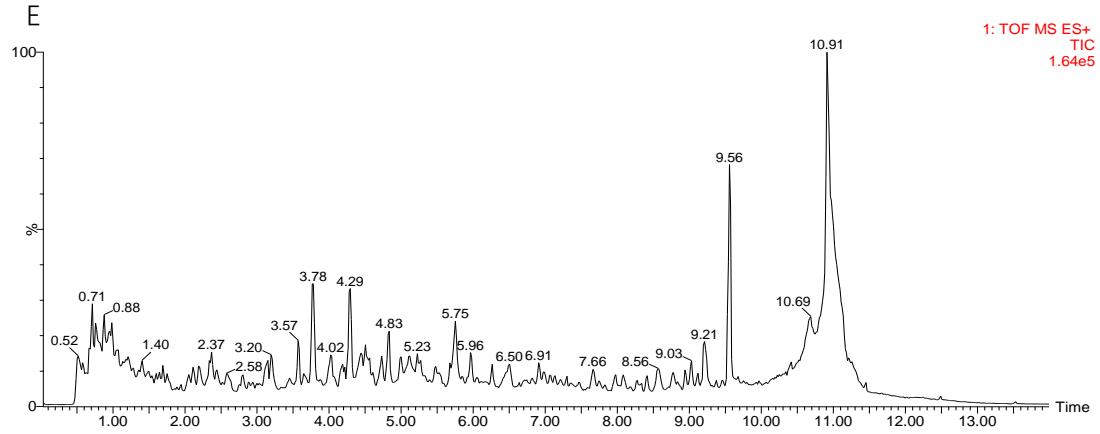


Figure S2 TIC chromatograms on positive ion mode

Notes:

A. Sham-operated Group

B. CNP Model Group

C. Levofloxacin Treatment Group

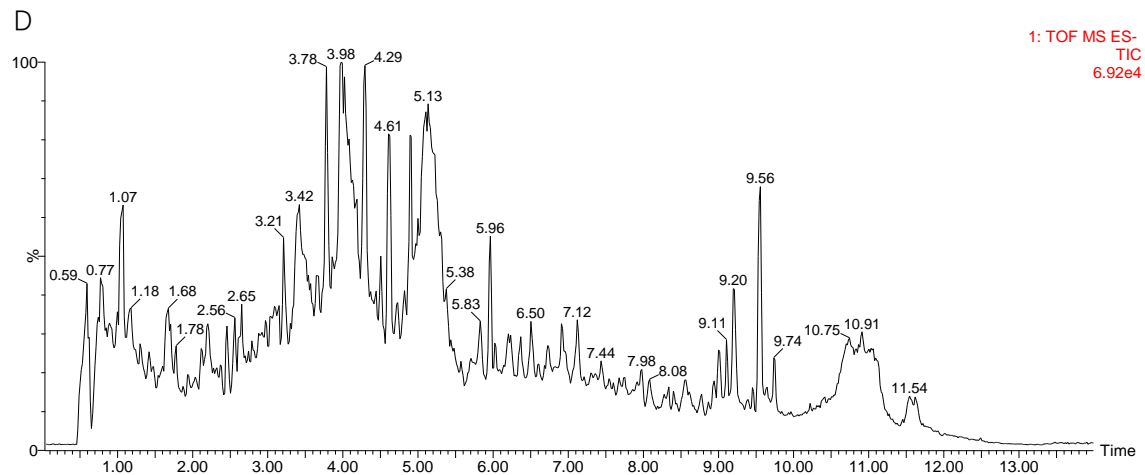
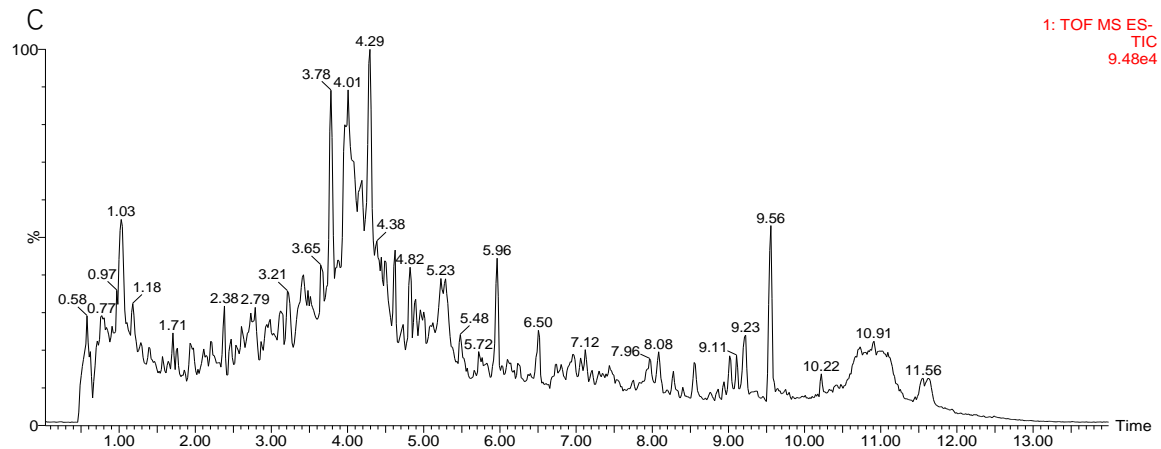
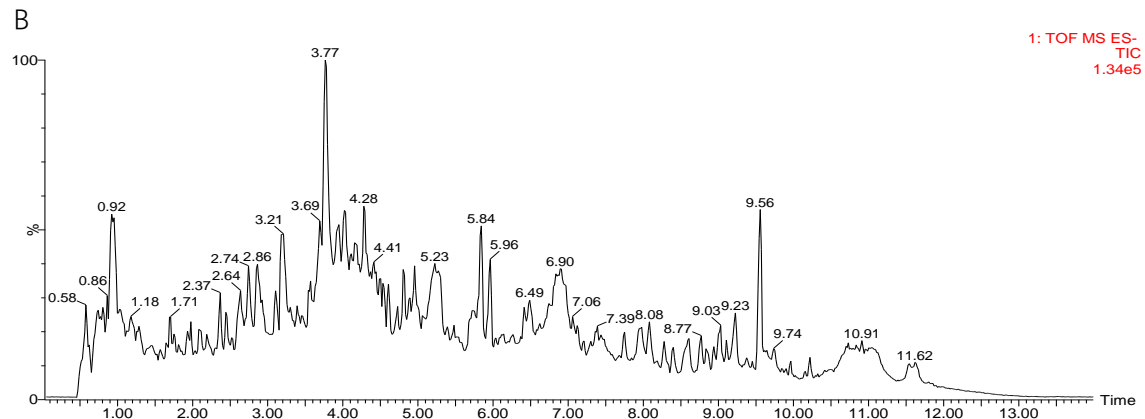
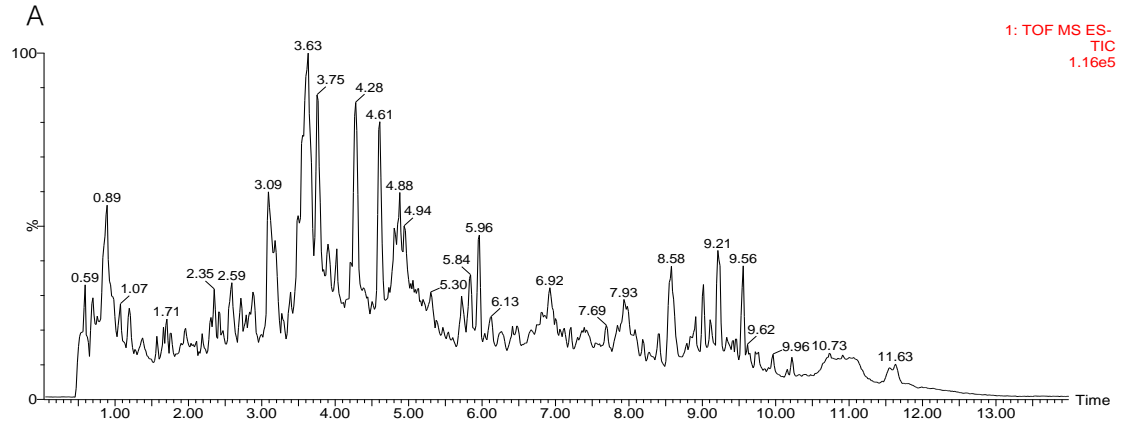
D. Pule' an Tablet Treatment Group

E. Water Decoction Treatment Group

F. Essential Oil Treatment Group

G. Polysaccharide Treatment Group

H. Supernatant Treatment Group



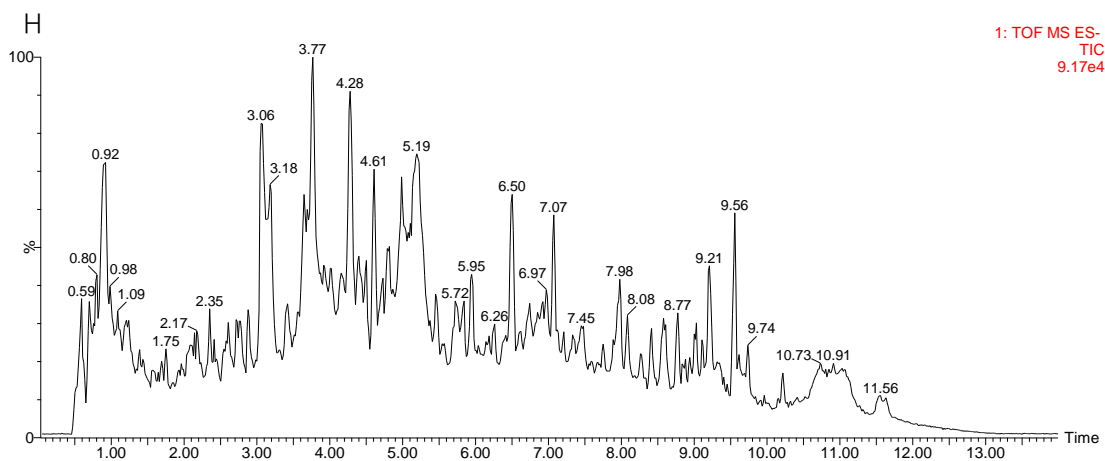
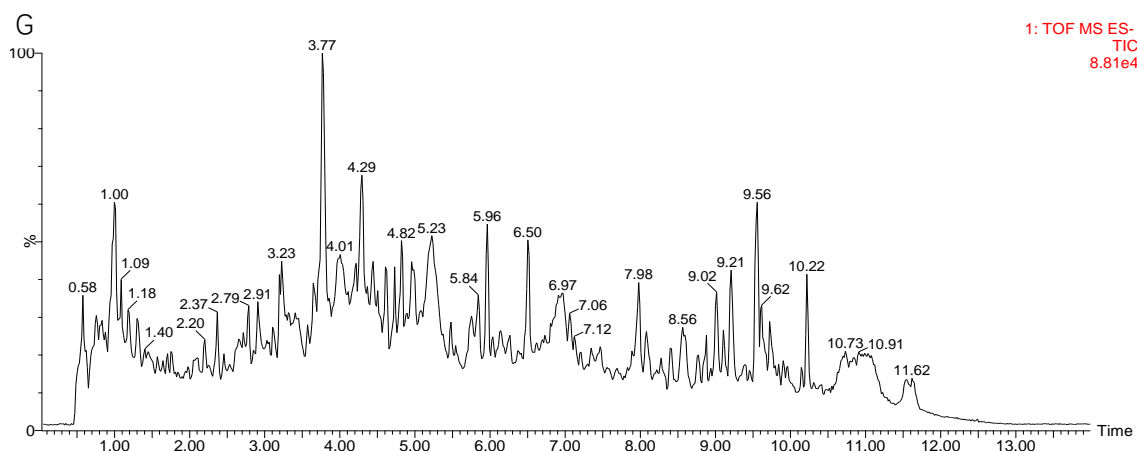
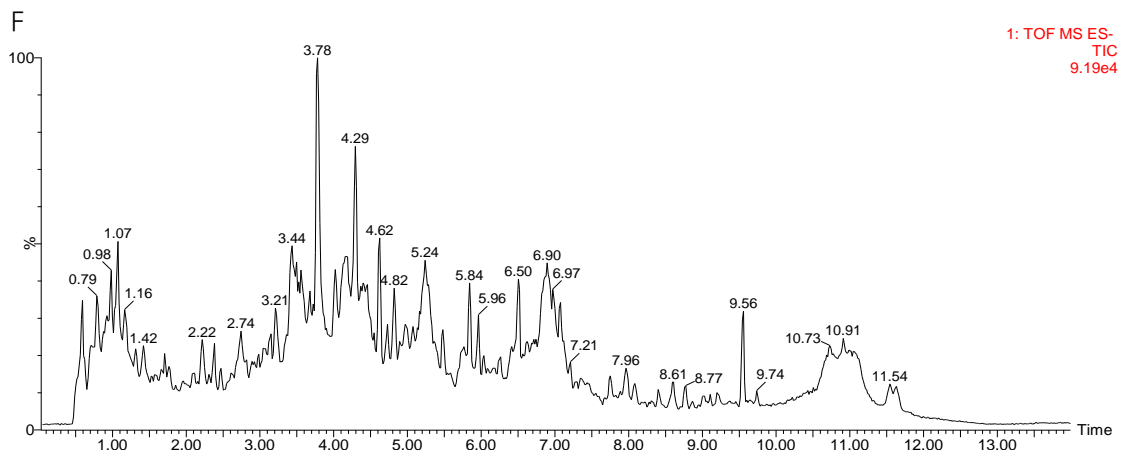
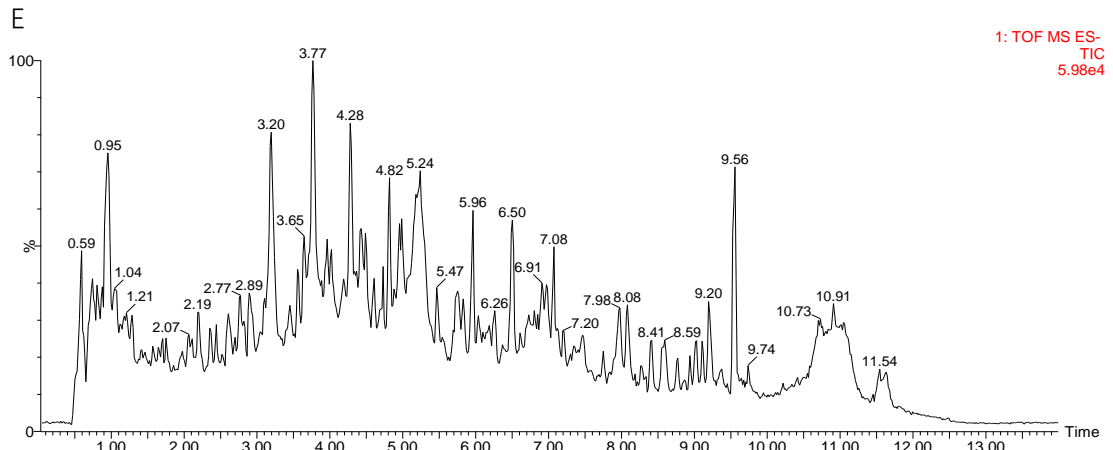


Figure S3 TIC chromatograms on negative ion mode

Notes:

A. Sham-operated Group

B. CNP Model Group

C. Levofloxacin Treatment Group

D. Pule' an Tablet Treatment Group

E. Water Decoction Treatment Group

F. Essential Oil Treatment Group

G. Polysaccharid Treatment Group

H. Supernatant treatment Group

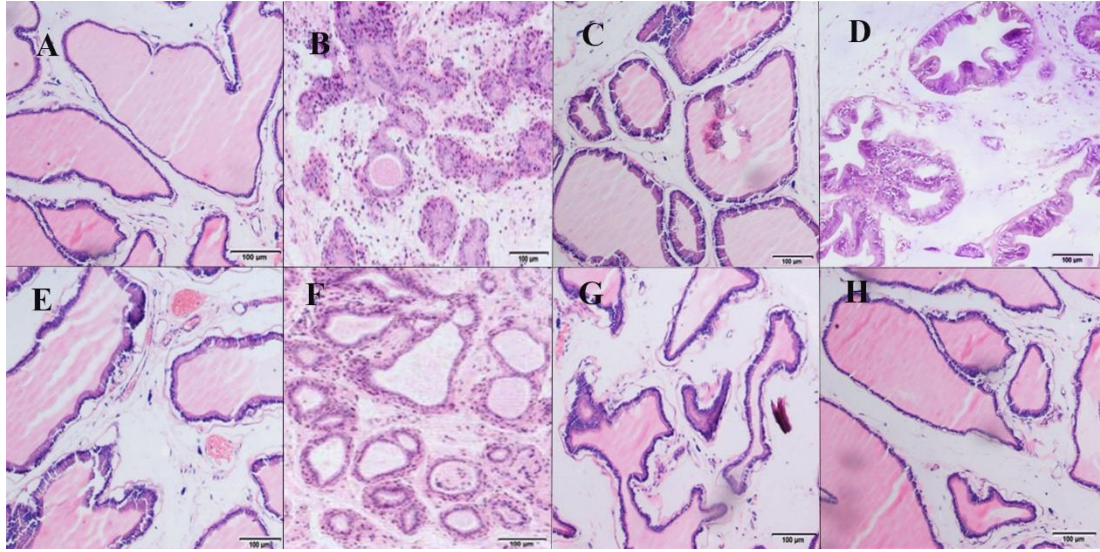


Figure S4 Histological analysis of prostate

Notes:

A. Sham-operated Group

B. CNP Model Group

C. Levofloxacin Treatment Group

D. Pule'an Tablet Treatment Group

E. Water Decoction Treatment Group

F. Essential Oil Treatment Group

G. Polysaccharid Treatment Group

H. Supernatant treatment Group

Table S1 Potential targets of active compounds

| Compound | Target | Uniprot ID | Gene Code | Probability | |
|---|---|---|-----------|-------------|------|
| KQCR1 | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 0.86 | |
| | Muscleblind-like protein 1 | Q9NR56 | MBNL1 | 0.67 | |
| | Muscleblind-like protein 2 | Q5VZF2 | MBNL2 | 0.67 | |
| | Muscleblind-like protein 3 | Q9NUK0 | MBNL3 | 0.67 | |
| | Adenosine receptor A1 | P30542 | ADORA1 | 0.6 | |
| | Arachidonate 5-lipoxygenase | P09917 | ALOX5 | 0.56 | |
| | Arachidonate 15-lipoxygenase | P16050 | ALOX15 | 0.56 | |
| | Arachidonate 12-lipoxygenase | P18054 | ALOX12 | 0.56 | |
| | Arachidonate 15-lipoxygenase B | O15296 | ALOX15B | 0.56 | |
| | Arachidonate 12-lipoxygenase | O75342 | ALOX12B | 0.56 | |
| | Epidermis-type lipoxygenase 3 | Q9BYJ1 | ALOXE3 | 0.56 | |
| | Multidrug resistance-associated protein 1 | P33527 | ABCC1 | 0.53 | |
| | Canalicular multispecific organic anion transporter 2 | O15438 | ABCC3 | 0.53 | |
| | Canalicular multispecific organic anion transporter 1 | Q92887 | ABCC2 | 0.53 | |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 0.51 | |
| | KQCR2 | Aldose reductase | P15121 | AKR1B1 | 0.97 |
| | | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.97 |
| Aldo-keto reductase family 1 member B10 | | O60218 | AKR1B10 | 0.97 | |
| Alcohol dehydrogenase [NADP(+)] | | P14550 | AKR1A1 | 0.96 | |
| Dual specificity tyrosine-phosphorylation-regulated kinase 1A | | Q13627 | DYRK1A | 0.96 | |
| 15-anhydro-D-fructose reductase | | Q96JD6 | AKR1E2 | 0.96 | |
| Tyrosyl-DNA phosphodiesterase 1 | | Q9NUW8 | TDP1 | 0.96 | |
| Alpha-2A adrenergic receptor | | P08913 | ADRA2A | 0.95 | |
| Alpha-2C adrenergic receptor | | P18825 | ADRA2C | 0.95 | |
| NADPH oxidase 4 | | Q9NPH5 | NOX4 | 0.95 | |
| Alpha-2B adrenergic receptor | | P18089 | ADRA2B | 0.95 | |
| Ribosylidihyronicotinamide dehydrogenase [quinone] | | P16083 | NQO2 | 0.91 | |
| NAD(P)H dehydrogenase [quinone] 1 | | P15559 | NQO1 | 0.91 | |
| Prostaglandin G/H synthase 1 | | P23219 | PTGS1 | 0.87 | |
| Prostaglandin G/H synthase 2 | | P35354 | PTGS2 | 0.87 | |
| KQCR5 | | Aldose reductase | P15121 | AKR1B1 | 0.98 |
| | | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.98 |
| | Aldo-keto reductase family 1 member B10 | O60218 | AKR1B10 | 0.98 | |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 0.98 | |
| | Alcohol dehydrogenase [NADP(+)] | P14550 | AKR1A1 | 0.96 | |
| | 5-anhydro-D-fructose reductase | Q96JD6 | AKR1E2 | 0.96 | |
| | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 0.94 | |

| | | | | |
|--------|--|--------|---------|------|
| | Ribosyldihydrionicotinamide dehydrogenase [quinone] | P16083 | NQO2 | 0.94 |
| | NAD(P)H dehydrogenase [quinone] 1 | P15559 | NQO1 | 0.94 |
| | Alpha-2A adrenergic receptor | P08913 | ADRA2A | 0.93 |
| | Alpha-2C adrenergic receptor | P18825 | ADRA2C | 0.93 |
| | NADPH oxidase 4 | Q9NPH5 | NOX4 | 0.93 |
| | Alpha-2B adrenergic receptor | P18089 | ADRA2B | 0.93 |
| | Muscleblind-like protein 1 | Q9NR56 | MBNL1 | 0.89 |
| | Muscleblind-like protein 2 | Q5VZF2 | MBNL2 | 0.89 |
| KQCR6 | Aldose reductase | P15121 | AKR1B1 | 0.94 |
| | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.94 |
| | Aldo-keto reductase family 1 member B10 | O60218 | AKR1B10 | 0.94 |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 0.94 |
| | Alcohol dehydrogenase [NADP(+)] | P14550 | AKR1A1 | 0.93 |
| | 5-anhydro-D-fructose reductase | Q96JD6 | AKR1E2 | 0.93 |
| | Ribosyldihydrionicotinamide dehydrogenase [quinone] | P16083 | NQO2 | 0.92 |
| | NAD(P)H dehydrogenase [quinone] 1 | P15559 | NQO1 | 0.92 |
| | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 0.9 |
| | Alpha-2A adrenergic receptor | P08913 | ADRA2A | 0.89 |
| | Alpha-2C adrenergic receptor | P18825 | ADRA2C | 0.89 |
| | NADPH oxidase 4 | Q9NPH5 | NOX4 | 0.89 |
| | Alpha-2B adrenergic receptor | P18089 | ADRA2B | 0.89 |
| | Prostaglandin G/H synthase 1 | P23219 | PTGS1 | 0.86 |
| | Prostaglandin G/H synthase 2 | P35354 | PTGS2 | 0.86 |
| KQCR9 | Adenosine receptor A1 | P30542 | ADORA1 | 0.84 |
| | Aldose reductase | P15121 | AKR1B1 | 0.83 |
| | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.83 |
| | Aldo-keto reductase family 1 member B10 | O60218 | AKR1B10 | 0.83 |
| | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 0.82 |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 0.69 |
| | Alpha-2A adrenergic receptor | P08913 | ADRA2A | 0.65 |
| | Alpha-2C adrenergic receptor | P18825 | ADRA2C | 0.65 |
| | Alpha-2B adrenergic receptor | P18089 | ADRA2B | 0.65 |
| | Alcohol dehydrogenase [NADP(+)] | P14550 | AKR1A1 | 0.65 |
| | 5-anhydro-D-fructose reductase | Q96JD6 | AKR1E2 | 0.65 |
| | Muscleblind-like protein 1 | Q9NR56 | MBNL1 | 0.65 |
| | Muscleblind-like protein 2 | Q5VZF2 | MBNL2 | 0.65 |
| | Muscleblind-like protein 3 | Q9NUK0 | MBNL3 | 0.65 |
| | NADPH oxidase 4 | Q9NPH5 | NOX4 | 0.6 |
| KQCR11 | Cytochrome P450 1A2 | P05177 | CYP1A2 | 1 |
| | Multidrug resistance protein 1 | P08183 | ABCB1 | 1 |

| | | | | |
|--------|---|--------|---------|------|
| | Arachidonate 5-lipoxygenase | P09917 | ALOX5 | 1 |
| | Estradiol 17-beta-dehydrogenase 1 | P14061 | HSD17B1 | 1 |
| | Aldose reductase | P15121 | AKR1B1 | 1 |
| | Arachidonate 15-lipoxygenase | P16050 | ALOX15 | 1 |
| | Arachidonate 12-lipoxygenase | P18054 | ALOX12 | 1 |
| | Multidrug resistance-associated protein 1 | P33527 | ABCC1 | 1 |
| | Aryl hydrocarbon receptor | P35869 | AHR | 1 |
| | Estradiol 17-beta-dehydrogenase 2 | P37059 | HSD17B2 | 1 |
| | Xanthine dehydrogenase/oxidase | P47989 | XDH | 1 |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 1 |
| | Cytochrome P450 1B1 | Q16678 | CYP1B1 | 1 |
| | NADPH oxidase 4 | Q9NPH5 | NOX4 | 1 |
| | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 1 |
| KQCR12 | Aldose reductase | P15121 | AKR1B1 | 0.94 |
| | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.94 |
| | Aldo-keto reductase family 1 member B10 | O60218 | AKR1B10 | 0.94 |
| | Dual specificity tyrosine-phosphorylation-regulated kinase 1A | Q13627 | DYRK1A | 0.94 |
| | Alcohol dehydrogenase [NADP(+)] | P14550 | AKR1A1 | 0.93 |
| | 5-anhydro-D-fructose reductase | Q96JD6 | AKR1E2 | 0.93 |
| | Ribosylidihyronicotinamide dehydrogenase [quinone] | P16083 | NQO2 | 0.92 |
| | NAD(P)H dehydrogenase [quinone] 1 | P15559 | NQO1 | 0.92 |
| | Tyrosyl-DNA phosphodiesterase 1 | Q9NUW8 | TDP1 | 0.9 |
| | Alpha-2A adrenergic receptor | P08913 | ADRA2A | 0.89 |
| | Alpha-2C adrenergic receptor | P18825 | ADRA2C | 0.89 |
| | NADPH oxidase 4 | Q9NPH5 | NOX4 | 0.89 |
| | Alpha-2B adrenergic receptor | P18089 | ADRA2B | 0.89 |
| | Prostaglandin G/H synthase 1 | P23219 | PTGS1 | 0.86 |
| | Prostaglandin G/H synthase 2 | P35354 | PTGS2 | 0.86 |
| KQCY6 | Arachidonate 5-lipoxygenase | P09917 | ALOX5 | 0.8 |
| | Arachidonate 15-lipoxygenase | P16050 | ALOX15 | 0.8 |
| | Arachidonate 12-lipoxygenase | P18054 | ALOX12 | 0.8 |
| | Arachidonate 15-lipoxygenase B | O15296 | ALOX15B | 0.8 |
| | Epidermis-type lipoxygenase 3 | Q9BYJ1 | ALOXE3 | 0.8 |
| | Arachidonate 12-lipoxygenase | O75342 | ALOX12B | 0.75 |
| | Aldo-keto reductase family 1 member B10 | O60218 | AKR1B10 | 0.71 |
| | Aldose reductase | P15121 | AKR1B1 | 0.71 |
| | Aldo-keto reductase family 1 member B15 | C9JRZ8 | AKR1B15 | 0.71 |
| | Estrogen receptor | P03372 | ESR1 | 0.69 |
| | Estrogen receptor beta | Q92731 | ESR2 | 0.69 |
| | Adenosine receptor A1 | P30542 | ADORA1 | 0.65 |
| | Microtubule-associated protein tau | P10636 | MAPT | 0.63 |

| | | | |
|-----------------------------------|--------|--------|------|
| FAD-linked sulfhydryl oxidase ALR | P55789 | GFER | 0.61 |
| Adenosine receptor A3 | P33765 | ADORA3 | 0.61 |

Table S2 Relevant target genes of prostatitis

| No. | Gene Symbol | Gene ID | Inference Score | No. | Gene Symbol | Gene ID | Inference Score |
|-----|-------------|---------|-----------------|-----|-------------|---------|-----------------|
| 1 | TP53 | 7157 | 68.8 | 278 | PCNA | 5111 | 33.82 |
| 2 | FOLH1 | 2346 | 62.39 | 279 | CLU | 1191 | 33.81 |
| 3 | RNASEL | 6041 | 59.66 | 280 | EGR1 | 1958 | 33.79 |
| 4 | HPCAL1 | 3241 | 57.51 | 281 | PAK1IP1 | 55003 | 33.72 |
| 5 | ELAC2 | 60528 | 56.68 | 282 | COL1A1 | 1277 | 33.7 |
| 6 | KLF6 | 1316 | 54.42 | 283 | IFIT1 | 3434 | 33.64 |
| 7 | GNRH1 | 2796 | 53.1 | 284 | GAL | 51083 | 33.64 |
| 8 | ER | 246870 | 52.78 | 285 | SRC | 6714 | 33.63 |
| 9 | IGF1R | 3480 | 51.87 | 286 | CDC25B | 994 | 33.59 |
| 10 | HOXB13 | 10481 | 51.87 | 287 | P4HB | 5034 | 33.58 |
| 11 | MSR1 | 4481 | 51.03 | 288 | COL18A1 | 80781 | 33.53 |
| 12 | PRLR | 5618 | 50.68 | 289 | TNFRSF1A | 7132 | 33.52 |
| 13 | HMGB2 | 3148 | 50.55 | 290 | PFKFB3 | 5209 | 33.48 |
| 14 | PIM1 | 5292 | 50.49 | 291 | MSMB | 4477 | 33.48 |
| 15 | AR | 367 | 49.04 | 292 | CCNT2 | 905 | 33.48 |
| 16 | AKT1 | 207 | 48.09 | 293 | BRCA2 | 675 | 33.48 |
| 17 | CCND1 | 595 | 47.79 | 294 | BAX | 581 | 33.48 |
| 18 | FOS | 2353 | 47.42 | 295 | STC2 | 8614 | 33.38 |
| 19 | PSCA | 8000 | 47.17 | 296 | PBK | 55872 | 33.38 |
| 20 | COL3A1 | 1281 | 46.29 | 297 | GJB2 | 2706 | 33.38 |
| 21 | PGR | 5241 | 46.27 | 298 | MPP6 | 51678 | 33.37 |
| 22 | MKLN1 | 4289 | 45.85 | 299 | DDX60 | 55601 | 33.37 |
| 23 | GADD45A | 1647 | 45.81 | 300 | CETN3 | 1070 | 33.37 |
| 24 | CYP2E1 | 1571 | 45.77 | 301 | CRHR2 | 1395 | 33.36 |
| 25 | DNMT3B | 1789 | 45.4 | 302 | BUB1 | 699 | 33.28 |
| 26 | EPHB2 | 2048 | 45.29 | 303 | AP1G1 | 164 | 33.25 |
| 27 | CEBPA | 1050 | 45.18 | 304 | HDAC8 | 55869 | 33.14 |
| 28 | FADD | 8772 | 45.08 | 305 | CCDC86 | 79080 | 33.14 |
| 29 | HNF1B | 6928 | 44.76 | 306 | SELENBP1 | 8991 | 33.13 |
| 30 | GHR | 2690 | 44.71 | 307 | GAS6 | 2621 | 33.13 |
| 31 | TGFB3 | 7043 | 44.53 | 308 | EFNA1 | 1942 | 33.13 |
| 32 | TP63 | 8626 | 44.5 | 309 | FASLG | 356 | 33.11 |
| 33 | ODC1 | 4953 | 44.42 | 310 | CYP11A1 | 1583 | 33.09 |
| 34 | PIK3CA | 5290 | 44.27 | 311 | BAD | 572 | 33.09 |
| 35 | MXI1 | 4601 | 43.83 | 312 | HSPB8 | 26353 | 33.08 |
| 36 | FGF2 | 2247 | 43.82 | 313 | KIF14 | 9928 | 33.04 |
| 37 | CYP1A1 | 1543 | 43.81 | 314 | FXYD3 | 5349 | 33.04 |
| 38 | HIF1A | 3091 | 43.67 | 315 | ADIPOR1 | 51094 | 33.04 |
| 39 | NKX3-1 | 4824 | 43.38 | 316 | PGPEP1 | 54858 | 33.03 |
| 40 | TMPRSS2 | 7113 | 43.34 | 317 | GOLIM4 | 27333 | 33.03 |
| 41 | EHBP1 | 23301 | 43.31 | 318 | TIPARP | 25976 | 32.93 |

| | | | | | | | |
|----|-------------|-------|-------|-----|-----------|--------|-------|
| 42 | TH | 7054 | 43.28 | 319 | PHTF2 | 57157 | 32.93 |
| 43 | PDGFA | 5154 | 43.16 | 320 | NPM1 | 4869 | 32.93 |
| 44 | LHB | 3972 | 43.09 | 321 | HDAC1 | 3065 | 32.93 |
| 45 | TNFSF10 | 8743 | 43.03 | 322 | BMP2K | 55589 | 32.93 |
| 46 | THOC1 | 9984 | 42.91 | 323 | UGT2B1 | 71773 | 32.89 |
| 47 | EGFR | 1956 | 42.75 | 324 | SAT1 | 6303 | 32.89 |
| 48 | TSKU | 25987 | 42.63 | 325 | OLR139 | 293278 | 32.86 |
| 49 | CYP1B1 | 1545 | 42.06 | 326 | SAMD9 | 54809 | 32.82 |
| 50 | CDK2 | 1017 | 42.06 | 327 | RPL22L1 | 200916 | 32.82 |
| 51 | PIK3R1 | 5295 | 42.02 | 328 | NMI | 9111 | 32.82 |
| 52 | TIMP3 | 7078 | 41.98 | 329 | MYOD1 | 4654 | 32.82 |
| 53 | ABCG2 | 9429 | 41.82 | 330 | INPP5A | 3632 | 32.82 |
| 54 | ABCC1 | 4363 | 41.76 | 331 | HR | 55806 | 32.82 |
| 55 | CFLAR | 8837 | 41.67 | 332 | FANCC | 2176 | 32.82 |
| 56 | ANGPT1 | 284 | 41.56 | 333 | ADAMTS2 | 9509 | 32.82 |
| 57 | ECE1 | 1889 | 41.48 | 334 | XDH | 7498 | 32.8 |
| 58 | CDKN1A | 1026 | 41.47 | 335 | IRS2 | 8660 | 32.79 |
| 59 | ID1 | 3397 | 41.38 | 336 | CDC6 | 990 | 32.79 |
| 60 | BCL2L1 | 598 | 41.38 | 337 | NAT2 | 10 | 32.75 |
| 61 | CDK6 | 1021 | 41.29 | 338 | MKI67 | 4288 | 32.75 |
| 62 | CENPE | 1062 | 41.18 | 339 | IFNG | 3458 | 32.75 |
| 63 | ATF3 | 467 | 41.15 | 340 | DHRS13A.2 | 447903 | 32.75 |
| 64 | TUBB6 | 84617 | 40.89 | 341 | STXBP6 | 29091 | 32.72 |
| 65 | TGFB2 | 7042 | 40.85 | 342 | SLC28A2 | 9153 | 32.72 |
| 66 | MAF | 4094 | 40.82 | 343 | PARP12 | 64761 | 32.72 |
| 67 | DNAJC3 | 5611 | 40.82 | 344 | IPO4 | 79711 | 32.72 |
| 68 | PRKCD | 5580 | 40.77 | 345 | HEG1 | 57493 | 32.72 |
| 69 | NRIP1 | 8204 | 40.68 | 346 | CYP24A1 | 1591 | 32.61 |
| 70 | ACE | 1636 | 40.62 | 347 | PTEN | 5728 | 32.6 |
| 71 | PLA2G2A | 5320 | 40.61 | 348 | PAGE4 | 9506 | 32.56 |
| 72 | CYP4B1 | 1580 | 40.61 | 349 | HPC3 | 408259 | 32.53 |
| 73 | SLC2A4 | 6517 | 40.58 | 350 | MMP16 | 4325 | 32.52 |
| 74 | PNPT1 | 87178 | 40.56 | 351 | INSL3 | 3640 | 32.52 |
| 75 | MYH14 | 79784 | 40.56 | 352 | MIR205 | 406988 | 32.51 |
| 76 | MAD1L1 | 8379 | 40.5 | 353 | NFKB1 | 4790 | 32.49 |
| 77 | CXCR4 | 7852 | 40.47 | 354 | MIR21 | 406991 | 32.44 |
| 78 | CDKN1B | 1027 | 40.45 | 355 | OPRL1 | 4987 | 32.43 |
| 79 | CCND2 | 894 | 40.36 | 356 | SRP9 | 6726 | 32.42 |
| 80 | PCA3 | 50652 | 40.35 | 357 | PCCA | 5095 | 32.42 |
| 81 | NBN | 4683 | 40.15 | 358 | EPB41L2 | 2037 | 32.42 |
| 82 | PHLDA3 | 23612 | 40.14 | 359 | ATP6V1B2 | 526 | 32.42 |
| 83 | CYP3A23/3A1 | 25642 | 40.14 | 360 | POR | 5447 | 32.38 |
| 84 | NR3C1 | 2908 | 40.11 | 361 | CEBPB | 1051 | 32.35 |
| 85 | BIRC5 | 332 | 39.93 | 362 | ENC1 | 8507 | 32.34 |

| | | | | | | | |
|-----|----------|--------|-------|-----|----------|--------|-------|
| 86 | KLK2 | 3817 | 39.89 | 363 | ADORA1 | 134 | 32.34 |
| 87 | ARMCX3 | 51566 | 39.88 | 364 | SLC44A4 | 80736 | 32.33 |
| 88 | CTNNB1 | 1499 | 39.86 | 365 | MND1 | 84057 | 32.33 |
| 89 | FGFR4 | 2264 | 39.83 | 366 | PLK1 | 5347 | 32.3 |
| 90 | PRKCA | 5578 | 39.82 | 367 | NCOA1 | 8648 | 32.3 |
| 91 | CCNB1 | 891 | 39.73 | 368 | CLDN1 | 9076 | 32.3 |
| 92 | SCNN1A | 6337 | 39.71 | 369 | CKB | 1152 | 32.3 |
| 93 | PLAU | 5328 | 39.51 | 370 | CDK4 | 1019 | 32.3 |
| 94 | SLC39A11 | 201266 | 39.5 | 371 | UBE2C | 11065 | 32.25 |
| 95 | EDN1 | 1906 | 39.31 | 372 | MAPK14 | 1432 | 32.25 |
| 96 | TCF21 | 6943 | 39.14 | 373 | PSPC1 | 55269 | 32.23 |
| 97 | IGF1 | 3479 | 39.12 | 374 | ITPR1 | 3708 | 32.21 |
| 98 | PHB2 | 11331 | 39.03 | 375 | SOX9 | 6662 | 32.17 |
| 99 | ELOVL1 | 64834 | 39.03 | 376 | ADGRG2 | 10149 | 32.15 |
| 100 | FSHB | 2488 | 38.92 | 377 | FGD4 | 121512 | 32.13 |
| 101 | AMH | 268 | 38.91 | 378 | ATXN3 | 4287 | 32.13 |
| 102 | LPIN1 | 23175 | 38.84 | 379 | ANGPTL2 | 23452 | 32.13 |
| 103 | LMNB1 | 4001 | 38.84 | 380 | PARP1 | 142 | 32.12 |
| 104 | PTPRN2 | 5799 | 38.8 | 381 | BID | 637 | 32.09 |
| 105 | JUN | 3725 | 38.8 | 382 | MIR145 | 406937 | 32.06 |
| 106 | NFIL3 | 4783 | 38.78 | 383 | MMP2 | 4313 | 32.04 |
| 107 | GPATCH4 | 54865 | 38.58 | 384 | ENPP2 | 5168 | 32.04 |
| 108 | ATP1B1 | 481 | 38.57 | 385 | ERBB2 | 2064 | 32.01 |
| 109 | CAT | 847 | 38.5 | 386 | ZFH3 | 463 | 32 |
| 110 | GJA1 | 2697 | 38.49 | 387 | SLC1A2 | 6506 | 32 |
| 111 | MCL1 | 4170 | 38.43 | 388 | GSN | 2934 | 32 |
| 112 | KLK3 | 354 | 38.41 | 389 | HPC14 | 1E+08 | 31.98 |
| 113 | PADI2 | 11240 | 38.37 | 390 | PCAP | 7834 | 31.95 |
| 114 | VEGFA | 7422 | 38.26 | 391 | PARP9 | 83666 | 31.95 |
| 115 | AHR | 196 | 38.26 | 392 | MACF1 | 23499 | 31.95 |
| 116 | TOP2A | 7153 | 38.22 | 393 | CCNA2 | 890 | 31.95 |
| 117 | DUSP1 | 1843 | 38.22 | 394 | AGR2 | 10551 | 31.95 |
| 118 | F2R | 2149 | 38.2 | 395 | KLF4 | 9314 | 31.92 |
| 119 | VCPKMT | 79609 | 38.19 | 396 | BMP4 | 652 | 31.91 |
| 120 | KDELR3 | 11015 | 38.16 | 397 | EPHA1 | 2041 | 31.87 |
| 121 | CCN2 | 1490 | 38.08 | 398 | CCT7 | 10574 | 31.87 |
| 122 | STAT1 | 6772 | 38.02 | 399 | SLC16A1 | 6566 | 31.79 |
| 123 | STAT3 | 6774 | 37.99 | 400 | CYP2A4 | 13086 | 31.79 |
| 124 | ESR1 | 2099 | 37.97 | 401 | FZD5 | 7855 | 31.78 |
| 125 | DNMT3A | 1788 | 37.96 | 402 | HSD17B12 | 51144 | 31.77 |
| 126 | AQP1 | 358 | 37.96 | 403 | TLR4 | 7099 | 31.72 |
| 127 | KISS1 | 3814 | 37.87 | 404 | CKAP4 | 10970 | 31.7 |
| 128 | MBP | 4155 | 37.76 | 405 | STARD13 | 90627 | 31.69 |
| 129 | MMP14 | 4323 | 37.71 | 406 | AKAP1 | 8165 | 31.69 |

| | | | | | | | |
|-----|---------|--------|-------|-----|------------|--------|-------|
| 130 | MED11 | 400569 | 37.69 | 407 | MIR221 | 407006 | 31.67 |
| 131 | HOPX | 84525 | 37.67 | 408 | SDR39U1 | 56948 | 31.64 |
| 132 | CD68 | 968 | 37.67 | 409 | HPC4 | 408260 | 31.63 |
| 133 | FADS2 | 9415 | 37.62 | 410 | AURKA | 6790 | 31.63 |
| 134 | KRT19 | 3880 | 37.57 | 411 | GAA | 2548 | 31.61 |
| 135 | TSC22D3 | 1831 | 37.53 | 412 | DMBT1 | 1755 | 31.61 |
| 136 | GOT1 | 2805 | 37.53 | 413 | IGFBP5 | 3488 | 31.59 |
| 137 | MDM2 | 4193 | 37.52 | 414 | HPC10 | 1E+08 | 31.57 |
| 138 | CCNE1 | 898 | 37.5 | 415 | SRD5A2 | 6716 | 31.52 |
| 139 | TK1 | 7083 | 37.48 | 416 | RUNX1T1 | 862 | 31.52 |
| 140 | JUND | 3727 | 37.43 | 417 | ACPP | 55 | 31.52 |
| 141 | UBQLN4 | 56893 | 37.24 | 418 | TNFRSF12A | 51330 | 31.51 |
| 142 | IL1R1 | 3554 | 37.21 | 419 | RSRC2 | 65117 | 31.44 |
| 143 | CXCL10 | 3627 | 37.18 | 420 | PPARGC1A | 10891 | 31.44 |
| 144 | STAR | 6770 | 37.1 | 421 | P2RY1 | 5028 | 31.44 |
| 145 | CYP17A1 | 1586 | 37.05 | 422 | NTRK2 | 4915 | 31.44 |
| 146 | ZYX | 7791 | 37.04 | 423 | FAM13A | 10144 | 31.44 |
| 147 | STAT2 | 6773 | 37.04 | 424 | TRPV6 | 55503 | 31.36 |
| 148 | HSDL2 | 84263 | 37.04 | 425 | SLC39A4 | 55630 | 31.36 |
| 149 | GSTP1 | 2950 | 37.04 | 426 | RCAN2 | 10231 | 31.36 |
| 150 | CYP1A2 | 1544 | 37.02 | 427 | CASP6 | 839 | 31.36 |
| 151 | GADD45G | 10912 | 36.94 | 428 | CASP2 | 835 | 31.36 |
| 152 | ARNT | 405 | 36.94 | 429 | MYC | 4609 | 31.35 |
| 153 | POLK | 51426 | 36.87 | 430 | EIF2S2 | 8894 | 31.35 |
| 154 | ATP2A2 | 488 | 36.86 | 431 | HSD3B1 | 3283 | 31.32 |
| 155 | RARA | 5914 | 36.81 | 432 | RGD1559459 | 501907 | 31.3 |
| 156 | HRAS | 3265 | 36.77 | 433 | DHX9 | 1660 | 31.29 |
| 157 | FOXA1 | 3169 | 36.71 | 434 | KLK5L | 408211 | 31.27 |
| 158 | ARPC1B | 10095 | 36.71 | 435 | FAM43A | 131583 | 31.27 |
| 159 | FOXO3 | 2309 | 36.65 | 436 | FKBP5 | 2289 | 31.25 |
| 160 | LXN | 56925 | 36.63 | 437 | ARG1 | 383 | 31.25 |
| 161 | TFF1 | 7031 | 36.61 | 438 | HPC5 | 619402 | 31.22 |
| 162 | MSMO1 | 6307 | 36.61 | 439 | UGT2B17 | 7367 | 31.2 |
| 163 | EGF | 1950 | 36.6 | 440 | TNF | 7124 | 31.2 |
| 164 | DDIT3 | 1649 | 36.55 | 441 | SYNJ2 | 8871 | 31.2 |
| 165 | SMC2 | 10592 | 36.54 | 442 | RAD23A | 5886 | 31.2 |
| 166 | SRD5A1 | 6715 | 36.52 | 443 | GNAO1 | 2775 | 31.2 |
| 167 | SREBF1 | 6720 | 36.48 | 444 | CEMIP2 | 23670 | 31.2 |
| 168 | PTK2 | 5747 | 36.48 | 445 | PHKG1 | 5260 | 31.19 |
| 169 | ID3 | 3399 | 36.44 | 446 | MAPK11 | 5600 | 31.19 |
| 170 | NUP133 | 55746 | 36.42 | 447 | TANGO2 | 128989 | 31.17 |
| 171 | RAD51 | 5888 | 36.4 | 448 | LGALS3 | 3958 | 31.17 |
| 172 | GSR | 2936 | 36.39 | 449 | AKR1CL | 70861 | 31.17 |
| 173 | PYGM | 5837 | 36.38 | 450 | HPCQTL19 | 347747 | 31.15 |

| | | | | | | | |
|-----|---------|--------|-------|-----|-----------|--------|-------|
| 174 | BRCA1 | 672 | 36.36 | 451 | CYP2C9 | 1559 | 31.14 |
| 175 | SMC4 | 10051 | 36.31 | 452 | TSPAN8 | 7103 | 31.12 |
| 176 | CD82 | 3732 | 36.27 | 453 | TRP53 | 22059 | 31.12 |
| 177 | SNW1 | 22938 | 36.24 | 454 | PRKD1 | 5587 | 31.12 |
| 178 | ATAD2 | 29028 | 36.23 | 455 | SQLE | 6713 | 31.1 |
| 179 | ALAS2 | 212 | 36.16 | 456 | TGFBR2 | 7048 | 31.06 |
| 180 | NR5A1 | 2516 | 36.15 | 457 | TNNC1 | 7134 | 31.04 |
| 181 | ESRRA | 2101 | 36.15 | 458 | SLC15A2 | 6565 | 31.04 |
| 182 | VIM | 7431 | 36.13 | 459 | PARP14 | 54625 | 31.04 |
| 183 | RPS6KA3 | 6197 | 36.08 | 460 | GDF10 | 2662 | 31.04 |
| 184 | IGF2 | 3481 | 36.08 | 461 | HSPH1 | 10808 | 31.02 |
| 185 | GLI1 | 2735 | 36.08 | 462 | MSMP | 692094 | 31.01 |
| 186 | DBH | 1621 | 36.08 | 463 | TGFA | 7039 | 30.99 |
| 187 | SMTNL2 | 342527 | 36.05 | 464 | PFN2 | 5217 | 30.97 |
| 188 | HSP90B1 | 7184 | 36.05 | 465 | PKP2 | 5318 | 30.96 |
| 189 | IL1B | 3553 | 36.02 | 466 | CLCN1 | 1180 | 30.96 |
| 190 | LY6E | 4061 | 36 | 467 | POC5 | 134359 | 30.95 |
| 191 | MET | 4233 | 35.97 | 468 | MORN2 | 729967 | 30.95 |
| 192 | CASP9 | 842 | 35.96 | 469 | KCNF1 | 3754 | 30.94 |
| 193 | SPAG5 | 10615 | 35.93 | 470 | CDC25C | 995 | 30.92 |
| 194 | GPX3 | 2878 | 35.93 | 471 | IL6 | 3569 | 30.9 |
| 195 | BDNF | 627 | 35.9 | 472 | CREB1 | 1385 | 30.9 |
| 196 | DNMT1 | 1786 | 35.89 | 473 | SLC38A4 | 55089 | 30.89 |
| 197 | MRPS27 | 23107 | 35.88 | 474 | COX5B | 1329 | 30.89 |
| 198 | MMD2 | 221938 | 35.88 | 475 | ANP32E | 81611 | 30.89 |
| 199 | PCLAF | 9768 | 35.86 | 476 | CYP3A2 | 266682 | 30.85 |
| 200 | CKS1B | 1163 | 35.86 | 477 | CYP19A1B | 60640 | 30.82 |
| 201 | CDH1 | 999 | 35.81 | 478 | BCL2 | 596 | 30.82 |
| 202 | ERG | 2078 | 35.76 | 479 | TNS3 | 64759 | 30.81 |
| 203 | SPDEF | 25803 | 35.71 | 480 | OAS1 | 4938 | 30.81 |
| 204 | ESPNP | 284729 | 35.64 | 481 | MGST1 | 4257 | 30.81 |
| 205 | APAF1 | 317 | 35.63 | 482 | STEAP2 | 261729 | 30.79 |
| 206 | IRS1 | 3667 | 35.6 | 483 | S100A9 | 6280 | 30.77 |
| 207 | CYP19A1 | 1588 | 35.59 | 484 | SIAH2 | 6478 | 30.74 |
| 208 | COL6A3 | 1293 | 35.57 | 485 | EFHD1 | 80303 | 30.74 |
| 209 | ATP2B1 | 490 | 35.57 | 486 | CPEB2 | 132864 | 30.74 |
| 210 | RAB12 | 201475 | 35.54 | 487 | ARHGAP18 | 93663 | 30.74 |
| 211 | PWP2 | 5822 | 35.54 | 488 | HIST1H2BO | 8348 | 30.72 |
| 212 | HNRNPH1 | 3187 | 35.5 | 489 | CYBA | 1535 | 30.71 |
| 213 | CCN1 | 3491 | 35.45 | 490 | SPSB1 | 80176 | 30.67 |
| 214 | PCBP3 | 54039 | 35.38 | 491 | S100G | 795 | 30.67 |
| 215 | ABCD3 | 5825 | 35.37 | 492 | S100A8 | 6279 | 30.67 |
| 216 | ACTA2 | 59 | 35.27 | 493 | IFIH1 | 64135 | 30.67 |
| 217 | MYO18A | 399687 | 35.22 | 494 | HBEGF | 1839 | 30.64 |

| | | | | | | | |
|-----|---------|--------|-------|-----|---------|--------|-------|
| 218 | CAMK2D | 817 | 35.17 | 495 | FSHR | 2492 | 30.61 |
| 219 | INSIG1 | 3638 | 35.14 | 496 | TIA1 | 7072 | 30.6 |
| 220 | CPE | 1363 | 35.1 | 497 | NUPR1 | 26471 | 30.6 |
| 221 | NUP107 | 57122 | 35.07 | 498 | CYBB | 1536 | 30.6 |
| 222 | LHCGR | 3973 | 35.04 | 499 | CRIP2 | 1397 | 30.6 |
| 223 | CTSD | 1509 | 35 | 500 | STARD4 | 134429 | 30.59 |
| 224 | NOS2 | 4843 | 34.97 | 501 | PADI1 | 29943 | 30.53 |
| 225 | RELA | 5970 | 34.95 | 502 | ENAM | 10117 | 30.53 |
| 226 | TIMP2 | 7077 | 34.93 | 503 | DLC1 | 10395 | 30.53 |
| 227 | FUCA2 | 2519 | 34.92 | 504 | CLMN | 79789 | 30.53 |
| 228 | ASB13 | 79754 | 34.92 | 505 | LRRFIP1 | 9208 | 30.52 |
| 229 | CGA | 1081 | 34.91 | 506 | FANCI | 55215 | 30.52 |
| 230 | MUC1 | 4582 | 34.84 | 507 | EIF2S3 | 1968 | 30.52 |
| 231 | GSK3B | 2932 | 34.82 | 508 | CDH11 | 1009 | 30.52 |
| 232 | C3 | 718 | 34.73 | 509 | MAFF | 23764 | 30.47 |
| 233 | GBP2 | 2634 | 34.66 | 510 | VTG1 | 559475 | 30.46 |
| 234 | ECT2 | 1894 | 34.66 | 511 | KNSTRN | 90417 | 30.46 |
| 235 | ZP3 | 7784 | 34.64 | 512 | INS1 | 16333 | 30.45 |
| 236 | TWNK | 56652 | 34.63 | 513 | PXN | 5829 | 30.39 |
| 237 | WARS | 7453 | 34.6 | 514 | HPC7 | 1E+08 | 30.39 |
| 238 | KLHL24 | 54800 | 34.6 | 515 | ABHD2 | 11057 | 30.39 |
| 239 | SLC45A3 | 85414 | 34.58 | 516 | EPHA4 | 2043 | 30.38 |
| 240 | SRPRA | 6734 | 34.49 | 517 | MIR146A | 406938 | 30.36 |
| 241 | CBFA2T3 | 863 | 34.49 | 518 | WDR60 | 55112 | 30.35 |
| 242 | SLC6A6 | 6533 | 34.48 | 519 | MIR222 | 407007 | 30.34 |
| 243 | NFKBIA | 4792 | 34.48 | 520 | CRYAB | 1410 | 30.34 |
| 244 | DLGAP5 | 9787 | 34.48 | 521 | SDK1 | 221935 | 30.33 |
| 245 | RXRA | 6256 | 34.38 | 522 | EIF3K | 27335 | 30.33 |
| 246 | CD44 | 960 | 34.38 | 523 | TM4SF1 | 4071 | 30.32 |
| 247 | WWC2 | 80014 | 34.35 | 524 | HAO2 | 51179 | 30.32 |
| 248 | DGKH | 160851 | 34.35 | 525 | DTL | 51514 | 30.32 |
| 249 | VCAM1 | 7412 | 34.34 | 526 | PGRMC1 | 10857 | 30.31 |
| 250 | IGFBP6 | 3489 | 34.3 | 527 | RRM2 | 6241 | 30.3 |
| 251 | NR4A1 | 3164 | 34.26 | 528 | IGFBP1 | 3484 | 30.3 |
| 252 | SLC29A1 | 2030 | 34.24 | 529 | GPX1 | 2876 | 30.3 |
| 253 | PROM1 | 8842 | 34.24 | 530 | CHEK2 | 11200 | 30.3 |
| 254 | ESR2 | 2100 | 34.22 | 531 | ALB | 213 | 30.3 |
| 255 | LAMC2 | 3918 | 34.19 | 532 | CDH2 | 1000 | 30.27 |
| 256 | AHNAK | 79026 | 34.19 | 533 | PSRC1 | 84722 | 30.25 |
| 257 | HMOX1 | 3162 | 34.14 | 534 | PAWR | 5074 | 30.25 |
| 258 | IL2 | 3558 | 34.1 | 535 | NOLC1 | 9221 | 30.25 |
| 259 | RORA | 6095 | 34.02 | 536 | MX2 | 4600 | 30.25 |
| 260 | MUC5B | 727897 | 33.97 | 537 | ELF3 | 1999 | 30.25 |
| 261 | TGFB1 | 7040 | 33.96 | 538 | TLR2 | 7097 | 30.24 |

| | | | | | | | |
|-----|----------|--------|-------|-----|----------|--------|-------|
| 262 | RALGAPA1 | 253959 | 33.96 | 539 | SOCS3 | 9021 | 30.21 |
| 263 | PPARG | 5468 | 33.96 | 540 | HPC6 | 1E+08 | 30.21 |
| 264 | MRPL33 | 9553 | 33.96 | 541 | HPC15 | 1E+08 | 30.21 |
| 265 | MEN1 | 4221 | 33.96 | 542 | EPOR | 2057 | 30.18 |
| 266 | IFT88 | 8100 | 33.96 | 543 | GH | 14599 | 30.16 |
| 267 | GUSB | 2990 | 33.96 | 544 | SLC7A6OS | 84138 | 30.15 |
| 268 | FAM110C | 642273 | 33.96 | 545 | LAS1L | 81887 | 30.15 |
| 269 | NQO1 | 1728 | 33.94 | 546 | ZBTB22 | 9278 | 30.14 |
| 270 | CASP8 | 841 | 33.94 | 547 | PCGEM1 | 64002 | 30.12 |
| 271 | HSD17B1 | 3292 | 33.91 | 548 | SP1 | 6667 | 30.11 |
| 272 | CD80 | 941 | 33.91 | 549 | ME1 | 4199 | 30.08 |
| 273 | CD38 | 952 | 33.91 | 550 | CYCS | 54205 | 30.06 |
| 274 | MCM7 | 4176 | 33.9 | 551 | OPTN | 10133 | 30.05 |
| 275 | BCL3 | 602 | 33.9 | 552 | MYH10 | 4628 | 30.05 |
| 276 | SERPINE1 | 5054 | 33.88 | 553 | ITPR3 | 3710 | 30.05 |
| 277 | MTHFD2 | 10797 | 33.85 | 554 | MIR34A | 407040 | 30.01 |

Table S3 The information of merging gene

| No. | Gene | Gene ID | Gene Name |
|-----|---------|---------|---|
| 1 | XDH | 7498 | xanthine dehydrogenase(XDH) |
| 2 | CYP1B1 | 1545 | cytochrome P450 family 1 subfamily B member 1(CYP1B1) |
| 3 | HSD17B1 | 3292 | hydroxysteroid 17-beta dehydrogenase 1(HSD17B1) |
| 4 | ESR1 | 2099 | estrogen receptor 1(ESR1) |
| 5 | ABCC1 | 4363 | ATP binding cassette subfamily C member 1(ABCC1) |
| 6 | ESR2 | 2100 | estrogen receptor 2(ESR2) |
| 7 | CYP1A2 | 1544 | cytochrome P450 family 1 subfamily A member 2(CYP1A2) |
| 8 | NQO1 | 1728 | NAD(P)H quinone dehydrogenase 1(NQO1) |
| 9 | ADORA1 | 134 | adenosine A1 receptor(ADORA1) |
| 10 | AHR | 196 | aryl hydrocarbon receptor(AHR) |

Table S4 Details of enriched pathways

| Term | Database | ID | Input number | Background number | P-Value | Corrected P-Value |
|--|---------------|------------|--------------|-------------------|----------|-------------------|
| Caffeine metabolism | KEGG PATHWAY | hsa00232 | 2 | 5 | 1.19E-06 | 3.36E-05 |
| omega-hydroxylase P450 pathway | Gene Ontology | GO:0097267 | 2 | 9 | 3.13E-06 | 6.38E-05 |
| ERBB signaling pathway | Gene Ontology | GO:0038127 | 3 | 145 | 5.95E-06 | 0.0001 |
| epoxygenase P450 pathway | Gene Ontology | GO:0019373 | 2 | 18 | 1.08E-05 | 0.000161 |
| Tryptophan metabolism | KEGG PATHWAY | hsa00380 | 2 | 40 | 4.87E-05 | 0.000493 |
| enzyme linked receptor protein signaling pathway | Gene Ontology | GO:0007167 | 4 | 942 | 5.96E-05 | 0.000577 |
| Prolactin signaling pathway | KEGG PATHWAY | hsa04917 | 2 | 72 | 0.000152 | 0.001114 |
| Estrogen signaling pathway | KEGG PATHWAY | hsa04915 | 2 | 99 | 0.000284 | 0.001809 |
| Sphingolipid signaling pathway | KEGG PATHWAY | hsa04071 | 2 | 121 | 0.00042 | 0.002448 |
| hormone-mediated signaling pathway | Gene Ontology | GO:0009755 | 2 | 214 | 0.001284 | 0.005838 |
| Metabolic pathways | KEGG PATHWAY | hsa01100 | 3 | 1243 | 0.003121 | 0.010098 |
| adenosine receptor signaling pathway | Gene Ontology | GO:0001973 | 1 | 12 | 0.003264 | 0.010218 |
| vascular endothelial growth factor signaling pathway | Gene Ontology | GO:0038084 | 1 | 24 | 0.006269 | 0.01554 |
| purinergic receptor signaling pathway | Gene Ontology | GO:0035587 | 1 | 31 | 0.008018 | 0.017868 |
| Thyroid hormone signaling pathway | KEGG PATHWAY | hsa04919 | 1 | 118 | 0.029526 | 0.044206 |
| G-protein coupled receptor signaling pathway | Gene Ontology | GO:0007186 | 2 | 1204 | 0.035176 | 0.050369 |
| cGMP-PKG signaling pathway | KEGG PATHWAY | hsa04022 | 1 | 167 | 0.041453 | 0.057463 |
| cAMP signaling pathway | KEGG PATHWAY | hsa04024 | 1 | 199 | 0.049172 | 0.065465 |
| Purine metabolism | KEGG PATHWAY | hsa00230 | 1 | 176 | 0.04363 | 0.05956 |

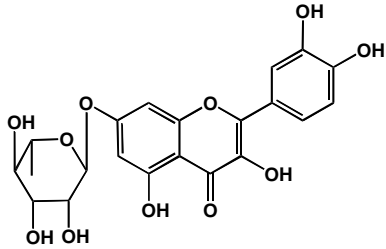
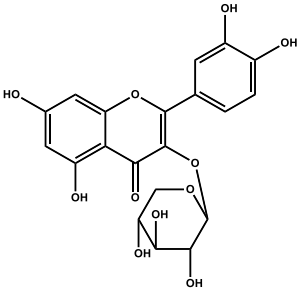
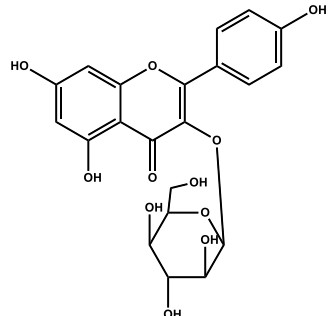
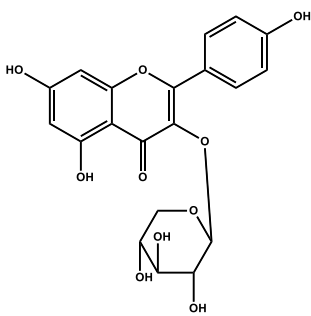
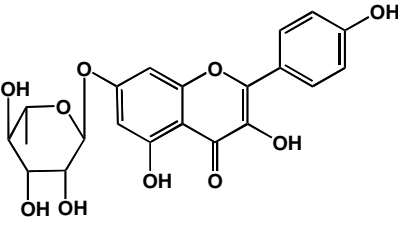
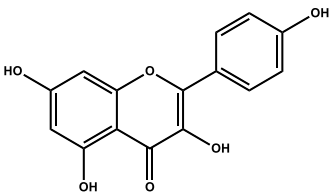
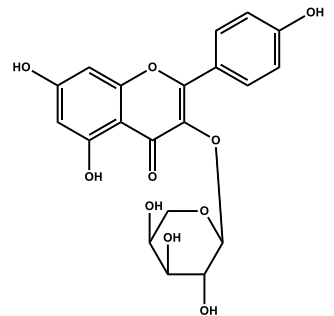
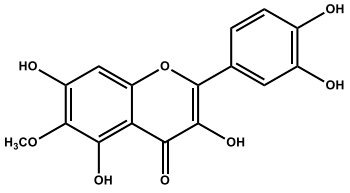
Table S5 Gradient elution program

| Time (min) | A% | B% | Curve |
|------------|------|------|---------|
| 0.00 | 98.0 | 2.0 | Initial |
| 8.00 | 60.0 | 40.0 | 6 |
| 10.00 | 2.0 | 98.0 | 6 |
| 12.00 | 98.0 | 2.0 | 6 |
| 14.00 | 98.0 | 2.0 | 6 |

Table S6 Markerlynx Software parameter settings

| Parameter | ESI(+) | ESI(-) |
|-------------------------------------|------------------|------------------|
| Function | 1 | 1 |
| Analysis type | Peak Detection | Peak Detection |
| Initial/Final Retention Time | 0.00/10.00min | 0.00/10.00min |
| Low/High Mass | 50.00/1200.00 Da | 50.00/1200.00 Da |
| XIC Window (Da) | 0.05 | 0.05 |
| Use relative retention time | NO | NO |
| Peak width at 5% Height (seconds) | 1.00 | 1.00 |
| Peak-to-Peak Baseline Noise | 0.00 | 0.00 |
| Apply Smoothing | NO | NO |
| Marker Intensity threshold (counts) | 100 | 100 |
| Mass window | 0.05 Da | 0.05 Da |
| Retention time window | 0.10 min | 0.10 min |
| Noise elimination level | 6.00 | 6.00 |
| Deisotope data | YES | YES |
| Replicate% Minimum | 0.00 | 0.00 |

Table S7 Structures of active compounds

| No | ID | Structure | No | ID | Structure |
|----|---------|--|----|---------|---|
| 1 | KQCR-1 |  Quercetin-7-O- α -L-rhamnopyranoside | 2 | KQCR-2 |  Quercetin-3-O- α -L-arabinopyranoside |
| 3 | KQCR-5 |  Kaempferol-3-O- β -D-glucopyranoside | 4 | KQCR-6 |  Kaempferol-3-O- β -D-xylopyranoside |
| 5 | KQCR-9 |  Kaempferol-3-O- α -L-rhamnopyranoside | 6 | KQCR-11 |  Kaempferol |
| 7 | KQCR-12 |  Kaempferol-3-O- α -L-arabinopyranoside | 8 | KQCY-6 |  Patuletin |