

Table S3 Gene symbol of target proteins interacts with non-volatile differential metabolites in flowers and leaves by network pharmacological analysis.

	Gene symbol
Flower	<p>NFKB1, APEX1, HIF1A, PSMB1, KLF5, GPR55, KDM1A, NR1I2, CNR1, NFE2L2, TLR4, NTRK3, PTGS1, TOP2A, CLK4, CHUK, SCN2A, SLC6A5, SCN3A, NR3C2, ADAM10, CDK1, PDGFRA, CTSD, DPP9, FPR2, CACNA1B, PIK3R1, DUSP3, C5AR1, RORB, TFPI, ADORA1, GRIN1, TRIM24, PRKCD, GRIA2, METAP2, CYP3A4, CFTR, AURKB, SCD, CSNK2B, PDE3A, CNR2, HSP90AA1, GRK5, RXFP1, NTSR2, PSMB9, ACHE, CACNA1H, WDR5, S1PR5, PLA2, CCR1, CCR2, CYSLTR2, ITK, AOC3, FPRL2, FPR1, SAE1, PRMT5, RPS6KA3, NR2E3, GPR6, MAP2K2, QRFPR, SCN4A, F13A1, AR, HDAC5, PRCP, PRSS1, AXL, CDC25C, GLRA1, CCNE1, KEAP1, PRKAA1, ITGB1, GRB2, CASP8, CAPN1, GPR17, MC4R, ACACA, CACNA1C, TNK1, NOTUM, TDP1, HSD17B10, ALOX12, THRA, TTR, MAOA, FFAR4, ANPEP, LDHB, GPBAR1, HPGD, HDAC2, BLM, PIN1, GUSB, KCNA5, MDM4, PDE11A, KDM4C, PTPN7, ACVRL1, AVPR1B, SLC2A1, CAMKK2, PDGFRB, KIF11, PRKCZ, DHODH, CBX4, CHKA, GLO1, ENPP1, KDM4A, SERPINE1, PLAT, FAAH, PDE3B, P2RX4, S1PR4, GLS, NOX1, TYRO3, PTPN11, HTR2C, NPC1, NAAA, DCUN1D1, PTGER1, NR4A1, MTOR, MIF, CREBBP, ESR2, HDAC8, DYRK1A, RPS6KA1, NLK, CXCR4, ZAP70, AKR1C1, ERN1, STAT1, MAPKAPK2, DRD1, GBA2, TBK1, CDK2, SLC1A3, ACVR1, DPP7, CDK5, LGALS3, CHRM2, RPS6KA6, ADRB1, FCGRT, MME, SLC1A1, CHEK1, ERAP1, HSP90AB1, ACE, AAK1, GCK, NQO2, MMP12, NOS2, PTGER2, CHRM1, ABCC1, SLC1A2, HDAC10, EGLN1, CYP19A1, MCHR1, CDC25B, TACR1, GSK3A, GABRA1, DNMT1, PPIA, XDH, ACVR1B, MELK, TNIK, EIF2AK1, CLK2, ALOX5, MC5R, YES1, BRDT, ACACB, AKR1B1, GBA, IMPDH2, HRH3, CHRM3, TBXA2R, PTPN1, PTPN2, ATG4B, TLR8, HDAC7, TACR2, SLC40A1, SLC9A1, AKR1C3, OPRK1, CHRM4, MAP3K14, STK3, ADK, PNMT, CHRNA4, CHRM5, PRKACA, KLK1, RAB9A, NT5E, TYMS, CLK1, PTGS2, HDAC11, TOP1, KDM5A, MINK1, HDAC9, SIRT1, PKN2, CHRNA2, FASN, ADORA2B, BMPR1A, PKN1, PARP2, CSNK1E, HDAC3, ULK3, TMPRSS6, GSTP1, NEK2, HSD11B1, CDK4, KLK7, ABCG2, NOS3, ULK1, KIT, PSMB2, PDE9A, HPRT1, APLNR, IL23R, SLC6A2, MAP4K4, HRH4, HSD11B2, CSNK2A2, MARK4, GPR35, PHF8, KDM5C, TYMP, TBXAS1, CHRNA7, RPS6KA5, PTGES, CA3, CDK7, TDO2, TRPM8, CHEK2, AKT3, MAP3K11, HDAC4, KLK5, CSNK1D, DYRK1B, KLKB1, FDP5, BRD2, PKMYT1, GRM2, MAOB, FYN, DUT, TAOK1, LNPEP, GHSR, STING1, CYP2A6, P2RX7, CTSS, LYN, ALK, HTR1A, FGR, DPP8, DAO, GSK3B, ADAM17, PYGL, CHRNA1, IRAK1, AKR1C2, CASP6, EPHB2, EPHB3, CETP, DOT1L, MAPK1, OPRD1, CCR5, OPRM1, PIK3CD, P2RY12, S1PR3, ARG2, SPHK1, BTK, AKT2, PIK3CB, FAP, ABL1, MAP3K5, SLC5A1, APH1A, PARP1, PLA2G2A, PRKCA, FBP1, TGFB2, F12, PAK4, APP, PDE4D, DPP4, ATR, NR1H4, NR3C1, CDC7, DCK, SLC6A4, STAT3, P2RY4, NOX4, FNTA, PRMT1, PDE5A, F2R, CFD, TGM2, PPARG, VDR, SIRT3, FLT1, CXCR6, PTK2B, SPHK2, DRD2, BMP2K, TYK2, RET, GAK, EZH2, HTR3A, KDM6B, PREP, KCNK9, and NAMPT.</p>
Leaf	<p>BLM, GPR55, TRIM24, PTGS1, NFKB1, CTSD, KDM1A, STAT3, APEX1, CYP3A4, NR3C2, PTPN2, CLK4, ADAM10, CDK5, HSD17B10, GLRA1, CSNK2B, HSP90AB1, NTRK3, FPR2, TLR4, NTSR2, PDE3A, CDC25B, SCN3A, PIK3R1, SCN2A, KLF5, TOP2A, GRIN1, AKR1C3, CNR2, AR, CLK1, PDGFRA, SLC9A1, FPR1, ITK, CACNA1B, TACR2, FPRL2, DPP9, GPR6, NR4A1, ADORA1, PROC, PRCP, CPT2, CYSLTR2, S1PR5, TERT, CHRM4, PLAT, CACNA1H, HDAC7, TLR8, QRFPR, RPS6KA1, CDC25C, AURKB, TFPI, MTOR, C5AR1, SAE1, PTK2B, CHRM1, PTGER1, PSMB9, STING1, DPP8, MARK4, SPHK1, CHRM5, SLC6A5, THRA.</p>

Table S3 Gene symbol of target proteins interacts with non-volatile differential metabolites in flowers and leaves by network pharmacological analysis (continued).

	Targets
Leaf	<p>ATG4B, CDK1, WDR5, AVPR1B, PLA1, PTGER2, CHRM2, FKBP1A, TDP1, MAOA, TTR, XDH, NR1I2, ABCC1, ALOX12, EGLN1, RPS6KA3, PSMB1, PRKCZ, DUSP3, DRD2, SLC2A1, OPRM1, GPR17, F13A1, ROCK1, GRM5, CDK2, OPRD1, CAPN1, FFAR4, CHRNA4, DRD1, AAK1, DNMT1, PRKACA, RORB, LGALS3, SERPINE1, LYN, SCN9A, IL23R, KEAP1, STAT1, RPS6KA6, DUT, CETP, ACVRL1, GLO1, MAP2K2, CASP8, ZAP70, HDAC5, FCGRT, RET, PKN1, CHUK, FFAR2, ACACA, BRAF, STK3, SCD, ITGB1, ACE, FAAH, ERAP1, ABCB1, F2R, PTPN11, PIK3CB, ACVR1B, PIN1, GRB2, DRD3, HDAC11, YES1, KDM6B, ESR2, GRIA2, HIF1A, HPGD, GPBAR1, KDM4C, ANPEP, GUSB, NOS2, CXCR4, HSP90AA1, LDHB, PTPN7, METAP2, CFTR, NFE2L2, PDGFRB, CAMKK2, NPC1, GRK5, MME, HDAC2, CHKA, PDE3B, NT5E, DCUN1D1, NAAA, KDM4A, PDE11A, KIF11, CBX4, MIF, NOS3, HRH3, KCNA5, HTR2C, GABRA1, SCN4A, NLK, MC5R, AOC3, GPR35, ACHE, CHRM3, AKR1C1, RXFP1, ADRB1, P2RX4, TYRO3, CXCR6, S1PR4, TBXA2R, MDM4, ACACB, TACR1, TBK1, NOTUM, ENPP1, GBA, CCNE1, RAB9A, GLS, NOX1, GSTP1, PSMB2, MAOB, GBA2, CA3, PKN2, NQO2, TNIK, KLK5, FFAR1, RPS6KA5, TOP1, LNPEP, AKR1C2, FYN, CYP2A6, BRDT, TMPPRS6, KLK1, HTR7, PRSS1, MAP2K1, TAOK3, ULK1, TRPA1, PLK4, CCR1, CHEK1, ERN1, CCR2, PLA2G2A, EPHB2, SLC1A3, KLK7, FGR, KDR, PARP2, ADORA2A, DPP7, SLC1A1, CPT1B, SLC1A2, ADORA3, EPHX2, CASP6, FLT3, ITGB3, KIT, SOAT1, EPHB3, NR2E3, KCNK9, GRM4, CTSS, CHRNA1, MAP3K5, MAPK1, DOT1L, PIK3CD, P2RY12, ARG2, PTPN1, S1PR3, LTA4H, CCR5, CSNK2A2, CSNK2A1, CTSG, SLC40A1, F12, FAP, PARP1, OPRK1, ABL1, AKT2, TBXAS1, ST14, NAMPT, HTR2A, APLNR, CFD, MET, JAK2, PRKCA, IDE, AKT3, NR1H3, PRKCD, ADORA2B, HDAC8, SLC6A2, BMP2K, HDAC3, DYRK1B, PRKCQ, CDC7, PPIA, MAP3K11, FDPS, HDAC10, BCHE, CSK, CLK2, AXL, TYMS, HDAC9, ALOX5, HSD11B2, MC4R, F11, NTSR1, PREP, KCNH2, CDK7, CARM1, SLC6A4, PRMT6, MMP7, IKBKB, PAK4, TAOK1, HDAC4, ERAP2, NOS1, DYRK1A, EPHA4, ROCK2, DAO, ESR1, PKMYT1, HCAR2, BMPR1A, HSD11B1, GCK, MCHR1, P2RX7, NEK2, MAP4K4, IMPDH2, FLT1, ALK, CTSK, DCTPP1, HTR3A, CNR1, HDAC1, CDK4, F7, MAP3K14, CTSB, PIK3CA, FER, BCL6, UGT2B7, TEC, ICMT, IDO1, S1PR2, CTSL, PDPK1, P2RY2, TGM2, CD38, BCR, CAMK2D, PRMT1, PARG, ADAM17, PPARA, DPP4, IDH1, PIK3CG, RXRB, PRMT5, PRKAA1, VDR, MAP3K20, RIPK3, AHCY, SLC6A3, TDO2, TDP2, BRD4, ATAD2, SPHK2, EP300, F2, MARK3, GHSR, PDE7A, FABP4, RXRG, EGFR, TTK, ULK3, FKBP5, FBP1, GRM3, TGFBR2, MAPKAPK2, SLC5A1, SYK, PLK1, NMT1, APH1A, NTRK1, and MMP1.</p>

Table S4 Non-volatile metabolites for yellowhorn treat enuresis, hyperlipidemia, neurodegenerative diseases, and prostatitis.

Source	Name	Classification	No.	Degree
Flower	Zarzissine	Alkaloids	Flower25	61
	2-Aminopurine	Nucleotides and derivatives	Flower31	53
	Hispidulin (5,7,4'-Trihydroxy-6-methoxyflavone)	Flavonoids	Flower11	51
	Luteolin-3'-O-glucoside	Flavonoids	Flower13	47
	Naringenin (5,7,4'-Trihydroxyflavanone)	Flavonoids	Flower4	47
	Diosmetin (5,7,3'-Trihydroxy-4'-methoxyflavone)	Flavonoids	Flower9	47
	Luteolin-7-O-gentiobioside	Flavonoids	Flower15	46
	3,5,4'-Trihydroxy-7-methoxyflavone (Rhamnocitrin)	Flavonoids	Flower16	46
	Isorhamnetin-3-O-rutinoside (Narcissin)	Flavonoids	Flower18	46
	Kaempferol-3-O-sambubioside	Flavonoids	Flower21	46
	Luteolin-4'-O-glucoside	Flavonoids	Flower14	45
	Kaempferol-3-O-galactoside (Trifolin)	Flavonoids	Flower19	45
	Kaempferol-3-O-glucoside (Astragalin)	Flavonoids	Flower20	45
	Diosmetin-7-O-glucoside	Flavonoids	Flower10	43
	6-C-MethylKaempferol-3-glucoside	Flavonoids	Flower12	43
	Rhamnetin-3-O-Rutinoside	Flavonoids	Flower24	43
	Kaempferol-7-O-glucoside	Flavonoids	Flower22	42
	Quercetin-3-O-rhamnoside(Quercitrin)	Flavonoids	Flower23	42
	Guanosine	Nucleotides and derivatives	Flower32	42
	L-Homocystine	Amino acids and derivatives	Flower30	41
	Vidarabine	Nucleotides and derivatives	Flower33	41
	Adenosine	Nucleotides and derivatives	Flower34	41
	Persicoside	Flavonoids	Flower5	41
	Isorhamnetin-3-O-neohesperidoside	Flavonoids	Flower17	40
	isoscopoletin	Lignans and Coumarins	Flower27	40
	Scopoletin (7-Hydroxy-6-methoxycoumarin)	Lignans and Coumarins	Flower28	38
	Gallic acid	Phenolic acids	Flower29	37
	Chrysoeriol-7-O-glucoside	Flavonoids	Flower8	37
	Savinin	Lignans and Coumarins	Flower26	36
	Hesperetin-7-O-glucoside	Flavonoids	Flower3	35
	Oleanolic acid-3-O-glucoside	Terpenoids	Flower7	35
	3,5,7-Trihydroxyflavanone (Pinobanksin)	Flavonoids	Flower6	34
	Shanzhiside methyl ester	Terpenoids	Flower1	32
	Oleanolic acid-3-O-glucoside	Terpenoids	Flower2	29
Leaf	Jujubogenin	Terpenoids	Leaf3	81
	Serotonin	Alkaloids	Leaf21	54
	Tryptamine	Alkaloids	Leaf19	48
	L-Lysine	Amino acids and derivatives	Leaf33	48
	Apigenin-7-O-neohesperidoside (Rhoifolin)	Flavonoids	Leaf10	47
	Epigallocatechin	Flavonoids	Leaf8	47

Table S4 Non-volatile metabolites for yellowhorn treat enuresis, hyperlipidemia, neurodegenerative diseases, and prostatitis (continued).

Source	Name	Classification	No.	Degree
Leaf	Galocatechin	Flavonoids	Leaf9	47
	Apigenin-7-O-rutinoside (Isorhoifolin)	Flavonoids	Leaf11	46
	N-Methyltryptamine	Alkaloids	Leaf20	46
	Quercetin-3,7-Di-O-rhamnoside	Flavonoids	Leaf14	45
	DL-2-Aminoadipic acid	Alkaloids	Leaf18	44
	L-Valine	Amino acids and derivatives	Leaf31	44
	Myricetin-3-O-galactoside	Flavonoids	Leaf12	43
	Cannabicitrin	Flavonoids	Leaf13	42
	L-Glutamine	Amino acids and derivatives	Leaf32	42
	Catechin	Flavonoids	Leaf6	42
	Epicatechin	Flavonoids	Leaf7	42
	N-Feruloylagmatine	Alkaloids	Leaf16	40
	Acetaminophen	Alkaloids	Leaf17	40
	Cis-Coutaric acid	Phenolic acids	Leaf26	38
	5-Glucosyloxy-2-Hydroxybenzoic acid methyl ester	Phenolic acids	Leaf28	38
	3-O-p-Coumaroylquinic acid	Phenolic acids	Leaf30	38
	Acetryptine	Alkaloids	Leaf22	36
	Isofraxetin	Lignans and Coumarins	Leaf24	36
	4-(3,4,5-Trihydroxybenzoxy)benzoic acid	Phenolic acids	Leaf29	36
	Hederagenin	Terpenoids	Leaf4	36
	Fraxetin-8-O-glucoside (Fraxin)	Lignans and Coumarins	Leaf23	34
	p-Coumaric acid-4-O-glucoside	Phenolic acids	Leaf25	33
	2-Nitrophenol	Phenolic acids	Leaf27	33
	Pomolic acid	Terpenoids	Leaf1	32
	30-Norhederagenin	Terpenoids	Leaf5	32
	2-Phenylethylamine	Alkaloids	Leaf15	31
	Corosolic acid	Terpenoids	Leaf2	29

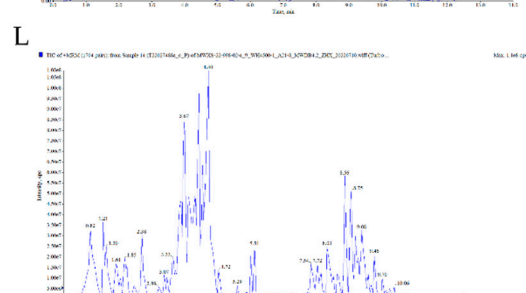
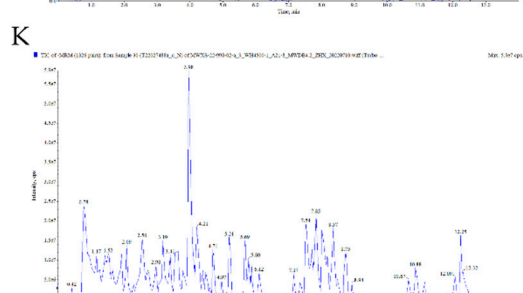
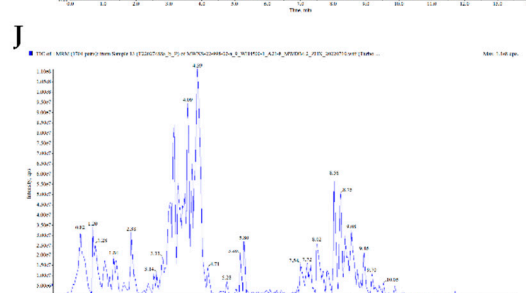
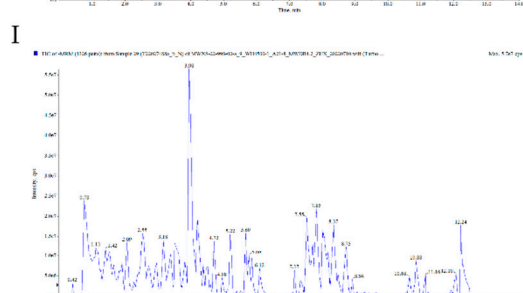
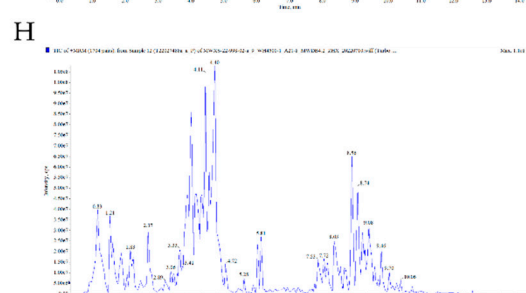
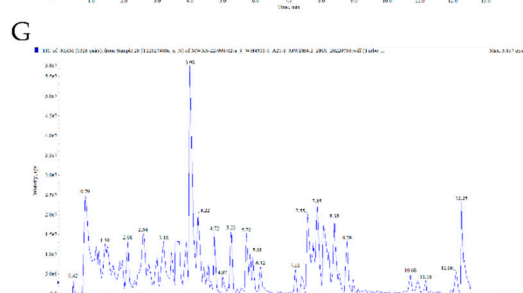
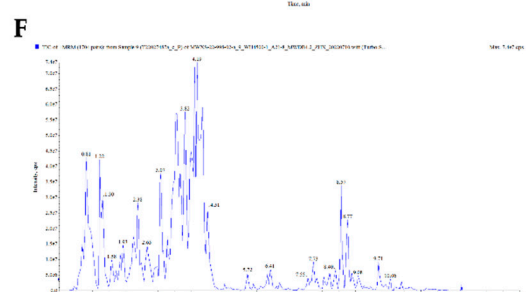
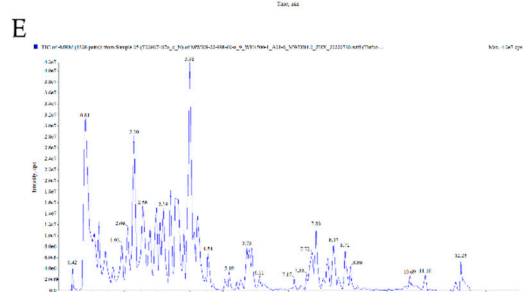
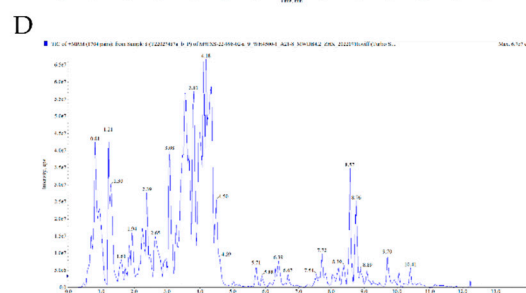
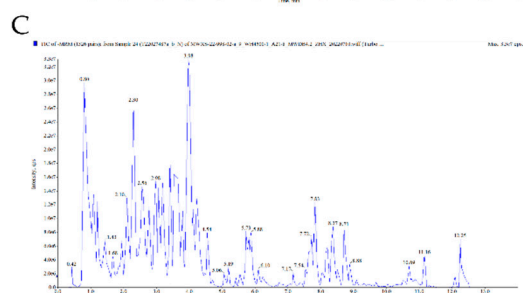
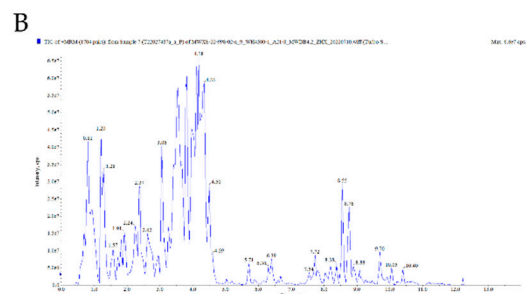
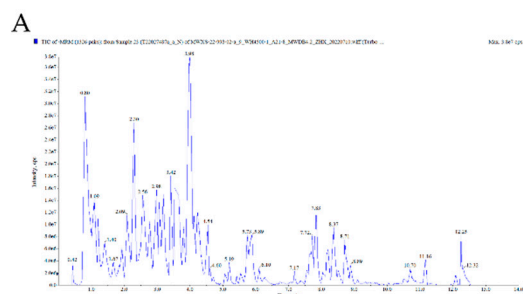
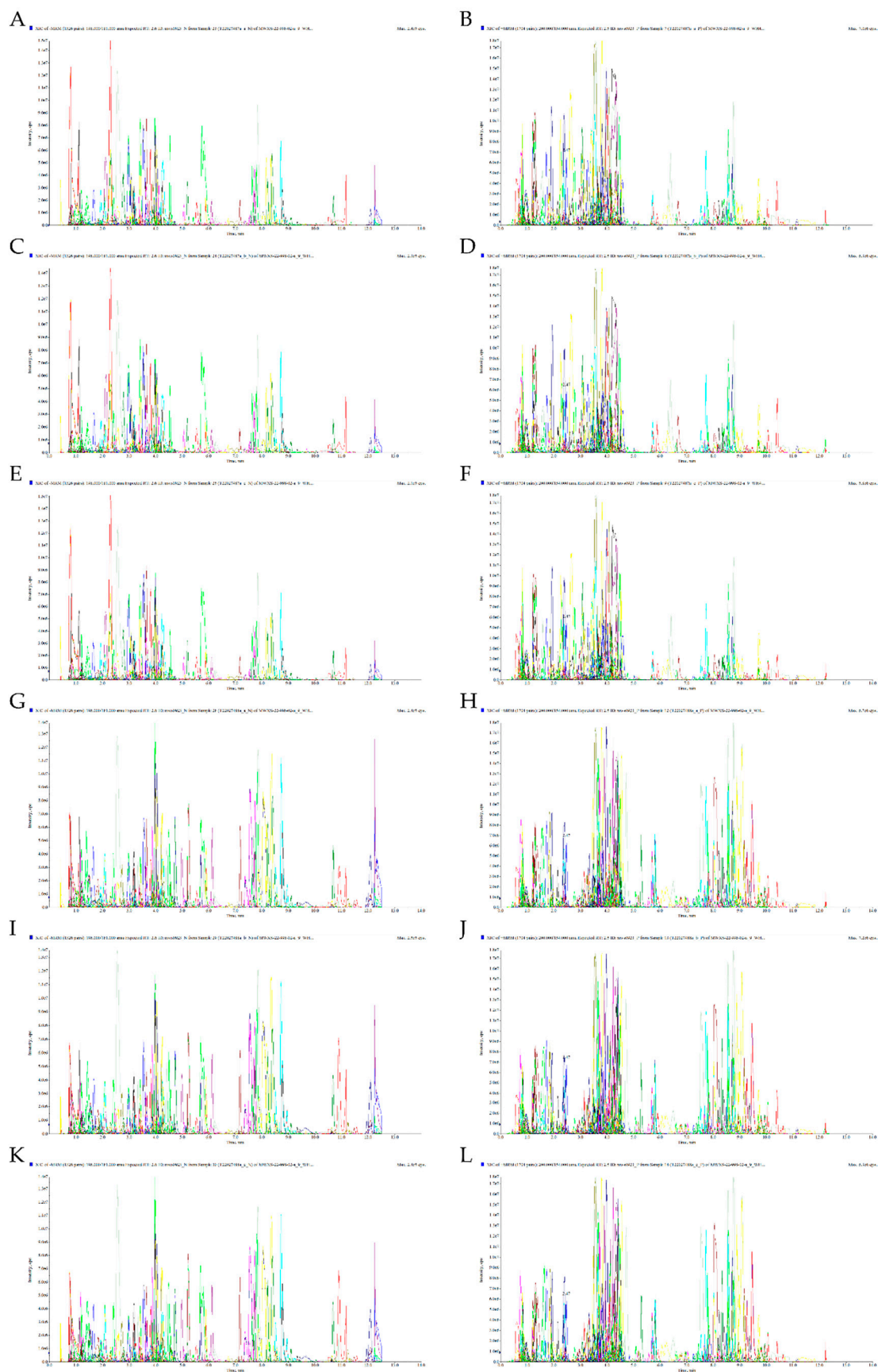


Figure S1 Total ions current of non-volatile metabolites in yellowhorn Leaf (A-F) and flower (G-L). (A, C, E, G, I, and K) Negative ion mode; (B, D, F, H, J, and L) positive ion mode.



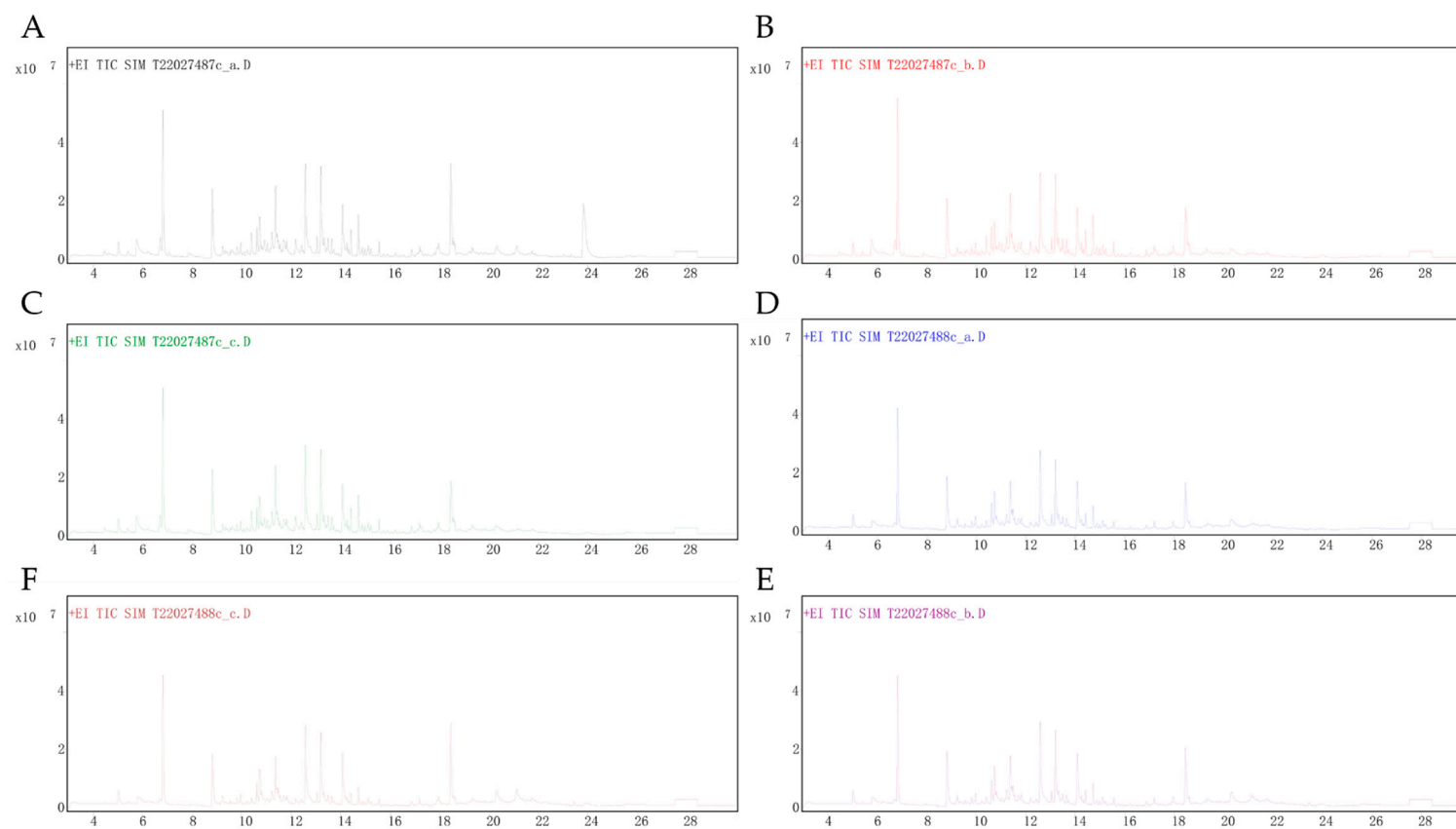


Figure S3. Total ions current of volatile metabolites in yellowhorn Leaf (A-B) and flower (D-E).

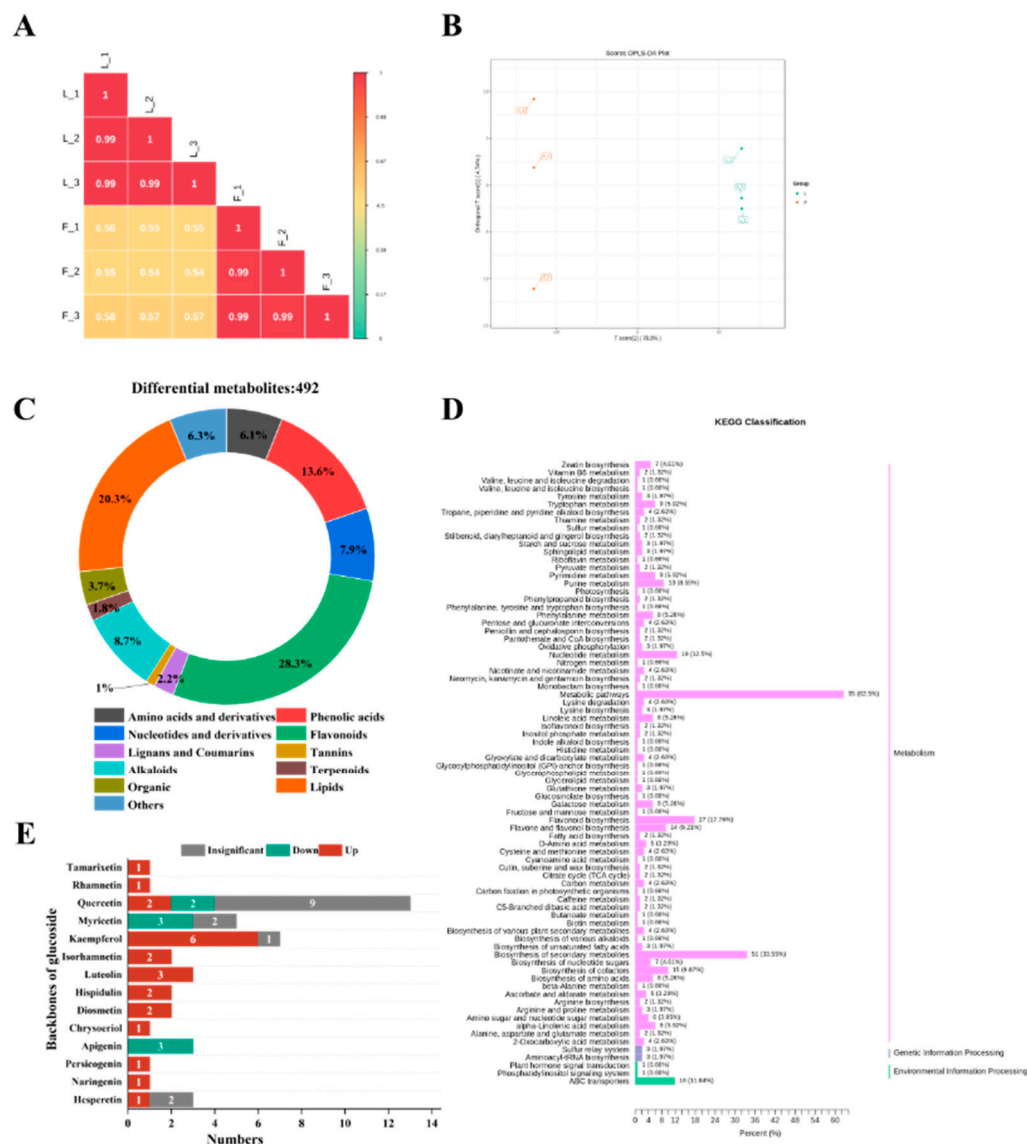


Figure. S4 Screening of significantly differentially expressed non-volatile metabolites in yellowhorn leaf and flower. (A) Correlation heat map of non-volatile metabolites of yellowhorn leaves and flowers; (B) Scores plots of OPLS-DA; (C) Proportion of different classes of differentially expressed non-volatile metabolites; (D) KEGG annotate ions and enrichment results of the differentially expressed non-volatile metabolites; (E) Differentially expressed non-volatile metabolites of yellowhorn leaves and flowers.