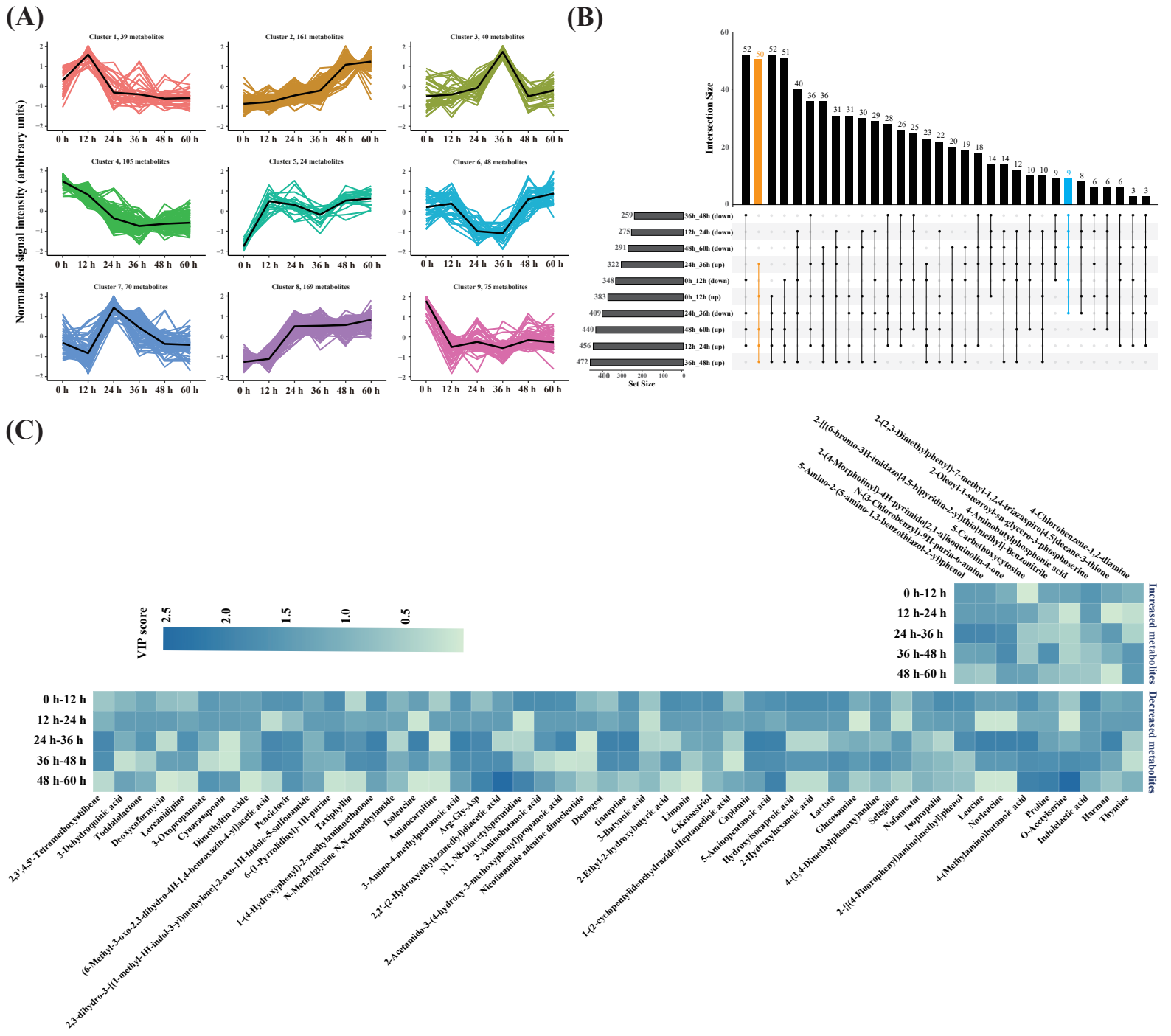
(A)
Cluster 1, 39 metabolites
Cluster 2, 161 metabolites
Cluster 3, 40 metabolites
Cluster 4, 105 metabolites
Cluster 5, 24 metabolites
Cluster 6, 48 metabolites
Cluster 7, 70 metabolites
Cluster 8, 169 metabolites
Cluster 9, 75 metabolites
Normalized signal intensity (arbitrary units)
0 h 12 h 24 h 36 h 48 h 60 h
(B)
Intersection Size
52 50 52 51 40 36 36 31 31 30 29 28 26 25 23 22 20 19 18 14 14 12 10 10 9 9 8 6 6 6 3 3
36h_48h (down)
12h_24h (down)
48h_60h (down)
24h_36h (up)
0h_12h (down)
0h_12h (up)
24h_36h (down)
48h_60h (up)
12h_24h (up)
36h_48h (up)
259 275 291 322 348 383 409 440 456 472
400 300 200 100 0
Set Size
(C)
VIP score
2.5 2.0 1.5 1.0 0.5
2-[(6-bromo-3H-imidazo[4,5-b]pyridin-2-yl)thio]methyl]-Benzonitrile
2-(4-Morpholinyl)-4H-pyrimido[2,1-a]isoquinolin-4-one
5-Amino-2-(5-amino-1,3-benzothiazol-2-yl)phenol
2-(2,3-Dimethylphenyl)-7-methyl-1,2,4-triazaspiro[4.5]dec-3-ene-1,4-dione
2-Oleoyl-1-stearoyl-sn-glycero-3-phosphoserine
4-Aminobutylphosphonic acid
5-Carbethoxycytosine
N-(3-Chlorobenzyl)-9H-purin-6-amine
4-Chlorobenzene-1,2-diamine
0 h-12 h
12 h-24 h
24 h-36 h
36 h-48 h
48 h-60 h
Increased metabolites
Decreased metabolites
2,3',4,5'-Tetramethoxystilbene
3-Dehydrocrominic acid
Toddalolactone
Deoxyeoformycin
Lercanidipine
3-Oxopropanoate
C-narasaponin
Dimethylfolin oxide
Penciclovir
(6-Methyl-3-oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)acetic acid
2,3-dihydro-3-[(1-methyl-1H-indol-3-yl)methylene]-2-oxo-1H-Indole-5-sulfonamide
6-(1-Pyrrolidinyl)-1H-purine
Taxiphyllin
1-(4-Hydroxyphenyl)-2-methylaminoethanone
N-Methylglycine
N,N-dimethylamide
Isoleucine
Aminocaranitine
3-Amino-4-methylpentanoic acid
Arg-Gly-Asp
2,2'-(2-Hydroxyethylazanediyl)diacetic acid
N1,N8-Diacetylspermidine
3-Aminobutanoic acid
2-Acetamido-3-(4-hydroxy-3-methoxyphenyl)propanoic acid
Nicotinamide adenine dinucleotide
Dienogest
tianeptine
3-Butynoic acid
2-Ethyl-2-hydroxybutyric acid
Limonin
6-Ketoestriol
1-(2-cyclopentylidenehydrazide)Heptanedioic acid
Caplamin
5-Aminopentanoic acid
Hydroxyisocaproic acid
2-Hydroxyhexanoic acid
Lactate
Glucosamine
4-(3,4-Dimethylphenoxy)aniline
Selegiline
Nafamostat
Isopropalin
2-[[(4-Fluorophenyl)amino]methyl]phenol
Leucine
Norleucine
4-(Methylamino)butanoic acid
Proline
O-Acetylserine
Indolelactic acid
Harman
Thymine