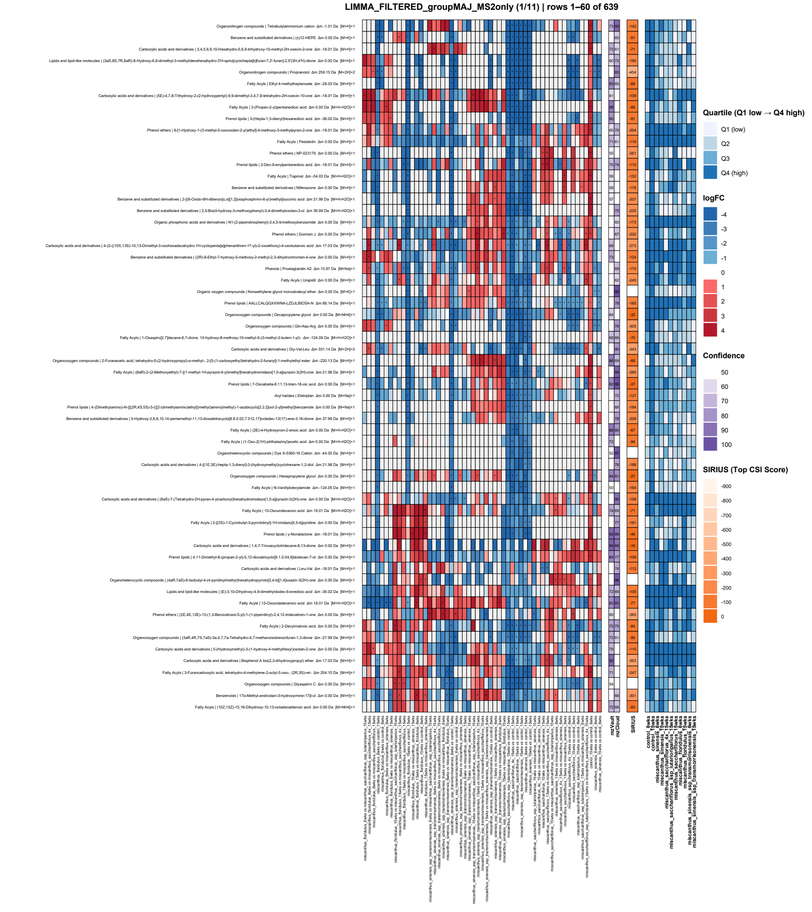
LIMMA_FILTERED_groupMAJ_MS2only (1/11) | rows 1–60 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Organonitrogen compounds | Tetrabutylammonium cation Δm -1.01 Da [M+]+
Benzene and substituted derivatives | (±)-12-HEPE Δm 0.00 Da [M+]+
Carboxylic acids and derivatives | 3,4,5,6,8,10-Hexadecatrienoic-6,8,9-trihydroxy-10-methyl-(9-cis-semi)-Lone Δm -18.01 Da [M+]+
Lipids and lipid-like molecules | (3aS,6S,7R,8aR)-8-Hydroxy-6,8-dimethyl-3-methylidenehexahydro-2H-spiro[cyclohepta[b]furan-7,2'-furan]-2,3'(3'H),4'(5'-dione Δm 0.00 Da [M+]+
Organonitrogen compounds | Propranolol Δm 259.15 Da [M+2H]+2
Fatty Acyls | Ethyl 4-methylheptanoate Δm -28.03 Da [M+]+
Carboxylic acids and derivatives | (5E)-4,7,8-Trihydroxy-2-(2-hydroxyperoxy)-6,9-dimethyl-3,4,7,8-tetrahydro-2H-oxecin-10-one Δm -18.01 Da [M+]+
Fatty Acyls | 3-(Propan-2-yl)pentanedioic acid Δm 0.00 Da [M+H+NH3]+
Prenol lipids | 3-Prenyl-7,3-dien-(2hexanedioic acid Δm -36.02 Da [M+]+
Phenol ethers | 6(21-Hydroxy-1,2-methyl-5-oxooxazin-2-yl)ethyl-4-methoxy-3-methylbiyan-2-one Δm -18.01 Da [M+]+
Fatty Acyls | Pestalotin Δm 0.00 Da [M+]+
Phenol ethers | NP-023176 Δm 0.00 Da [M+]+
Prenol lipids | 2-Oxo-3-oxo(pentanedioic acid Δm -18.01 Da [M+]+
Fatty Acyls | Tagonal Δm -44.03 Da [M+H+NH3]+
Benzene and substituted derivatives | Nifenazone Δm 0.00 Da [M+]+
Benzene and substituted derivatives | (2-[(8-Cholic-6H-dibenzo[b,d]]7,2)oxaphosphirin-6-yl)methylsuccinic acid Δm 21.98 Da [M+H+NH3]+
Benzene and substituted derivatives | 2,5,6-Bis(4-hydroxy-3-methoxyphenyl)-3,4-dimethylsoolan-3-ol Δm 38.99 Da [M+H+NH3]+
Organic phosphoric acids and derivatives | N1-(2-piperidinoethyl)-3,4,5,6-trimethoxybenzamide Δm 0.00 Da [M+]+
Phenol ethers | Somion J Δm 0.00 Da [M+]+
Carboxylic acids and derivatives | 4(-2-[(1S5,135)-10,13-Dimethyl-3-oxohexadecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-oxoethoxy)-4-oxobutanoic acid Δm 17.03 Da [M+]+
Benzene and substituted derivatives | (2R)-8-Ethyl-7-hydroxy-5-methoxy-2-methyl-2,3-dihydroichromen-4-one Δm 0.00 Da [M+]+
Phenols | Prostaglandin A2 Δm 15.97 Da [M+Na]+
Fatty Acyls | Unapidil Δm 0.00 Da [M+]+
Organic oxygen compounds | Nonaethylene glycol monododecyl ether Δm 0.00 Da [M+]+
Prenol lipids | AALLCALQGXXRNA-LZDLBCSA-N Δm 86.14 Da [M+]+
Organooxygen compounds | Decaoxypropylene glycol Δm 0.00 Da [M+NH4]+
Organooxygen compounds | Gln-Asp-Arg Δm 0.00 Da [M+]+
Fatty Acyls | 1-Oxaspiro[2.7]decane-6,7-dione, 10-hydroxy-8-methoxy-10-methyl-9-(3-methyl-2-butten-1-yl) Δm -124.09 Da [M+H+NH3]+
Carboxylic acids and derivatives | Gly-Val-Leu Δm 331.14 Da [M+2H]+2
Organooxygen compounds | 2-Furanoacetic acid, tetrahydro-5-(2-hydroxyprop)-(±-methyl-, 2-[5-(1-carboxyethyl)tetrahydro-2-furanyl]-1-methylethyl ester Δm -220.13 Da [M+]+
Fatty Acyls | (5aR)-2-(2-Methoxyethyl)-7-[(1-methyl-1H-pyrazol-4-yl)methyl]hexahydroindazol-5-algonyn-3(2H)-one Δm 21.98 Da [M+]+
Prenol lipids | 7-Oxocalabra-8,11,13-trien-18-oic acid Δm 0.00 Da [M+]+
Acyl halides | Elektriplan Δm 0.00 Da [M+Na]+
Prenol lipids | 4-(Dimethylamino)-N-[(3R,4S,5S)-5-[[2-(dimethylamino)ethyl]methylamino]methyl]-1-azabicyclo[2.2.2]oct-2-yl]methyl]benzamide Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | 5-Hydroxy-2,6,8,10,14-pentamethyl-11,13-dioxabicyclo[8.6.0.0(2,7.0(12,17)]octadec-12(17)-ene-3,16-dione Δm 37.96 Da [M+]+
Fatty Acyls | (3E)-4-Hydroxyoxo-2-enoic acid Δm 0.00 Da [M+H+NH3]+
Fatty Acyls | (1-Oxo-2(10)-phthalazin)acetic acid Δm 0.00 Da [M+H+NH3]+
Organoheterocyclic compounds | Dye A-6380-16 Cation Δm -44.05 Da [M+]+
Carboxylic acids and derivatives | 4-[(1E,3E)-Heptie-1,3-dien]-3,5-(hydroxymethyl)cyclohexane-1,2-diol Δm 21.98 Da [M+]+
Organooxygen compounds | Hexapropylene glycol Δm 0.00 Da [M+]+
Fatty Acyls | N-Vanillylnicotinamide Δm -124.05 Da [M+]+
Carboxylic acids and derivatives | (8aS)-7-(Tetrahydro-2H-pyran-4-yl)carbonyl]hexahydromoxazo[3,-5-algonyn-3(2H)-one Δm 0.00 Da [M+H+NH3]+
Fatty Acyls | 10-Decenedioxoic acid Δm 18.01 Da [M+H+NH3]+
Fatty Acyls | 2-[(3S)-1-Cyclobutyl-3-(cyrrolidinyl)-1H-imidazol]-3,5-algonyn Δm 0.00 Da [M+]+
Prenol lipids | γ-Nonalactone Δm -18.01 Da [M+]+
Carboxylic acids and derivatives | 1,4,7-Trioxacyclotridecane-8,13-dione Δm 0.00 Da [M+]+
Prenol lipids | 4,11-Dimethyl-8-(propan-2-yl)-5,12-dioxabicyclo[8.1.0.04,6]dodecan-7-ol Δm 0.00 Da [M+]+
Carboxylic acids and derivatives | Leu-Val Δm -18.01 Da [M+]+
Organoheterocyclic compounds | (4aR,7aS)-6-butoxy-4-(4-pyridylmethyl)hexahydropyrazo[3,4-b]1-Glycazin-3(2H)-one Δm 0.00 Da [M+]+
Lipids and lipid-like molecules | (2E)-5,10-Dihydroxy-8,8-dimethyldodec-6-enedioic acid Δm -36.02 Da [M+]+
Fatty Acyls | 13-Oxooctadecanoic acid Δm 18.01 Da [M+H+NH3]+
Phenol ethers | [(2E,4E,12E)-13-(1,3-Benzodioxol-5-yl)-1-(1-piperidinyl)-2,4,12-tridecatrien-1-one Δm 0.00 Da [M+]+
Fatty Acyls | 2-Decylmaleic acid Δm 0.00 Da [M+]+
Organooxygen compounds | (3aR,4R,7S,7aS)-3a,4,7,7a-Tetrahydro-5,7-methanoisobenzofuran-1,3-dione Δm -27.99 Da [M+]+
Carboxylic acids and derivatives | 5-(Hydroxymethyl)-3-(1-hydroxy-4-methylhexy)oxolan-2-one Δm 0.00 Da [M+]+
Carboxylic acids and derivatives | Bisphenol A bis(2,3-dihydroxypropyl) ether Δm 17.03 Da [M+]+
Fatty Acyls | 3-Furanoacetic acid, tetrahydro-6-methylene-2-oxo(-5-oxo-, (2R,3S)-rel- Δm 254.10 Da [M+]+
Organooxygen compounds | Glycopeptin C Δm 0.00 Da [M+]+
Benzenediol | 17α-Methyl-androstan-3-hydroxyimine-17β-ol Δm 0.00 Da [M+]+
Fatty Acyls | (15Z,13Z)-10,16-Dihydroxy-10,13-oxoladecadienoic acid Δm 0.00 Da [M+NH4]+
precCharge
Charge
Source
Target
Target_Description
Target_Source
Target_Type
Target_Subtype
Target_Chemical_Formula
Target_Molecular_Weight
Target_Pubchem_CID
Target_Chemical_Structure
Target_Chemical_Formula_Source
Target_Molecular_Weight_Source
Target_Pubchem_CID_Source
Target_Chemical_Structure_Source
Target_Chemical_Formula_Target
Target_Molecular_Weight_Target
Target_Pubchem_CID_Target
Target_Chemical_Structure_Target
Target_Interaction_Type
Target_Interaction_Pubmed_Id
Target_Interaction_Description
Target_Interaction_Source
Target_Interaction_Type_Source
Target_Interaction_Pubmed_Id_Source
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Target_Interaction_Type_Target
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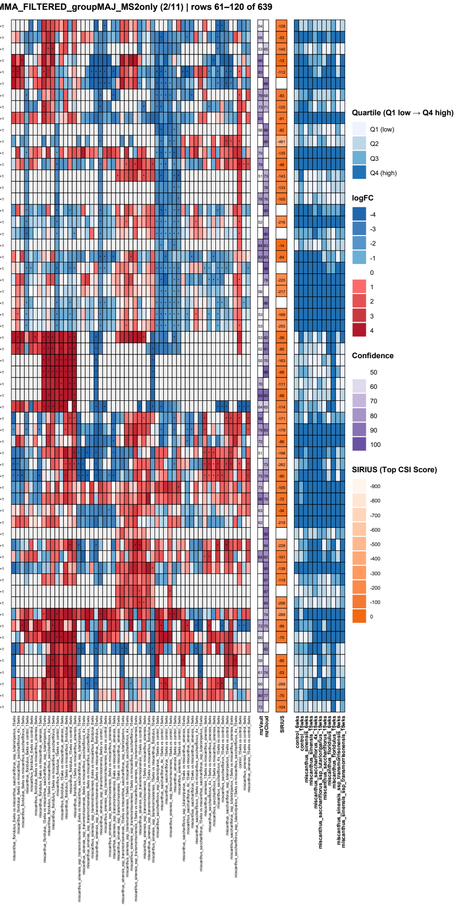
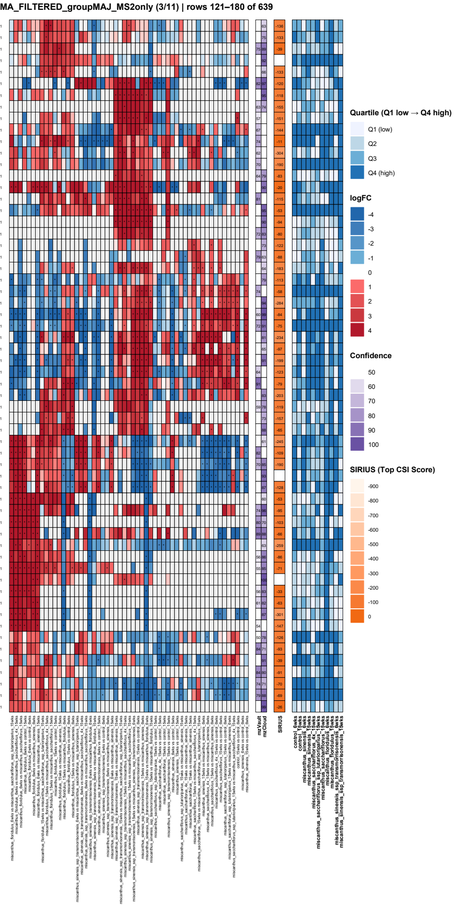
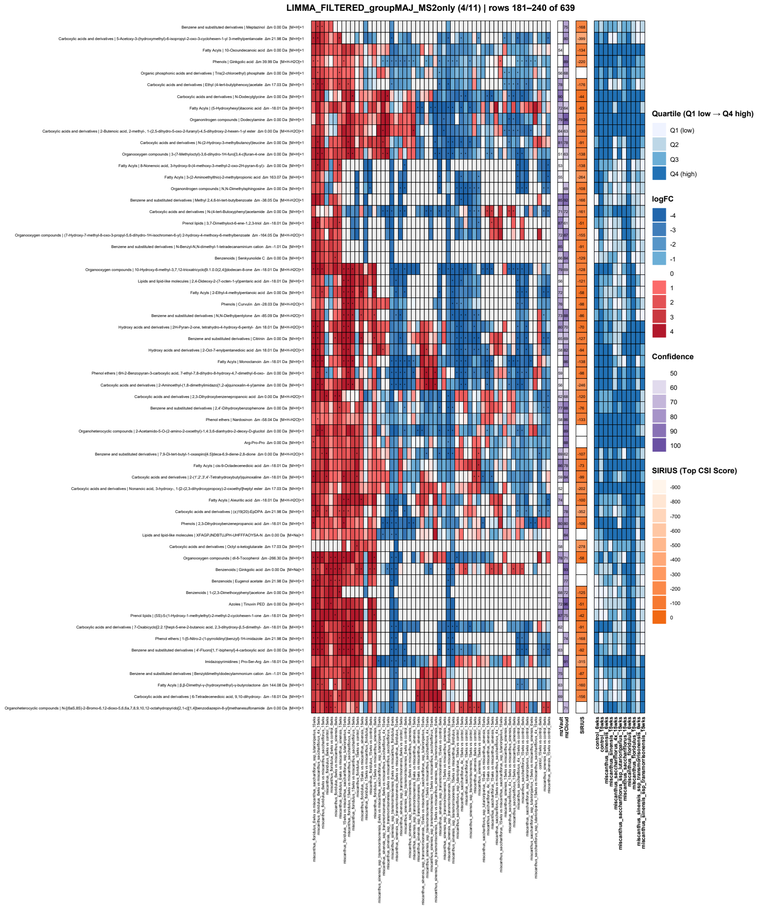
Target_Interaction_Source_Target


LIMMA_FILTERED_groupMAJ_MS2only (2/11) | rows 61–120 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Fatty Acyls | trans-Vaccenic acid Δm 0.00 Da [M+H]+
Fatty Acyls | 10,(Acetyloxy)decyl acetate Δm 0.00 Da [M+H]+
Isosorbamide | Bis(2-hydroxyethyl) phthalate Δm -62.04 Da [M+H]+
Organic metal salts | Tetraki(acetoxymethyl)cyclohexylsiloxane Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Cocamidopropyl betaine Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | Spinosade B Δm 0.00 Da [M+H]+
Fatty Acyls | 16-Hydroxyheadecanoic acid Δm -18.01 Da [M+H]+
Fatty Acyls | 17-Epoxandrolone Δm 0.00 Da [M+H]+
Fatty Acyls | 2E(),3-Dimethyl-2-octenedioic acid Δm 0.00 Da [M+NH4]+
Naphthalenes | 4-(3-Hydroxyphenyl)phenol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Tip-Asn-Arg Δm 0.00 Da [M+Na]+
Fatty Acyls | 4,11-Dioxabicyclo[8.2.1]undecan-3-one, 7-hydroxy-5-(2-hydroxypentyl)-2,2-dimethyl- Δm 0.00 Da [M+H-H2O]+
Organooxygen compounds | 2-(Tetradecylamino)ethanol Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 4,7-Dimethoxy-5,6-dimethyl-8-(3-O-(pseudopyranosyl)coumarin (to be confirmed) Δm -162.05 Da [M+H]+
Organooxygen compounds | N-[(2R,3E,4R,5S),3,4-Dihydroxy-5-[2-(4-methyl-1-piperidinyl)-2-oxoethyl]tetrahydro-2-furanyl]methylbenzenesulfonamide Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | 11-Hydroxyundecanoic acid Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | 1-Ethyl-3-[(1S,4S,6S)-6-isopropyl-3-methyl-4-([5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl)-2-cyclohexen-1-yl]methylurea Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Syringaresinol diglucoside Δm -324.11 Da [M+H]+
Organoheterocyclic compounds | 3-Hexadec-15-en-7-yn(-4-hydroxy-5-methylcoxan-2-one Δm 21.98 Da [M+H]+
Organooxygen compounds | Octaprazolene glycol Δm 0.00 Da [M+NH4]+
Fatty Acyls | Dimethyl succinate Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | (3E,5E,10E,14E)-6,9,13-trihydroxy-2,4,6,8,10,12,14-heptamethylhexadeca-2,6,10,14-tetraenal Δm 21.98 Da [M+H]+
Carboxylic acids and derivatives | (8aR)-N-Isopropyl-3-oxo-2-(2-pyridinylmethyl)hexahydroimidazo[1,5-a]pyrazine-7(1H)-carboxamide Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Phomalone Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | (1R,2S,3R,4R)-2-[(4-Methoxybenzoyl)amino]-4-phenyl-1,2-cyclopentanediol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3-[(E)-(3,4-Dihydroxy-3,5-dimethylhept-1-enyl)-7,8-dihydroxy-7-methyl-6,8a-dihydro-1H-isochromen-6-one Δm -66.07 Da [M+H]+
Phenols | 3-Hydroxy-3-methyl-5-oxo-5-[(2R,3E,4S,5R,6S)-3,4,5-trihydroxy-6-(4-(4-(4-hydroxy-3,5-dimethoxyphenyl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl)-2,6-dimethoxyphenoxy)tetrahydro-2H-pyran-2-yl]methoxy]pentanoic acid Δm -306.10 Da [M+H]+
Benzene and substituted derivatives | 2,4-Di-tert-butyl-6-[[(dimethylamino)methyl]phenol Δm -45.06 Da [M+H]+
Organooxygen compounds | 3-7-Methylocta(1,3,5-dihydro-1H-furo[3,4-c]furan-4-one Δm -84.08 Da [M+H]+
Benzene and substituted derivatives | Lauryloxytoctone B Δm -46.01 Da [M+H]+
Coumarins and derivatives | 7,7-Dihydroxy-4-methylcoumarin Δm 0.00 Da [M+H]+
Prenol lipids | (5Z)-3-Hydroxy-5-dodecenoic acid Δm -18.01 Da [M+H]+
Prenol lipids | (2R,8aS)-Decahydro-2-naphthalenol Δm 0.00 Da [M+H-H2O]+
Benzenoids | 3-[(1E,3E)-Heptre-1,3-dienyl]pentanedioic acid Δm -18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Ernno-Dihydrobupropion Δm 0.00 Da [M+H]+
Organooxygen compounds | N,N-Dimethyl-3,4-DMA Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3-Hydroxy-2-[(2-oxo-3-oxolanylidene)amino]pentanoic acid Δm -18.01 Da [M+NH4]+
Organic phosphonic acids and derivatives | 4-Ethyl-5-(cyclobe-4-carbonyl)-2,3-dihydro-1H-imidazol-2-one Δm 0.00 Da [M+H]+
Organic phosphonic acids and derivatives | 1-[4-[(3-[(5-Ivdodyl)-1,2-oxazol-3-yl]methyl)-3-oxetanyl]piperazi-1-yl]piperidin-1-yl]ethanone Δm 0.00 Da [M+H-H2O]+
Prenol lipids | 20-Hydroxyarachidonic acid Δm 0.00 Da [M+H]+
Fatty Acyls | 2-Octanevoctanoic acid, 5-hydroxy-3-oxo(r Δm 0.00 Da [M+H-H2O]+
Fatty Acyls | 2-Pentenedioic acid, 2-octyl- Δm -46.01 Da [M+H]+
Organonitrogen compounds | 2-(Hexadecylamino)ethanol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 8-Acetoxnido-2-methyl-7-oxononanoic acid Δm 0.00 Da [M+H]+
Benzenoids | 5,7-(4-Tetradecene-1,4-diyl)bis(1,3-benzenediol) Δm 21.98 Da [M+H]+
Coumarins and derivatives | 4-(2-(E)-Amino-3-(4-methoxyphenyl)-1-oxo-2-propenyl)pentanoyl)-6-[[methylsulfonyl]oxy]phenyl-1-piperidinyl)-6-oxobutanoic acid Δm 0.00 Da [M+H]+
Phenol ethers | O-Benzyl-L-tyrosine methyl ester Δm -60.02 Da [M+H]+
Fatty Acyls | (Rac)-Ibrexofen acid Δm 0.00 Da [M+NH4]+
Peptidomimetics | Avosulane 1-valdate Δm 21.98 Da [M+H]+
Organoheterocyclic compounds | 5-Butyl-6-(hydroxymethyl)-4-methoxy-2H-pyran-2-one Δm 18.01 Da [M+H-H2O]+
Organic phosphonic acids and derivatives | [(2S)-1-Iodobutyl-3-pyrrolidinyl]-5-(2-methoxyphenyl)-1,3,4-oxadiazole Δm 0.00 Da [M+H]+
Organooxygen compounds | [(3R,4S,6R)-6-[[6-(Dihydroxymethyl)-1H-1,2,3-triazol-1-yl]methyl]-5-azabicyclo[2.2.2]oct-3-yl]-N-morpholinylmethanone Δm 0.00 Da [M+H]+
Phenol ethers | Propanoic acid, 2-hydroxy-3-[(1-(4-methoxy-6-methyl-2-oxo-2H-pyran-5-yl)butyl)thio]- Δm -122.00 Da [M+H]+
Pyrone | Mirabotide A Δm -18.01 Da [M+H]+
Organoheterocyclic compounds | Senkyunolide G Δm 0.00 Da [M+Na]+
Fatty Acyls | 3-(1-Oxoeicy)dihydro-2,5-furandione Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | 4,6-(Methoxycarbonyl)benzoic acid Δm 0.00 Da [M+H]+
Fatty Acyls | Benzenethanamine, 3,5-dimethoxy-α-methyl-4-propoxy- Δm 0.00 Da [M+H]+
Cinnamic acids and derivatives | 10-Hydroxy-8-methyl-3,7,12-trioxatricyclo[9.1.0.02,4]dodecan-8-one Δm -36.02 Da [M+H-H2O]+
Fatty Acyls | NP-012808 Δm -162.05 Da [M+H]+
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina
pHSCDNA
CLASS
SUBCLASS
Tissue_Adipose
Tissue_Adrenal_Gland
Tissue_Blood_Vessel
Tissue_Brain
Tissue_Breast
Tissue_Colon
Tissue_Esophagus
Tissue_Heart
Tissue_Kidney
Tissue_Liver
Tissue_Lung
Tissue_Muscle
Tissue_Nerve
Tissue_Pancreas
Tissue_Pituitary
Tissue_Prostate
Tissue_Salivary_Gland
Tissue_Skin
Tissue_Small_Intestine
Tissue_Spleen
Tissue_Stomach
Tissue_Testis
Tissue_Thyroid
Tissue_Uterus
Tissue_Vagina


LIMMA_FILTERED_groupMAJ_MS2only (3/11) | rows 121–180 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Carboxylic acids and derivatives | Vindoscoagelatrazinone -Δm 0.00 Da [M+H]+
Fatty Acyls | Monosaspirin -Δm -16.01 Da [M+H]+
Benzene and substituted derivatives | 3,4-Dihydroquinolin-1(2H)-yl(4-propoxyphenyl)methanone -Δm -133.00 Da [M+H]+
Organic acids and derivatives | Tropic acid -Δm 0.00 Da [M+Na]+
Fatty Acyls | 1,16-Hexadecanediolic acid -Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-2-hydroxybenzaldehyde -Δm 0.00 Da [M+H]+
Organonitrogen compounds | N,N-Dimethylsecylamine N-oxide -Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | NP-021192 -Δm -134.06 Da [M+H]+
Fatty Acyls | 1-Linoleoylglycerol -Δm 0.00 Da [M+H]+
Organonitrogen compounds | 1,7-(Octylazanediyl)bis(propan-2-ol) -Δm 0.00 Da [M+H]+
Organooxygen compounds | Tetraethylene glycol -Δm 0.00 Da [M+H]+
Fatty Acyls | 2H-Pyran-2-propanoic acid, 3,6-dihydro-a-hydroxy-a,2,4-trimethyl-6-oxo- -Δm 17.03 Da [M+H]+
Benzene and substituted derivatives | 2,4,6-Trimethylbenzenesulfonamide -Δm 199.07 Da [M+H]+
Organooxygen compounds | 3-Hydroxy-2,7-dimethylcoumarin -Δm -64.03 Da [M+H]+
Oxacyclic compounds | Benzidine -Δm 37.96 Da [M+H]+
Fatty Acyls | (2E)-2,7-Dimethyl-2-octenedioic acid -Δm 18.01 Da [M+H-H2O]+
Organonitrogen compounds | 2-Amino-1,3,4-octadecanetriol -Δm 0.00 Da [M+H]+
Organooxygen compounds | Hydroxyjasmonic acid -Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 2,6-Di-tert-butyl-4-(2E-[(3,5-di-tert-butyl-4-hydroxyphenyl)methylidene]amino-1-phenylethyl)phenol -Δm -384.25 Da [M+H]+
Fatty Acyls | Arg-Val-Val -Δm -16.01 Da [M+H]+
Fatty Acyls | 4-Hydroxydodecanoic acid -Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | 1-[(1R,4S,8S)-6-Isopropyl-3-methyl-8-[(5-methyl-1H-benzimidazol-2-yl)methyl]-2-cyclohexen-1-yl]methanamine -Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 4-(4-Methylphenyl)pentanoic acid -Δm 0.00 Da [M+H-H2O]+
Organonitrogen compounds | Tridecan-1-amine -Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | N-[(1S,4S,8S)-6-Isopropyl-4-(2-[(4-methoxybenzyl)amino]-2-oxoethyl)-3-methyl-2-cyclohexen-1-yl]methyl]-2-furamide -Δm 0.00 Da [M+Na]+
Organonitrogen compounds | Pentadecylamine -Δm 0.00 Da [M+H]+
Organonitrogen compounds | Tetradecylamine -Δm 0.00 Da [M+H]+
Organic phosphoric acids and derivatives | 1-[(1S,4S,8S)-6-Isopropyl-3-methyl-8-[(5-methyl-1H-benzimidazol-2-yl)methyl]-2-cyclohexen-1-yl]methanamine -Δm 18.01 Da [M+H-H2O]+
Organooxygen compounds | 1-[(1S,4S,8S)-4-(1H-Benzimidazol-2-ylmethyl)-6-isopropyl-3-methyl-2-cyclohexen-1-yl]methanamine -Δm 0.00 Da [M+H]+
Organonitrogen compounds | Kalexite -Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Carpinopinoid -Δm -138.02 Da [M+H]+
Prenol lipids | cis,cis-9,12-Octadecadien-1-ol -Δm -16.01 Da [M+H]+
Carboxylic acids and derivatives | 2-(7-Hydroxy-6-methylbutyl)-2H-iran-5-one -Δm 21.98 Da [M+H]+
Prenol lipids | Bicyclo[8.1.0]undec-5-ene-2,9-diol, 3-(hydroxymethyl)-3,5,10-trimethyl- -Δm -36.02 Da [M+H]+
Prenol lipids | 1-[(1S,4S,8S)-6-Isopropyl-3-methyl-4-[(4-methyl-1H-benzimidazol-2-yl)methyl]-2-cyclohexen-1-yl]-N,N-dimethylmethanamine -Δm 0.00 Da [M+H]+
Prenol lipids | Perhexiline -Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Valethamate -Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Bis(2-hydroxyethyl) phthalate -Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Pentiludol -Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | UFEZCKBFRMLAY-DBDKQAFGSA-N -Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | AALLCALQGXXKNA-LZOLBGSA-N -Δm 68.13 Da [M+H]+
Fatty Acyls | N,N-Diethyl-3-[(E5,5aS,8aR)-1-methyl-5-oxodecahydroquinolin]-2,4[1H]-dipiperazin-2-yl]propanamide -Δm 21.98 Da [M+H]+
Carboxylic acids and derivatives | 3,5-Di-tert-butyl-2-hydroxybenzaldehyde -Δm 18.01 Da [M+H-H2O]+
Fatty Acyls | Cyclohexanepentanoic acid -Δm 0.00 Da [M+H]+
3,4-dihydrocoumarins | 3,4-Dihydrocoumarin -Δm 0.00 Da [M+H]+
Organooxygen compounds | Ametoctradin -Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | 4-Methylbisphenidone -Δm -13.03 Da [M+H-H2O]+
Flavonoids | 10-hydroxydjalon (mixture of A and B) -Δm -16.01 Da [M+H]+
Organic nitrogen compounds | Cetrimonium -Δm 0.00 Da [M+H]+
Diarylheptanoids | Muricarpone B -Δm 0.00 Da [M+H]+
Benzenoids | trans-3-Coumarin acid -Δm -16.01 Da [M+H]+
Alkylcyclopentanones | Kelotiffen -Δm 0.00 Da [M+H]+
Fatty Acyls | NP-021107 -Δm -16.01 Da [M+H-H2O]+
Carboxylic acids and derivatives | Ethyl 2-cyanoacrylate -Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | 2-Furanacetic acid, tetrahydro-5-[(2-hydroxypropyl)-o-methyl-, 2-[(1,1-carboxyethyl)tetrahydro-2-furanyl]-1-methylethyl ester -Δm -202.12 Da [M+H-H2O]+
Benzene and substituted derivatives | Triphenylphosphine oxide -Δm 0.00 Da [M+H]+
Fatty Acyls | 9,12-Dihydroxy-10-dodecenoic acid -Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | Cyclobexylfaturyl -Δm 0.00 Da [M+H]+
Phenylpropanoic acids | 1-(3-Hydroxy-2-(2-hydroxypropan-2-yl)-2,3-dihydro-1-benzofuran-5-yl)ethanone -Δm -54.06 Da [M+H-H2O]+
Flavonoids | Isoscoparin -Δm 0.00 Da [M+H]+
Healthy
Healthy
Healthy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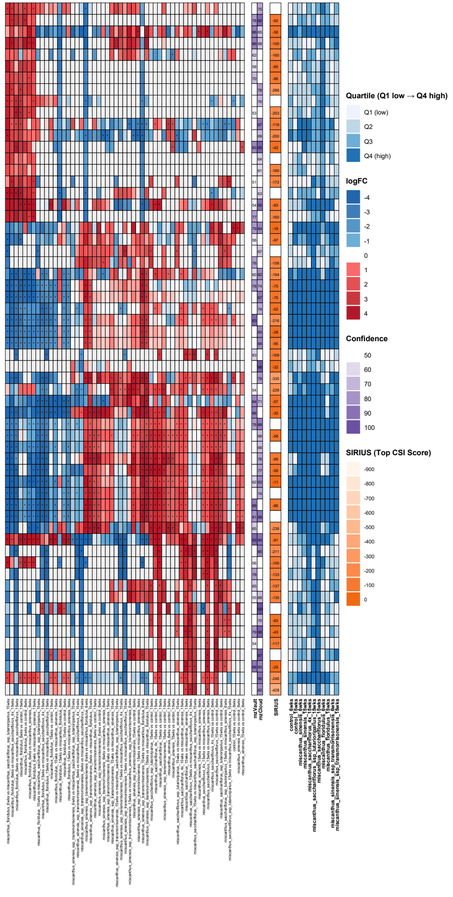
Benzene and substituted derivatives | Meptazinol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 5-Acetoxy-3-(hydroxymethyl)-5-isopropyl-2-oxo-3-cyclohexen-1-yl 3-methylpentanoate Δm 21.98 Da [M+H]+
Fatty Acyls | 16-Oxooctadecanoic acid Δm 0.00 Da [M+H]+
Phenols | Ortho(p)-acid Δm 39.99 Da [M+H+NO]+
Organo phosphonic acids and derivatives | Tris(2-chloroethyl) phosphate Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Ethyl (4-tert-butylphenoxy)acetate Δm 17.03 Da [M+H]+
Carboxylic acids and derivatives | N-Dodecylglycine Δm 0.00 Da [M+H]+
Fatty Acyls | (5-Hydroxyhexyl)tacrine acid Δm -16.01 Da [M+H]+
Organonitrogen compounds | Dodecylamine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-Butenoic acid, 2-methyl-, 1-(2,5-dihydro-5-oxo-3-furanyl)-4,5-dihydroxy-2-hexen-1-yl ester Δm 0.00 Da [M+H+NO]+
Carboxylic acids and derivatives | N-(2-Hydroxy-3-methylfulacinyl)leucine Δm 0.00 Da [M+H]+
Organooxygen compounds | 3-(7-Methylvalyl)-3,6-dihydro-1H-furo[3,4-c]tacan-4-one Δm 0.00 Da [M+H]+
Fatty Acyls | 8-Nonenoic acid, 3-hydroxy-9-(4-methoxy-3-methyl-2-oxo-2H-pyran-6-yl)- Δm 0.00 Da [M+H]+
Fatty Acyls | 3-(2-Aminoethylthio)-2-methylpropanoic acid Δm 163.07 Da [M+H]+
Organonitrogen compounds | N,N-Dimethylhydrogenine Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Methyl 2,4,6-tri-tert-butylbenzoate Δm -38.05 Da [M+H+NO]+
Carboxylic acids and derivatives | N-(4-tert-Butoxyphenyl)acetamide Δm 0.00 Da [M+H]+
Prenol lipids | 3,7-Dimethylcis-6-nine-1,2,3-trol Δm -16.01 Da [M+H]+
Organooxygen compounds | (7-Hydroxy-7-methyl-6-oxo-3-propyl-5,6-dihydro-1H-isochromen-8-yl) 2-hydroxy-4-methoxy-6-methylbenzoate Δm -164.05 Da [M+H+NO]+
Benzene and substituted derivatives | N-Benzyl-N,N-dimethyl-1-tetradecanaminium cation Δm -1.01 Da [M+H]+
Benzenoids | Senkyunolide C Δm 0.00 Da [M+H]+
Organooxygen compounds | 10-Hydroxy-6-methyl-3,7,12-trioxatricyclo[8.1.0.02,4]dodecan-8-one Δm -16.01 Da [M+H+NO]+
Lipids and lipid-like molecules | 2,4-Octenoxy-(2-7-octen-1-yl)pentanic acid Δm -16.01 Da [M+H]+
Fatty Acyls | 2-Ethyl-4-methylpentanoic acid Δm 0.00 Da [M+H]+
Phenols | Curcolin Δm -28.03 Da [M+H+NO]+
Benzene and substituted derivatives | N,N-Dethylpentylone Δm -49.04 Da [M+H+NO]+
Hydroxy acids and derivatives | 2H-Pyran-2-one, tetrahydro-4-hydroxy-6-pentyl- Δm 18.01 Da [M+H+NO]+
Benzene and substituted derivatives | Citrinin Δm 0.00 Da [M+H]+
Hydroxy acids and derivatives | 2-Oxo-7-ecdysteroid acid Δm 18.01 Da [M+H+NO]+
Fatty Acyls | Monosilanum Δm -16.01 Da [M+H]+
Phenol ethers | (6H-2-Benzopyran-3-carboxylic acid, 7-ethyl-7,8-dihydro-8-hydroxy-4,7-dimethyl-6-oxo- Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-Aminethyl-(1,8-dimethylindolyl)-2,-(alpiscovalin-4-yl)amine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2,3-Dihydroxybenzenepropanoic acid Δm 0.00 Da [M+H+NO]+
Benzene and substituted derivatives | 2,4'-Dihydroxybenzophenone Δm 0.00 Da [M+H]+
Phenol ethers | Nardosinon Δm -58.04 Da [M+H+NO]+
Organoheterocyclic compounds | 2-Acetamido-5-O-(2-amino-2-oxoethyl)-1,4,3,6-dianhydro-2-deoxy-D-glucitol Δm 0.00 Da [M+H]+
Arg-Pro-Pro Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione Δm 0.00 Da [M+H+NO]+
Fatty Acyls | cis-9-Octadecenedioic acid Δm -16.01 Da [M+H]+
Carboxylic acids and derivatives | 2-(1',2',2',4'-Tetrahydroxybutyl)pteroxaline Δm -16.01 Da [M+H]+
Carboxylic acids and derivatives | Nonanoic acid, 3-hydroxy-, 1-[2-(3-dihydroxypropoxy)-2-oxoethyl]hepty ester Δm 17.03 Da [M+H]+
Fatty Acyls | Arkeritic acid Δm -16.01 Da [M+H+NO]+
Carboxylic acids and derivatives | (±)-N(20)-EpDPA Δm 21.98 Da [M+H]+
Phenols | 2,3-Dihydroxybenzenepropanoic acid Δm -16.01 Da [M+H]+
Lipids and lipid-like molecules | KFASP,INDBTLIPH-LHFFFAOYSA-N Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | Octyl α-ketoglutarate Δm 17.03 Da [M+H]+
Organooxygen compounds | dl-δ-Tocopherol Δm -286.30 Da [M+H]+
Benzenoids | Ortho(p)-acid Δm 0.00 Da [M+Na]+
Benzenoids | Eugenol acetate Δm 21.98 Da [M+H]+
Benzenoids | 1-(2,3-Dimethoxyphenyl)acetone Δm 0.00 Da [M+H]+
Azoles | Trovorin PEO Δm 0.00 Da [M+H]+
Prenol lipids | (3S)-6,7-Hydroxy-1-methylethyl)-2-dodecyl-1-one Δm -16.01 Da [M+H]+
Carboxylic acids and derivatives | 7-Oxabicyclo[2.2.1]hept-5-ene-2-butanoic acid, 2,3-dihydroxy-2,5-dimethyl- Δm -16.01 Da [M+H]+
Phenol ethers | 1-(6-Methoxy-2-(pyrrolidinyl)benzo[b 1H-imidazole Δm 21.98 Da [M+H]+
Benzene and substituted derivatives | 4'-Fluoro[1,1'-biphenyl]-4-carboxylic acid Δm 0.00 Da [M+H]+
Imidazopyrimidines | Pro-Ser-Arg Δm -16.01 Da [M+H]+
Benzene and substituted derivatives | Benzyldimethylidodecylammonium cation Δm -1.01 Da [M+H]+
Fatty Acyls | 2,[2-Dimethyl-γ-(hydroxymethyl)-γ-butyrolactone Δm 144.08 Da [M+H]+
Carboxylic acids and derivatives | 6,7-Tetradecanedioic acid, 9,10-dihydroxy- Δm -16.01 Da [M+H]+
Organoheterocyclic compounds | N-[(5aS,8S)-2-Bromo-6,8,8a,7,8,9,10,10-octahydropyrazino[2,1-c][1,4]benzodiazepin-8-yl]methanesulfonamide Δm 0.00 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0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Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Lipids and lipid-like molecules | 3,7-Dihydroxy-8,11-eremophiladien-8-one Δm -18.01 Da [M+H]+
Fatty Acyls | (11E,15Z)-9,10,13-Trihydroxyoctadeca-11,15-dienoic acid Δm -36.02 Da [M+H]+
Fatty Acyls | Palmitic acid Δm 0.00 Da [M+H]+
Fatty Acyls | 8-Hydroxycytarenic acid Δm 0.00 Da [M+H-H2O]+
Coumarins and derivatives | Bartosiside Δm -36.02 Da [M+H]+
Fatty Acyls | NP-024160 Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | Benzyldimethylstearylammonium cation Δm -29.04 Da [M+H]+
Carboxylic acids and derivatives | Ile-Tyr-Lys Δm 0.00 Da [M+H]+
Organic acids and derivatives | N-(2-Furylmethyl)-3-[(25,5a5,8aR)-1-methyl-8-(4-methylbenzyl)-5-oxodecahydropyrazino[2,3-f][2,4]diazepin-2-yl]propanamide Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | 5,15-Dioxo-6,8-octadecadienoic acid Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | (+)-(8S)-EET Ethanolamide Δm -30.04 Da [M+NH4]+
Organooxygen compounds | Imazamethabenz-methyl Δm 0.00 Da [M+H]+
Cinnamic acids and derivatives | L-Tyrosine, O,O,1-trimethylethyl- Δm -73.08 Da [M+H]+
Lipids and lipid-like molecules | (6E,16E)-3-(methoxymethyl)-5,10-dimethyl-3a,4,5,8,9,11a-hexahydro-3H-cyclotetradf[oxa-2-one Δm 21.98 Da [M+H]+
Cinnamic acids and derivatives | Primicarb-desmethyl Δm 37.96 Da [M+H]+
Benzene and substituted derivatives | 1H,3H-Furo[3,4-c]furan-1-one, 6-heptyl-4,5-dihydro- Δm 0.00 Da [M+H]+
Organic oxygen compounds | Decanophenone Δm 0.00 Da [M+H]+
Fatty Acyls | Ethyl trans-4-hydroxycyclohexanecarboxylate Δm 18.01 Da [M+H-H2O]+
Fatty Acyls | Dodecanamide,N-[3-(dimethylamino)propyl]- Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Benzophenone Δm 0.00 Da [M+H]+
Fatty Acyls | 4,4'-Oxydibenzene-1,2-diamine Δm 0.00 Da [M+H]+
Organic acids and derivatives | 1-(4-benzylpiperazino)-2-(pyridin-2-ylamino)propan-1-one Δm -15.98 Da [M+H]+
Organooxygen compounds | 8-Hydroxy-8-methoxy-3-methyl-3,4-dihydroisocromen-1-one Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 11H-Dibenz[b,e][1,4]oxazepin-7-carboxylic acid, 4-formyl-3,8-dihydroxy-8-(methoxymethyl)-1,6-dimethyl-11-oxo- Δm -14.01 Da [M+H-H2O]+
Fatty Acyls | 5-Amino-2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)-5-oxopentanoic acid Δm 21.98 Da [M+H-H2O]+
Fatty Acyls | 3-methyl-3,8-methyl-1,2,3-trioxabicyclo[4.4.0]-nonadecanoic/suyanide Δm 0.00 Da [M+H]+
Organometallic compounds | N3-(2-Mercapto-4-oxo-3,4-dihydroquinazolin-3-yl)nicotinamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Decamethylcyclopentasiloxane Δm -37.96 Da [M+H]+
Organometallic compounds | 3-Methylxanthine Δm 0.00 Da [M+H-H2O]+
Organonitrogen compounds | 3-Methylxanthine Δm 17.03 Da [M+H]+
Organic sulfonic acids and derivatives | 4-[4-(Hydroxydiso(Bis(phenyl)methyl)methylamino)benzene-1-sulfinic/sulfuric acid Δm -60.04 Da [M+H]+
Organonitrogen compounds | N-(4-Fluorophenyl)acetamiprid-1-carboxamide Δm 0.00 Da [M+H]+
Benzenoids | Arg-Thr-Tyr Δm 0.00 Da [M+Na]+
Organonitrogen compounds | DOPR Δm 0.00 Da [M+H]+
Organooxygen compounds | Ethanone, 1-[2-(1-hydroxy-1-methylethyl)phenyl] Δm 0.00 Da [M+H-H2O]+
Organometallic compounds | Octamethylcyclotetrasiloxane Δm 0.00 Da [M+H]+
Organometallic compounds | Hexamethylcyclotrisiloxane Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | [(3,5-bis(trifluoromethyl)phenyl)(4'-hydroxyprop-2-enimidamide Δm 0.00 Da [M+H-H2O]+
Phenylpropanoids and polyketides | (E)-3-(8-hydroxy-6-methoxy-1-oxoisochromen-3-yl)prop-2-enoic acid Δm 0.00 Da [M+H]+
Fatty Acyls | N11-(1-Adamantyl)[(2,2-[bis(3-tyl)-3-chlorobenzamide Δm 0.00 Da [M+H]+
Organometallic compounds | Butoxin Δm 0.00 Da [M+H]+
Organic metal salts | Octadecamethylcyclohexasiloxane Δm 0.00 Da [M+H]+
Organoheterocyclic compounds | Pyridoki Δm 0.00 Da [M+H]+
Organometallic compounds | 4-(4-Chlorophenyl)-2,6-piperidinedione Δm 17.03 Da [M+H]+
Organometallic compounds | Hexamethylcyclotrisiloxane Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 8-(2-Chlorophenyl)-7,8-dihydro[1,3]dioxolo[4,5-g]quinolin-6(5H)-one Δm 217.03 Da [M+2H]+2
Glycerolipids | 1-Palmitoylglycerol Δm 0.00 Da [M+H]+
Organic sulfuric acids and derivatives | 5-nitro-N-(5a1,3,5-oxadiazole-2-yl)phenyl]furan-2-carboxamide Δm 0.00 Da [M+H-H2O]+
Organonitrogen compounds | Pheniprax 1-carboxamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 2,5-Di-tert-butyl-1,4-benzoquinone Δm 0.00 Da [M+H]+
Organonitrogen compounds | 16-Hepta(decyn-4-one, 1,2-dihydroxy- Δm -21.98 Da [M+Na]+
Phenol ethers | (2E,5E)-3,5,7,7-tetrethyloxa-2,5-dienedioic acid Δm -18.01 Da [M+H]+
Phenylpropanoids and polyketides | Kaempferol Δm 0.00 Da [M+H]+
Benzoquinones | Hymenoxone Δm 0.00 Da [M+H]+
Linear 1,3-diarylpropanoids | Liquiritigenin Δm 0.00 Da [M+H]+
Organic phosphonic acids and derivatives | 2-Chloro-4,5-dimethoxyferrocic acid Δm 0.00 Da [M+H]+
Benzenoids | 2-Chloro-1,3,8-trihydroxy-6-(hydroxymethyl)anthraquinone Δm 0.00 Da [M+H]+
Organooxygen compounds | D-(+)-Cellobiose Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | Trigenox 1006 Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | [(2-Methyl-1,3-dioxoid-4-yl)-5-(8-(trifluoromethyl)phenyl)-1,3,4-oxadiazole Δm 0.00 Da [M+H]+
Tetrahydrocannabinol (THC) | Tetrahydrocannabinol (THC) | Tetrahydrocannabinol (THC) |

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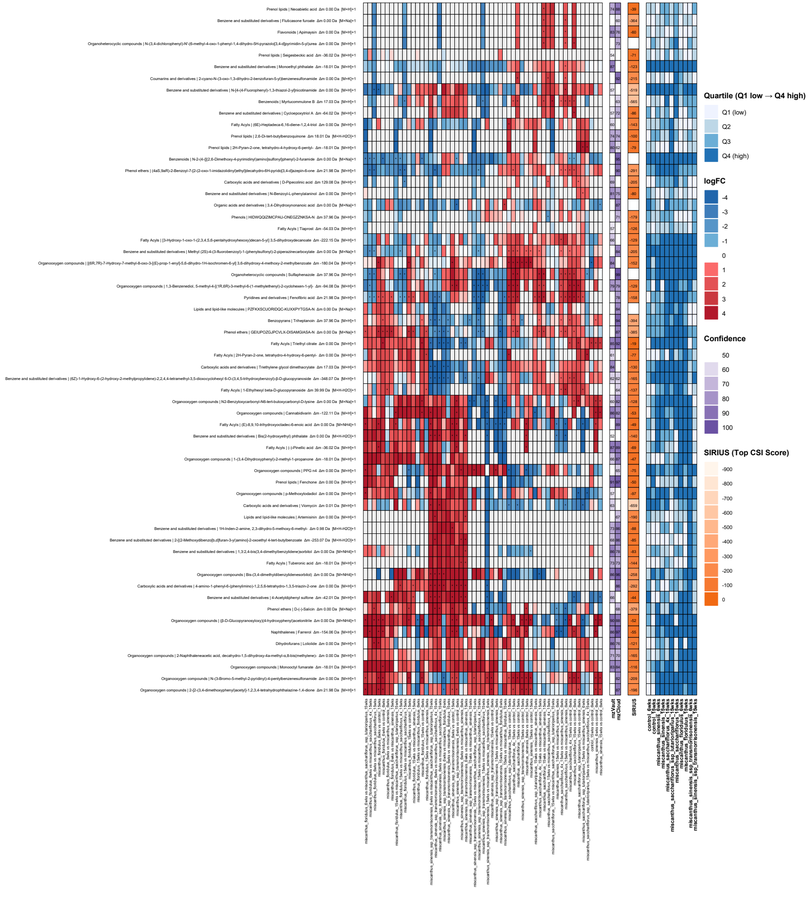

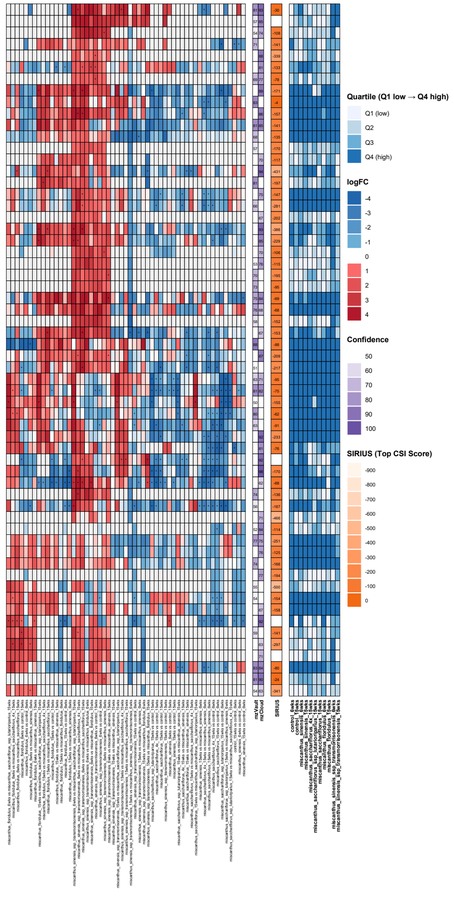
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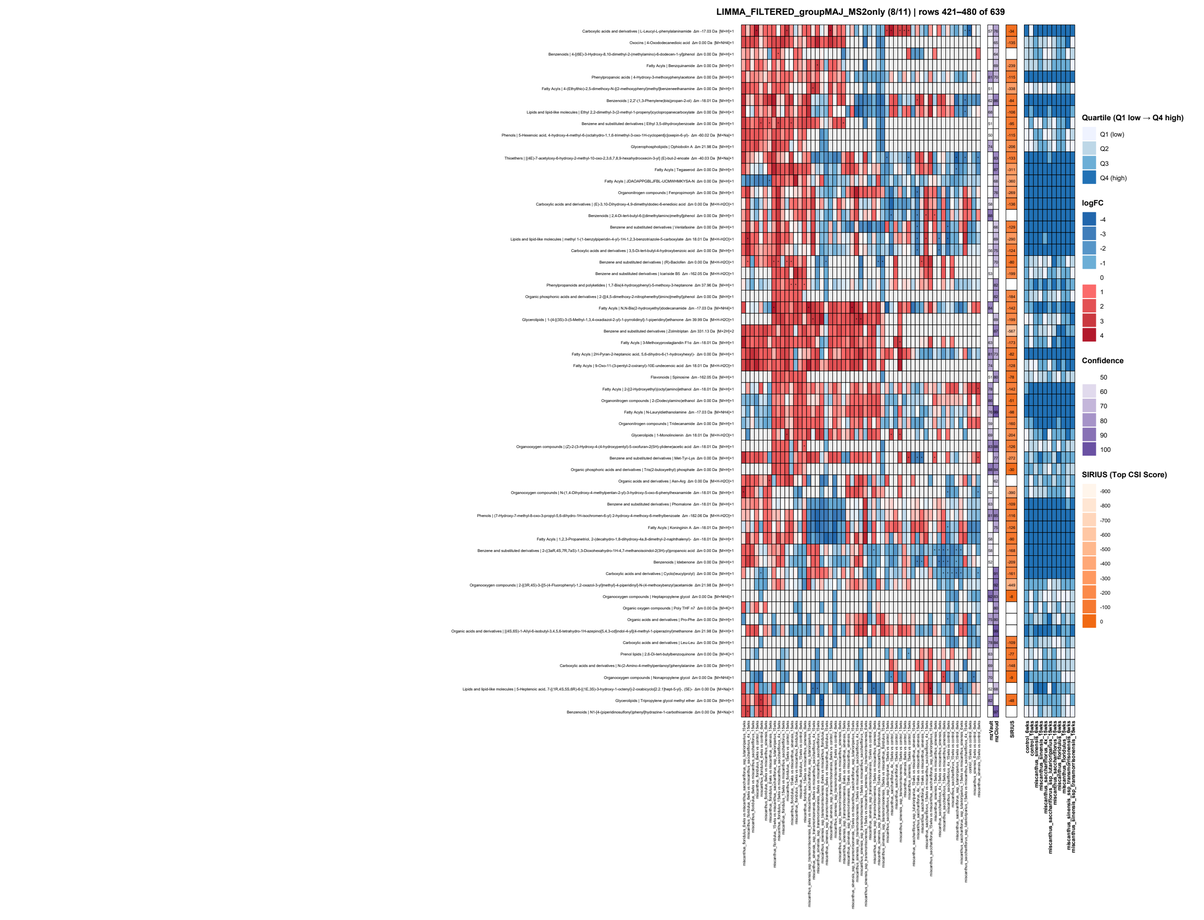
Cinnamic acids and derivatives | (2Z)-2-[(6-D-Glucopyranosyloxy)-3-phenyl-2-propenoxy] acid Δm -162.05 Da [M+H-H2O]+
Organic acids and derivatives | Nα-Acetyl-L-citrulline Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | 3,3-Diaminosuccinatoline Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Methyl 4-tert-butylbenzoate Δm 18.01 Da [M+H-H2O]+
Carboxylic acids and derivatives | (4S,8S)-N-[2-(Dimethylamino)ethyl]-5-isobutyl-1-(4-pyridinylmethyl)-3,4,5,6-tetrahydro-1H-azepino[5,4,3-cd]indole-4-carboxamide Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | Aureofaramine Δm 0.00 Da [M+H]+
Phenols | L-Tyrosine, O,O,1-dimethylethyl-, Δm -73.09 Da [M+H]+
Lipids and lipid-like molecules | (8aR)-(2-(2-Pyridinylmethyl)-7-(tetrahydro-2H-pyran-4-yl)hexahydroimidazo[1,5-a]pyrazin-3(2H)-one Δm 21.98 Da [M+H]+
Organooxygen compounds | L-Ulitol Δm 0.00 Da [M+H-H2O]+
Phenol ethers | 1-[5-Nitro-2-(1-pyrrolidinyl)benzyl]- 1H-imidazole Δm 21.98 Da [M+H]+
Glycerolipids | Monosaprin Δm 0.00 Da [M+H-H2O]+
Fatty Acyls | Myristoyl ethanolamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Diethyl cyclopentane-4,5-dione-1,3-dicarboxylate Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | (7E)-12-Hydroxy-3-nedoxyl-13-methoxy-4,5,8-trimethyl-3,3a,4,8a,9,10,11,12,13,14-decahydro-1H-cyclooctadecaf[d]pyrandion-1-10(2H)-dione Δm 0.00 Da [M+Na]+
Pteridines and derivatives | Sepiomod Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Decamethylcyclopentasilaxane Δm -37.96 Da [M+H-H2O]+
Benzenoids | Filiberenin Δm 0.00 Da [M+H]+
Organooxygen compounds | NP-008265 Δm 17.03 Da [M+H]+
Organooxygen compounds | Ala-Val-Phe Δm 97.95 Da [M+H]+
Benzene and substituted derivatives | Mitoxantrone Δm 21.98 Da [M+H]+
Phenol ethers | (((R)-6-((S)-Methyl-2-pyrrolidinyl)oxo)- 1,4-oxazepan-4-yl)(2-pyrazinyl)methanone Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | 6-(2,3-Dihydroxy-3-methylbutyl)-7-methoxycoumarin Δm 18.01 Da [M+H-H2O]+
Fatty Acyls | Chromomonic acid B Δm 18.01 Da [M+H-H2O]+
Lipids and lipid-like molecules | (9E,11Z)-8-Hydroxyoctadeca-9,11-dienoic acid Δm 21.98 Da [M+H]+
Fatty Acyls | 3-(5-5-Dihydroxyhexyl)-4-methyl-2H-furan-5-one Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | 4-(2-Butoxyethoxy)benzoic acid Δm -56.06 Da [M+H]+
Carboxylic acids and derivatives | 3,6,9-Trihydroxy-10-propyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | Methyl 7-acetyl-2,2,3-dihydroxy-8-methyl-6-oxabicyclo[3.2.1]octane-1-carboxylate Δm -18.01 Da [M+H]+
Coumarins and derivatives | 7-O-Methylsaginol Δm 18.01 Da [M+H-H2O]+
Hydroxy acids and derivatives | 2,5-Propyl-4-pentenoic acid Δm 18.01 Da [M+H-H2O]+
Carboxylic acids and derivatives | ((((R)-4-((S-Methyl-2-pyrrolidinyl)oxo)- 1,4-oxazepan-4-yl)(2-pyrazinyl)methanone Δm 39.99 Da [M+H-H2O]+
Benzenoids | 1-O-α-[(3E,4E)-5-(2′R,3S,5S,6S)-3,5-Dihydroxy- 1,5-dimethyl-6-oxabicyclo[2.2.1]octan-6-yl]-3-methylpentta-2,4-dienoyl]-β-D-glucopyranosan Δm -36.02 Da [M+H]+
Fatty Acyls | 1,1,3-Ethyl-2,4-dihydroxy-6-methoxyphenyl)-1-butanone Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | L-Tyrosine tert-butyl ester Δm -17.03 Da [M+H]+
Benzenoids | (3E,5E)-2-(4-Methoxy-6-oxododylpiyone-3,5-dienoic acid Δm -50.04 Da [M+H]+
Benzene and substituted derivatives | 1-(4-Hydroxy-3-(3-methylbut-2-enyl)phenyl)ethanone Δm 0.00 Da [M+H]+
Fatty Acyls | 5,6-Dioxaspirohexadecane-7,10-dione Δm -54.06 Da [M+H]+
Carboxylic acids and derivatives | L-4-Anhydro-2,5-dideoxy-5-(cyanoiminoylamino)-2-[1-methyl-4-piperidinyl]amino]-D-arabinitol Δm 21.98 Da [M+H]+
Benzene and substituted derivatives | 1-(4-Methoxyphenyl)piperazine Δm 0.00 Da [M+H]+
Alkaloids and derivatives | (1R,9S)-5-(1-Benzylidenethiophen-2-yl)-11-(2-thienylcarbonyl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | N4-(4-chloro-2,5-dimethoxyphenyl)mesityloxide-α-carbothioamide Δm 21.98 Da [M+H]+
Fatty Acyls | Undecylenic acid Δm 0.00 Da [M+NH4]+
Prenol lipids | Lupinalol B2 Δm -162.05 Da [M+H]+
Tetrahydroisoquinolines | 1-(2-Methoxyethyl)-1H-indole-2-carboxylic acid Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Clindamycin Δm 0.00 Da [M+Na]+
Benzenoids | 1-Ethyl-6-methoxy-2(1H)-quinolinone Δm -28.03 Da [M+H]+
Benzene and substituted derivatives | 2,10-Cyclooctadecadien-1-one, 9-[(acetyloxy)methyl]-7-hydroxy-2-(hydroxymethyl)-5-methyl-8-methylene- Δm -21.98 Da [M+Na]+
Diazines | Anobarbine Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | 7,9-Dihydroxy-2,5,7-trimethyl-8,8a-dihydro-1H-naphthoxanol-6-one Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | O-Arachidonoyl ethanolamine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-[2-(2,2,2-Trifluoroethoxy)ethoxy]ethan-1-amine Δm 235.08 Da [M+2H]+2
Fatty Acyls | Spiculisporic acid Δm -18.01 Da [M+H]+
Fatty Acyls | Embelic Δm 18.01 Da [M+NH4]+
Carboxylic acids and derivatives | CH3CHZCHZCHZCHNCHZCCLSA/A Δm 0.00 Da [M+Na]+
Benzopyranes | 6-Glucosyl-3,4′,5,7-tetrahydroxyflavanone Δm -120.04 Da [M+H]+
Fatty Acyls | Glycocholic acid Δm -11.02 Da [M+NH4]+
Organoheterocyclic compounds | HYKXRXOUIT,ZRAKJ-LHFITFACYSA-N Δm 21.98 Da [M+H]+
Benzene and substituted derivatives | Bis(2-hydroxyethyl) phthalate Δm -18.01 Da [M+H]+
Diarylheptanoids | Platiphylloneol Δm 0.00 Da [M+H]+
Prenol lipids | N-(8-AP(OE) Farnesyl Δm 21.98 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0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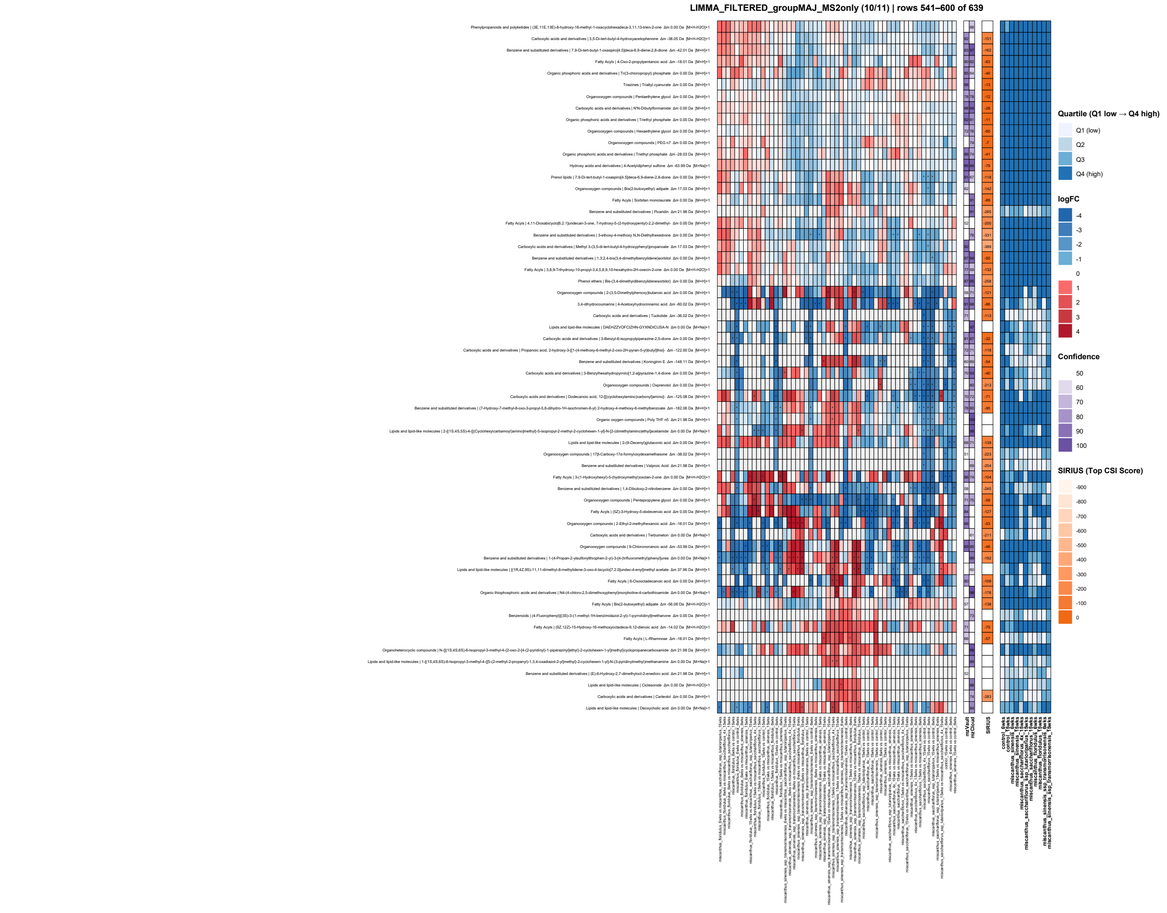
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
pmzCluster
MS2size
SIRIUS

LIMMA_FILTERED_groupMAJ_MS2only (9/11) | rows 481–540 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Fatty Acyls | 2-Pentenedioic acid, 2-octyl- Δm -27.99 Da [M+H-H2O]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm -56.06 Da [M+H]+
Lipids and lipid-like molecules | Naphtho[1,2-c]furan-1(3H)-one, 3a,5a,6,7,8,9,9a,9b-octahydro-8-hydroxy-3,7,9b-trimethyl-3,7-nonibutyl-, Δm 0.03 Da [M+H]+
Lipids and lipid-like molecules | Glycerol phenylbutyrate Δm 0.00 Da [M+H]+
Organonitrogen compounds | n-Octadecylamine Δm 0.00 Da [M+H]+
Organonitrogen compounds | 1-Hexadecylamine Δm 0.00 Da [M+H]+
Fatty Acyls | Nonanedioic acid Δm 0.00 Da [M+H]+
Flavonoids | (1S)-1,5-Anhydro-2-O-(6-deoxy-α-L-mannopyranosyl)-1-(3,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl)-D-glucitol Δm -146.06 Da [M+H]+
Acyl halides | Tris(1,3-dichloro-2-propyl) phosphite Δm 2.00 Da [M+H]+
Oxazolines | N-Octyl-2-pyrrolidone Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | NP-024319 Δm -162.05 Da [M+H]+
Phenols | 3-Allyl-4-ethoxy-5-methoxybenzaldehyde Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | ABRLZQFRHWMRY-UHFFFAOYSA-N Δm -18.01 Da [M+H]+
Lipids and lipid-like molecules | 1-Heptadecene-4,6-diyne-3,8,9,10-tetrol Δm 0.00 Da [M+H]+
Prenol lipids | 7,8-Dihydro-α-ionone Δm 0.00 Da [M+H]+
Organooxygen compounds | Decazphosmalone Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 1,2-Diethylbis-α-cyanoene Δm -36.05 Da [M+H-H2O]+
Benzene and substituted derivatives | Ethanone, 1-[2-(1-hydroxy-1-methylethyl)phenyl] Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Procaine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | (2)-Tyrosine tert-butyl ester Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm 18.01 Da [2M+NH4]+
Piperidines | Butaline A Δm 0.00 Da [M+H]+
Organooxygen compounds | 6-Chloro-7-hydroxy-4-(mosphoton-4-yimethyl)-2H-chromen-2-one Δm -115.06 Da [M+H]+
Fatty Acyls | Anandamide (AEA) Δm 6.01 Da [M+H]+
Fatty Acyls | 8-(3-Octyl-2-oxiranyl)octanoic acid Δm -18.01 Da [M+H]+
Flavonoids | Hispidulin Δm 0.00 Da [M+H]+
Organonitrogen compounds | Betaxolol Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | N-Desmethylbrainardol Δm 0.00 Da [M+H]+
Anthracenes | 5,7-Dihydroxy-2-phenyl-6-[(2,5,6-trihydroxy-6-(hydroxymethyl)oxan-2-yl)-6-(3,4,5-trihydroxyoxan-2-yl)chromen-4-one Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | N'-(4-Cyano-3-methylphenyl)-2,2-dipenzimidazo-1-yl)-N,N-dimethylbrimoformamide Δm 18.01 Da [M+H-H2O]+
Organooxygen compounds | 5(21-Deoxo)Bufotin-2,5-hexadecine Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | 9,12-Dihydroxy-10-dodecenoic acid Δm 0.00 Da [M+H-H2O]+
Organooxygen compounds | Hemycoside Δm 0.00 Da [M+Na]+
Fatty Acyls | 3-Nitro-2,6-dipiperidinopyridine Δm 0.00 Da [M+H]+
Benzenoids | (2S)-3,(5-Methoxy-1H-benzimidazol-2-yl)-N-phenyl-1-pyrrolidinecarboxamide Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | N-α-(tert-Butoxycarbonyl)-L-lysine Δm 0.00 Da [M+H]+
Organonitrogen compounds | Hexadecanamide Δm 0.00 Da [M+H]+
Hydroxy acids and derivatives | 3,8,9,12,15-Pentacosanoxacosan-1-oic acid Δm -196.22 Da [M+H]+
Benzene and substituted derivatives | Magnosch Δm -274.12 Da [M+Na]+
Fatty Acyls | 3-(5,6-Dihydroxyhepty)-4-methyl-2H-furan-5-one Δm 0.00 Da [M+NH4]+
Benzene and substituted derivatives | 4-Ethyl-N,N-dimethylcalithione Δm -27.06 Da [M+H-H2O]+
Benzene and substituted derivatives | Diisobutyl phthalate Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3-Cyclohexyl-1,1-dimethylurea Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 8-Aminoquanine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | N'-(1-(2-(1-Benzoyl-3-(3,4-dichlorophenyl)piperidin-3-yl)propyl)-4-phenylpiperidin-4-yl)-N,N-dimethylurea Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-(2B-Nitro-1H-indazol-1-yl)ethanol Δm 0.00 Da [M+H]+
Organooxygen compounds | (+)-(5S)-EET Ethanolamide Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Cyclopropy[][5]-(3-methyl-1H-benzimidazol-2-yl)-1-pyrrolidinylmethanone Δm 0.00 Da [M+H]+
Diarylheptanoids | (5-Hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-(4-hydroxyphenyl)-3-heptanone Δm 0.00 Da [M+H-H2O]+
Organoheterocyclic compounds | 1-adamantylf(4)piperidin)methanone Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | (±)-14(15)-EET Δm 0.00 Da [M+H]+
Fatty Acyls | Lomifaxanacid A Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Naagard-Ic, I Δm 17.03 Da [M+H]+
Organooxygen compounds | 2-(2-Butoxyethoxy)ethanol Δm 0.00 Da [M+H]+
Prenol lipids | 2-(4-Hydroxy-7-isopropyl-4,8-dimethyl-6-oxodecyl)[3,2-]pyran-1-yl)acetic acid Δm -18.01 Da [M+H]+
Phenols | 3,7-Dihydroxy-9,11-eremophladien-8-one Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | 1-Naphthol Δm 18.01 Da [M+H-H2O]+
Naphthalenes | 6-Chloro-N4-(1-methylethyl)pyrimidine-4,5-diamine Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Methyl (2E,4E)-5-(1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl)-3-methylpenta-2,4-dienoate Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm 18.01 Da [M+H-H2O]+
PHA2Chlor
PHA1Chlor
SHA8B
SHA8A
SHA7B
SHA7A
SHA6B
SHA6A
SHA5B
SHA5A
SHA4B
SHA4A
SHA3B
SHA3A
SHA2B
SHA2A
SHA1B
SHA1A
PHA8B
PHA8A
PHA7B
PHA7A
PHA6B
PHA6A
PHA5B
PHA5A
PHA4B
PHA4A
PHA3B
PHA3A
PHA2B
PHA2A
PHA1B
PHA1A
Hepatocytes, Chlorpyrifos, Hepatocytes
Hepatocytes, Chlorpyrifos, Hepatocytes
Hepatocytes, Chlorpyrifos, Hepatocytes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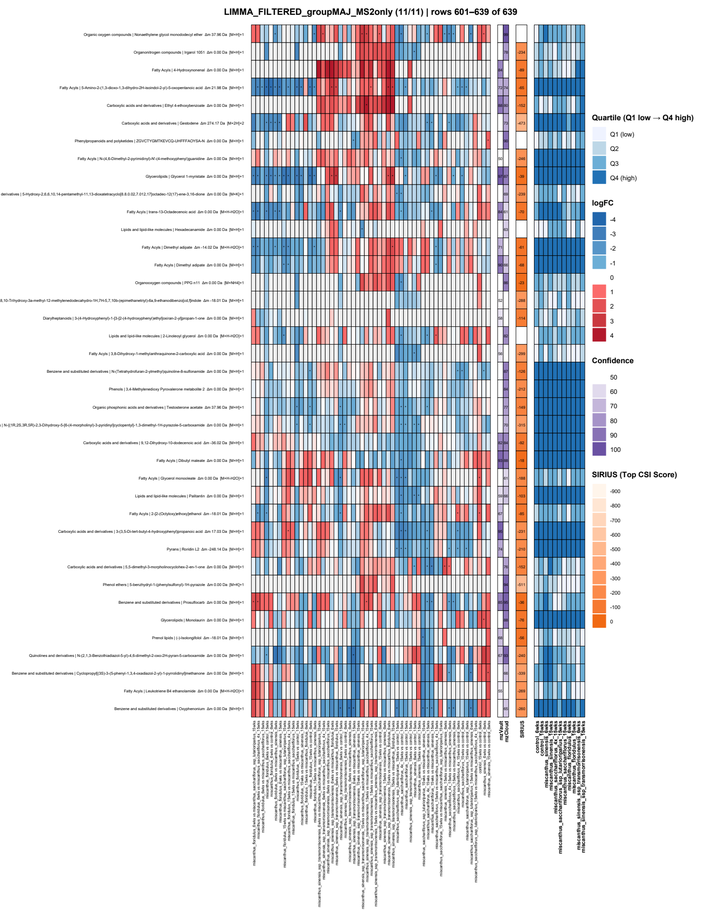
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Phenylpropanoids and polyketides | (3E,11E,13E)-8-hydroxy-16-methyl-1-oxacyclohexadeca-3,11,13-trien-2-one Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm -36.05 Da [M+H-H2O]+
Benzene and substituted derivatives | 7,8-Di-tert-butyl-1-oxaspiro[5.5]deca-6,9-diene-2,8-dione Δm -42.01 Da [M+H]+
Fatty Acyls | 4-Oxo-2-propylpentanoic acid Δm -18.01 Da [M+H]+
Organic phosphoric acids and derivatives | Tri(3-chloropropyl) phosphate Δm 0.00 Da [M+H]+
Triazines | Triallyl cyanurate Δm 0.00 Da [M+H]+
Organooxygen compounds | Pentaerithylene glycol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | N'N-Dibutylformamide Δm 0.00 Da [M+H]+
Organic phosphoric acids and derivatives | Triethyl phosphate Δm 0.00 Da [M+H]+
Organooxygen compounds | Hexaethylene glycol Δm 0.00 Da [M+H]+
Organooxygen compounds | PEG n7 Δm 0.00 Da [M+H]+
Organic phosphoric acids and derivatives | Triethyl phosphate Δm -28.03 Da [M+H]+
Hydroxy acids and derivatives | 4-Acetylphthalyl sulfone Δm -63.99 Da [M+Na]+
Prenol lipids | 7,9,20-tert-butyl-1-oxaspiro[5.5]deca-6,9-dione-2,8-dione Δm 0.00 Da [M+H]+
Organooxygen compounds | Bis(2-butoxyethyl) adipate Δm 17.03 Da [M+H]+
Fatty Acyls | Sorbitan monolaurate Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Picratrin Δm 21.98 Da [M+H]+
Fatty Acyls | 4,11-Dioxabicyclo[8.2.1]pentacan-3-one, 7-hydroxy-5-(2-hydroxypentyl)-2,2-dimethyl- Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 3-ethoxy-4-methoxy N,N-Diethylhexadrone Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoate Δm 17.03 Da [M+H]+
Benzene and substituted derivatives | 1,3-2,4-bis(3,4-dimethylbenzylidene)sorbitol Δm 0.00 Da [M+H]+
Fatty Acyls | 5,8,9-THydroxy-10-propyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one Δm 0.00 Da [M+H-H2O]+
Prenol ethers | Bis-(3,4-dimethylbenzylidene)sorbitol Δm 0.00 Da [M+H]+
Organooxygen compounds | (-)-3,5-Dimethylphenoxy)butanoic acid Δm 0.00 Da [M+H]+
3,4-dihydroxycinnamic | 4-Aminocinnamic acid Δm -60.02 Da [M+H]+
Carboxylic acids and derivatives | Tuberbilide Δm -36.02 Da [M+H]+
Lipids and lipid-like molecules | DHEHZZVQFCIZHN-GYXNDCUSA-N Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | 3-Benzyl-6-isopropylpiperazine-2,5-dione Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Propanoic acid, 2-hydroxy-3-[(1-(4-methoxy-6-methyl-2-oxo-2H-pyran-5-yl)buty]thio] Δm -122.00 Da [M+H]+
Benzene and substituted derivatives | Kontrigrion E Δm -148.11 Da [M+H]+
Carboxylic acids and derivatives | 3-Benzylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione Δm 0.00 Da [M+H]+
Organooxygen compounds | Oxiprenolol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Dodecanoic acid, 12-[[(cyclohexylamino)carbonyl]amino] Δm -125.08 Da [M+H]+
Benzene and substituted derivatives | (7-Hydroxy-7-methyl-8-oxo-3-propyl-5,8-dihydro-1H-isochromen-6-yl) 2-hydroxy-4-methoxy-6-methylbenzoate Δm -182.06 Da [M+H]+
Organic oxygen compounds | Poly THF n5 Δm 21.98 Da [M+H]+
Lipids and lipid-like molecules | 2-[(1S,4S,5S)-4-[[(Cyclohexylcarbamoyl)amino]methyl]-5-isopropyl-2-methyl-2-cyclohexen-1-yl]-N-[2-(dimethylamino)ethyl]acetamide Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | 2-(8-Decenoyl)glutaconic acid Δm 0.00 Da [M+H]+
Organooxygen compounds | (1*)-Carboxy-17α-formylcyclopseudomelhosine Δm -36.02 Da [M+H]+
Benzene and substituted derivatives | Valproic Acid Δm 21.98 Da [M+H]+
Fatty Acyls | 3-(1-Hydroxyheptyl)-5-(hydroxymethyl)oxolan-2-one Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | 1,4-Dibutoxy-2-nitrobenzene Δm 0.00 Da [M+H]+
Organooxygen compounds | Pentaepoxylipene glycol Δm 0.00 Da [M+H]+
Fatty Acyls | (3Z)-3-Hydroxy-5-dodecenoic acid Δm 0.00 Da [M+H]+
Organooxygen compounds | 2,6-Ethyl-2-methylheneoxo acid Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | Terbutrameton Δm 0.00 Da [M+Na]+
Organooxygen compounds | S-Chlorocinnamoic acid Δm -33.98 Da [M+H]+
Benzene and substituted derivatives | 1-(4-Propan-2-yloxifenylthio)phen-2-yl)-3-(2h-(trifluoromethyl)phenyl)urea Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | [(1R,4Z,9S)-11,11-dimethyl-8-methylidene-3-oxo-6-bicyclo[7.2.0]undec-4-enyl]methyl acetate Δm 37.96 Da [M+H]+
Fatty Acyls | N,Cinnoctylacetamide acid Δm 0.00 Da [M+H]+
Organic thiophosphoric acids and derivatives | N4-(4-chloro-2,5-dimethoxyphenyl)morpholine-4-carbothioamide Δm 0.00 Da [M+Na]+
Fatty Acyls | Bis(2-butoxyethyl) adipate Δm -56.06 Da [M+H-H2O]+
Benzenoids | (4-Fluorophenyl)[(3S)-3-(1-methyl-1H-benzimidazol-2-yl)-1-pyrrolidinyl]methanone Δm 0.00 Da [M+H]+
Fatty Acyls | (5E,12Z)-15-Hydroxy-16-methoxycleabea-8,12-dienoic acid Δm -14.02 Da [M+H-H2O]+
Fatty Acyls | L-Rhamnose Δm -18.01 Da [M+H]+
Organoheterocyclic compounds | N-[(1S,4S,6S)-6-Isopropyl-3-methyl-4-(2-oxo-2-(4-(2-pyridinyl)-1-piperazinyl)ethyl)-2-cyclohexen-1-yl]methyl]cyclopropanecarboxamide Δm 21.98 Da [M+H]+
Lipids and lipid-like molecules | 1-[(1S,4S,6S)-6-Isopropyl-3-methyl-4-[[(2-methyl-2-propanyl)-1,3,4-oxadiazol-2-yl]methyl]-2-cyclohexen-1-yl]-N-(3-pyridinylmethyl)methanamine Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | (E)-6-Hydroxy-2,7-dimethylsub-2-enebiss acid Δm 21.98 Da [M+H]+
Lipids and lipid-like molecules | Cickeoside Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | Carbetol Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | Deoxycholic acid Δm 0.00 Da [M+Na]+
Tissue_Tx_Cardiomyocyte_Treatment
Tissue_Tx_Cardiomyocyte_Treatment
Tissue_Tx_Cardiomyocyte_Treatment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Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0