

cec\_m1 for dss: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:NCGC00180518-02!2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3-dihydrochromen-4-one	3817.853742
w/o MS2:(2E)-3-(3,4-Dimethoxyphenyl)-N-[2-(3,4-dimethoxyphenyl)ethyl]prop-2-enamide	2307.12066
w/o MS2:Prostaglandin F2.alpha. dimethylamine	2101.962431
w/o MS2:Phe-Thr-Lys	882.419592
w/o MS2:N-(2-Phosphate-1R-methylethyl)-5Z,8Z,11Z,14Z-eicosatetraenamide	666.194185
w/o MS2:Bimatoprost diethylamide	582.308771
w/o MS2:1,3-Dihydroxy-4,4,6a,9,12b-pentamethyl-1,3,4,4a,5,6,6a,9,10,12,12a,12b-dodecahydro-2H,11H-benzo[f]pyrano[2,3-b]chromen-11-one	443.727825
w/o MS2:N-(2-Adamantyl)-N'-butylthiourea	407.501795
w/o MS2:N-Acetyldihydrosphingosine	380.150403
w/o MS2:L-Threonine	328.272015
w/o MS2:1-Methyl-4-(4-piperidiny)piperazine	321.027803
w/o MS2:3-[[2,2-Dimethyl-7-(2-methylbut-3-en-2-yl)-8H-pyrano[3,2-f]indol-6-yl]methyl]-2,3,6,7-tetrahydropyrrolo[1,2-a]pyrazine-1,4-dione	303.057828
w/o MS2:NCGC00160302-01!BELLADONNINE	301.146012
w/o MS2:NCGC00380909-01_C34H54O8_(1alpha,3alpha,7alpha,9xi,13alpha,17xi,20xi)-3,21,23-Trihydroxy-4,4,8-trimethyl-24,25-epoxycholest-14-ene-1,7-diyl diacetate	279.512553
w/o MS2:1-(4-Methylphenyl)cyclohexanecarbonitrile	237.211976

cec\_m1 dss: down reg by treatment, end up upreg

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Metabolite Name	
w/o MS2:12-Hydroxy-4',4a,6a,7-tetramethyldocosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-8,2'-pyran]-2-yl 6-O-hexopyranosylhexopyranoside	-4662.639117
w/o MS2:2-Cyclohexyl-N-(4-methoxyphenyl)acetamide	-1240.412044
w/o MS2:Thromboxane B2	-1126.532913
w/o MS2:8,14-Epoxy-3-hydroxycarda-16,20(22)-dienolide triglycoside	-880.593295
w/o MS2:Betaine aldehyde cation	-541.190923
w/o MS2:1H-Indole-5-sulfonamide, N-(3-chlorophenyl)-3-[[[3,5-dimethyl-4-[(4-methyl-1-piperazinyl)carbonyl]-1H-pyrrol-2-yl]methylene]-2,3-dihydro-N-methyl-2-oxo-, (3Z)-	-503.217788
w/o MS2:Nodularin	-436.912775
w/o MS2:Lisinopril	-343.390897
w/o MS2:1-[(1-Methylpiperidin-2-yl)methyl]-3-(1-naphthoyl)indole	-330.396796
w/o MS2:1-(1,2-Dihexanoylphosphatidyl)inositol-3,4-bisphosphate	-215.882877
w/o MS2:cis-13-Docosenoic acid	-200.988117
w/o MS2:Icariin	-189.55273
w/o MS2:NCGC00380898-01!(2E,4E,14E)-13-hydroperoxy-1-piperidin-1-ylcosa-2,4,14-trien-1-one	-154.384577
w/o MS2:N-(1-Acetylpiiperidin-4-yl)-N'-adamantan-1-ylurea	-154.021213
w/o MS2:N-Cyclohexyl-N'-(tetrahydro-2-furanylmethyl)urea	-149.853736

cec\_m1 for dss: up reg, end up down reg

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Metabolite Name	
w/o MS2:Pro-Pro-Lys	1217.385116
w/o MS2:NCGC00180733-02!(E)-9-(1,3-benzodioxol-5-yl)-1-piperidin-1-ylnon-8-en-1-one	860.473494
w/o MS2:1-O-Octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	739.622247
w/o MS2:4-Chloro-2-(trifluoromethyl)pyrimidine-5-carboxylic acid	558.419197

<b>w/o MS2:Palmitic acid</b>	497.318098
<b>w/o MS2:1,2-Dipalmitoylphosphatidylinositol-4,5-diphosphonate</b>	463.762928
<b>w/o MS2:3-[3-(Dimethylamino)propyl]-4-hydroxy-N-[4-(4-pyridyl)phenyl]benzamide</b>	420.263794
<b>w/o MS2:6,7-Dibromo-4-methoxy-1H-indole</b>	317.941229
<b>w/o MS2:7-Methoxy-2-propylquinolin-4-ol</b>	226.397948
<b>w/o MS2:6,6'-Benzene-1,2-diylbis(1,3,5-triazine-2,4-diamine)</b>	204.904094
<b>w/o MS2:3-Iodo-L-tyrosine</b>	194.666675
<b>w/o MS2:YRREAEDLQVGQVELGGGPGAGSLQPLALEGSLQKR/4</b>	160.828211
<b>w/o MS2:Ornibactin C6</b>	154.916986
<b>w/o MS2:Geraniol</b>	145.477275
<b>w/o MS2:Yohimbine</b>	140.480827

cec\_m1 dss: down reg, end up down reg

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<b>Metabolite Name</b>	
<b>w/o MS2:Blood Group A Tetrasaccharide</b>	-331.396077
<b>w/o MS2:DL-Norvaline</b>	-299.604677
<b>w/o MS2:Coproporphyrin I</b>	-263.014102
<b>w/o MS2:Benzo[h]-1,6-naphthyridin-2(1H)-one, 1-[4-[4-(1-oxopropyl)-1-piperazinyl]-3-(trifluoromethyl)phenyl]-9-(3-quinoliny)-</b>	-227.724386
<b>w/o MS2:Sodium 2,2'-methylene bis(4,6-di-tert-butylphenyl) phosphate</b>	-213.643618
<b>w/o MS2:Tetradecanamide, N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]-</b>	-192.985513
<b>w/o MS2:6-Ketoprostaglandin E1</b>	-154.626132
<b>w/o MS2:4-(Diphenylmethoxy)-1-[3-(1H-tetrazol-5-yl)propyl]piperidine</b>	-130.091423
<b>w/o MS2:Benamide, 5-bromo-2-[(2-chloro-4-iodophenyl)amino]-N-(cyclopropylmethoxy)-3,4-difluoro-</b>	-126.197175
<b>w/o MS2:NCGC00180698-03!(2S)-2-[(1S)-1-carboxyundecyl]-5-oxooxolane-2-carboxylic acid</b>	-114.918764
<b>w/o MS2:NCGC00169960-03!(2E,4E)-12-[(10E,12E)-13-carboxy-3-hydroxy-2-(hydroxymethyl)-8,10,12-trimethyltrideca-10,12-dienoyl]oxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid</b>	-109.207725
<b>w/o MS2:Phytic acid</b>	-97.125405
<b>w/o MS2:Hydrocodone</b>	-65.377275
<b>w/o MS2:Warfarin</b>	-62.015975
<b>w/o MS2:2-Methylbutyryl-L-carnitine</b>	-54.23719

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<b>Metabolite Name</b>	
<b>w/o MS2:NCGC00381282-01![5-hydroxy-2-[4-hydroxy-2,5-bis(hydroxymethyl)-3-(2-methylpropanoyloxy)oxolan-2-yl]oxy-4-(2-methylpropanoyloxy)-6-(2-methylpropanoyloxymethyl)oxan-3-yl] decanoate</b>	8274.107492
<b>w/o MS2:1-Naphthalenepentanoic acid, 5-carboxy-1,2,3,4,4a,7,8,8a-octahydro-7-hydroxy-.beta.,1,2,4a-tetramethyl-</b>	1939.552315
<b>w/o MS2:1-Lignoceroyl-2-hydroxy-sn-glycero-3-phosphocholine</b>	1350.498455
<b>w/o MS2:2,4-Bis(1,1-dimethylethyl)phenol phosphate</b>	732.908451
<b>w/o MS2:.beta.-Nicotinamide adenine dinucleotide phosphate</b>	728.457685
<b>w/o MS2:O-Isobutyrylthiamine disulfide</b>	613.187043
<b>w/o MS2:Oxazepam glucuronide</b>	586.489122
<b>w/o MS2:6-Nitro-2,3,4,9-tetrahydro-1H-carbazole</b>	538.473334
<b>w/o MS2:Ornibactin C6</b>	384.215293
<b>w/o MS2:Arvenin III</b>	363.27017
<b>w/o MS2:His-Ile-Arg</b>	353.035637
<b>w/o MS2:Ile-Thr-Lys</b>	336.459532
<b>w/o MS2:Halopemide</b>	300.991878

w/o MS2:Prostaglandin D2 serinolamide	279.420791
w/o MS2:17.alpha.-Ethinylestradiol	236.356604

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Metabolite Name	
w/o MS2:12-Hydroxy-4',4a,6a,7-tetramethyldocosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-8,2'-pyran]-2-yl 6-O-hexopyranosylhexopyranoside	-4661.424532
w/o MS2:2-Cyclohexyl-N-(4-methoxyphenyl)acetamide	-1240.906887
w/o MS2:Nodularin	-458.4404
w/o MS2:1H-Indole-5-sulfonamide, N-(3-chlorophenyl)-3-[[3,5-dimethyl-4-[(4-methyl-1-piperazinyl)carbonyl]-1H-pyrrol-2-yl]methylene]-2,3-dihydro-N-methyl-2-oxo-, (3Z)-	-452.032069
w/o MS2:Lisinopril	-340.518338
w/o MS2:Blood Group A Tetrasaccharide	-298.359985
w/o MS2:Coproporphyrin I	-262.988787
w/o MS2:Icariin	-188.880028
w/o MS2:N-Cyclohexyl-N'-(tetrahydro-2-furanylmethyl)urea	-152.00616
w/o MS2:Win 64821	-138.304072
w/o MS2:Phosphoric acid	-128.846869
w/o MS2:NCGC00169960-03!(2E,4E)-12-[(10E,12E)-13-carboxy-3-hydroxy-2-(hydroxymethyl)-8,10,12-trimethyltrideca-10,12-dienoyl]oxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid	-119.378219
w/o MS2:NCGC00180698-03!(2S)-2-[(1S)-1-carboxyundecyl]-5-oxoxolane-2-carboxylic acid	-117.073164
w/o MS2:Scytophycin D	-111.367193
w/o MS2:MLS000069478-01!CORTISONE ACETATE	-91.611385

cec\_m1 for ab: up reg, end up down reg

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Metabolite Name	
w/o MS2:2-Aminoethyl diphenylborinate	10816.740351
w/o MS2:Adefovir dipivoxil	3070.135625
w/o MS2:NCGC00169957-03_C30H51N5O7_3-sec-Butyl-16-isobutyl-6-isopropyl-5,8,9-trimethyldodecahydropyrrolo[1,2-d][1,4,7,10,13,16]oxapentaazacyclononadecine-1,4,7,10,14,17(11H,16H)-hexone	1000.902975
w/o MS2:2-(4-Hydroxy-7-methyl-5-oxo-2,3-dihydro-5H-furo[3,2-g]chromen-2-yl)propan-2-yl hexopyranoside	548.335707
w/o MS2:4-(2-Hydroxyethyl)piperazine-1-(2-hydroxypropanesulfonic acid)	398.189938
w/o MS2:cis-5-Dodecenoic acid	395.441462
w/o MS2:(1S,4R)-4-[[[(2S,3aS,4S)-4-Hydroxy-2-methyl-1-oxo-3,3a-dihydro-2H-imidazo[1,2-a]indol-4-yl]methyl]-1-methyl-2,4-dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-dione	377.011321
w/o MS2:Entecavir	362.856401
w/o MS2:Guanosine 5'-tetrphosphate	315.725171
w/o MS2:O-Desmethylgefitinib	304.350852
w/o MS2:Herniariasaponin 7	290.571955
w/o MS2:1-Palmitoyl-2-linoleoyl-rac-glycerol	267.594155
w/o MS2:Clarithromycin	235.109989
w/o MS2:4-Bromo-2-([(1-propyl-1H-benzimidazol-2-yl)amino]methyl}phenol	230.805313
w/o MS2:Benzenepropanoic acid, 5-(3-carboxybenzoyl)-2-[(5E)-6-(4-methoxyphenyl)-5-hexen-1-yl]oxy]-	219.74629

cec\_m1 ab: down reg, end up down reg

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Metabolite Name	
w/o MS2:Thromboxane B2	-1130.520033
w/o MS2:8,14-Epoxy-3-hydroxycarda-16,20(22)-dienolide triglycoside	-879.290482
w/o MS2:DL-Norvaline	-636.098505

<b>w/o MS2:Betaine aldehyde cation</b>	-542.391921
<b>w/o MS2:1-[(1-Methylpiperidin-2-yl)methyl]-3-(1-naphthoyl)indole</b>	-330.903402
<b>w/o MS2:1-(1,2-Dihexanoylphosphatidyl)inositol-3,4-bisphosphate</b>	-310.901081
<b>w/o MS2:Benzo[h]-1,6-naphthyridin-2(1H)-one, 1-[4-[4-(1-oxopropyl)-1-piperazinyl]-3-(trifluoromethyl)phenyl]-9-(3-quinolinyl)-</b>	-226.122087
<b>w/o MS2:Sodium 2,2'-methylene bis(4,6-di-tert-butylphenyl) phosphate</b>	-210.375619
<b>w/o MS2:Tetradecanamide, N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]-</b>	-192.37568
<b>w/o MS2:cis-13-Docosenoic acid</b>	-174.766641
<b>w/o MS2:N-(1-Acetylpiiperidin-4-yl)-N'-adamantan-1-ylurea</b>	-155.157731
<b>w/o MS2:6-Ketoprostaglandin E1</b>	-153.930808
<b>w/o MS2:NCGC00380898-01!(2E,4E,14E)-13-hydroperoxy-1-piperidin-1-yl-icos-2,4,14-trien-1-one</b>	-144.319676
<b>w/o MS2:4-(Diphenylmethoxy)-1-[3-(1H-tetrazol-5-yl)propyl]piperidine</b>	-135.090522
<b>w/o MS2:Benamide, 5-bromo-2-[(2-chloro-4-iodophenyl)amino]-N-(cyclopropylmethoxy)-3,4-difluoro-</b>	-127.445559

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<b>Metabolite Name</b>	
<b>w/o MS2:2,4-Bis(1,1-dimethylethyl)phenol phosphate</b>	1799.423895
<b>w/o MS2:Ritonavir</b>	876.265091
<b>w/o MS2:CSCKDMTDKECLNFCHQDVIW/3</b>	769.290036
<b>w/o MS2:Palmitic acid</b>	505.546074
<b>w/o MS2:NCGC00169102-02!2-[5-[2-[2-[5-[2-[2-[5-[2-[2-[5-(2-hydroxybutyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid</b>	393.844556
<b>w/o MS2:6-O-((2Z)-3-(4-Hydroxy-3-methoxyphenyl)prop-2-enoyl)-.beta.-D-fructofuranosyl 6-O-acetyl-.alpha.-D-glucopyranoside</b>	373.285293
<b>w/o MS2:2-Cyano-N-{3-[(cyanoacetyl)amino]propyl}acetamide</b>	234.294851
<b>w/o MS2:Chaetoglobosin A</b>	224.793853
<b>w/o MS2:4,6-Quinazolinediamine, N4-[2-(4-phenoxyphenyl)ethyl]-</b>	214.737227
<b>w/o MS2:G0F-2AB</b>	211.195897
<b>w/o MS2:Herniariasaponin 7</b>	205.741216
<b>w/o MS2:Isosilybin A</b>	195.797345
<b>w/o MS2:DL-Ethionine</b>	150.870009
<b>w/o MS2:NCGC00380113-01!2,3,14-trihydroxy-10,13-dimethyl-17-(2,3,6,7-tetrahydroxy-5,6-dimethylheptan-2-yl)-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one</b>	150.146506
<b>w/o MS2:YGGFMTLFFKNAIIKNAYKKGE/3</b>	133.262207

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<b>Metabolite Name</b>	
<b>w/o MS2:Thromboxane B2</b>	-1121.262077
<b>w/o MS2:8,14-Epoxy-3-hydroxycarda-16,20(22)-dienolide triglycoside</b>	-881.08414
<b>w/o MS2:Betaine aldehyde cation</b>	-542.659393
<b>w/o MS2:Nodularin</b>	-458.512548
<b>w/o MS2:Lisinopril</b>	-345.34884
<b>w/o MS2:1-[(1-Methylpiperidin-2-yl)methyl]-3-(1-naphthoyl)indole</b>	-329.955365
<b>w/o MS2:1-(1,2-Dihexanoylphosphatidyl)inositol-3,4-bisphosphate</b>	-327.373473
<b>w/o MS2:Coproporphyrin I</b>	-263.000338
<b>w/o MS2:cis-13-Docosenoic acid</b>	-188.554048
<b>w/o MS2:N-(1-Acetylpiiperidin-4-yl)-N'-adamantan-1-ylurea</b>	-155.065248
<b>w/o MS2:Tetradecanamide, N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]-</b>	-147.177271
<b>w/o MS2:NCGC00380898-01!(2E,4E,14E)-13-hydroperoxy-1-piperidin-1-yl-icos-2,4,14-trien-1-one</b>	-139.020814

w/o MS2:Phosphoric acid	-119.60516
w/o MS2:6-O-((2E)-2-Methylbut-2-enoyl)-.beta.-D-glucopyranosyl-(1->2)-6-O-((2E)-2-methylbut-2-enoyl)-.alpha.-D-glucopyranosyl 6-O-((2E)-2-methylbut-2-enoyl)-.beta.-D-glucopyranosyl-(1->2)-.alpha.-D-glucopyranoside	-111.86027
w/o MS2:Benzamide, 5-bromo-2-[(2-chloro-4-iodophenyl)amino]-N-(cyclopropylmethoxy)-3,4-difluoro-	-101.667607

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Metabolite Name	
w/o MS2:1H-Indazole-3-carboxamide, N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)-	1899.84318
w/o MS2:2-((1-(4-Nitrobenzoyl)propyl)amino)benzoic acid	1276.75515
w/o MS2:HSQGTFSDYSKYLDSRRAQDFVQWLMNTRNRNNIA/6	912.368736
w/o MS2:DKEAVYFAHLDIW/-2	607.357698
w/o MS2:Phosphatidylcholine 22:0-18:2	573.660392
w/o MS2:Oxasulfuron	512.954592
w/o MS2:Palmitoyl sphingomyelin	458.608183
w/o MS2:NCGC00384986-01!1-hydroxy-2-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxymethyl]oxan-2-yl]oxyanthracene-9,10-dione	438.683689
w/o MS2:Rimcazole	345.095931
w/o MS2:Ginsenoside Rh2	342.256644
w/o MS2:Aceroside VIII	278.714359
w/o MS2:NCGC00380734-01_C39H65NO10_2-{6-[5-Hydroxy-3-(2-hydroxy-2-propanyl)-6a,9b-dimethyldodecahydrocyclopenta[f]chromen-7-yl]-4a-methyl-3,4,4a,7,8,8a-hexahydro-2H-chromen-2-yl]-2-propanyl 2-acetamido-2-deoxy-6-O-methylhexopyranoside	177.030118
w/o MS2:Sapanisertib	171.86601
w/o MS2:NCGC00385199-01!2-[3,4-bis{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl]-5,7-dihydroxychromen-4-one	164.562875
w/o MS2:Neomycin	144.530752

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Metabolite Name	
w/o MS2:12-Hydroxy-4',4a,6a,7-tetramethyldocosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-8,2'-pyran]-2-yl 6-O-hexopyranosylhexopyranoside	-4655.737581
w/o MS2:2-Cyclohexyl-N-(4-methoxyphenyl)acetamide	-1239.211384
w/o MS2:DL-Norvaline	-636.0301
w/o MS2:1H-Indole-5-sulfonamide, N-(3-chlorophenyl)-3-[[3,5-dimethyl-4-[(4-methyl-1-piperazinyl)carbonyl]-1H-pyrrol-2-yl]methylene]-2,3-dihydro-N-methyl-2-oxo-, (3Z)-	-494.435593
w/o MS2:Blood Group A Tetrasaccharide	-319.699655
w/o MS2:Benzo[h]-1,6-naphthyridin-2(1H)-one, 1-[4-[4-(1-oxopropyl)-1-piperazinyl]-3-(trifluoromethyl)phenyl]-9-(3-quinolinyl)-	-228.582233
w/o MS2:Sodium 2,2'-methylene bis(4,6-di-tert-butylphenyl) phosphate	-212.924083
w/o MS2:Icariin	-180.690711
w/o MS2:N-Cyclohexyl-N'-(tetrahydro-2-furanylmethyl)urea	-157.634468
w/o MS2:6-Ketoprostaglandin E1	-152.705322
w/o MS2:Win 64821	-145.412823
w/o MS2:4-(Diphenylmethoxy)-1-[3-(1H-tetrazol-5-yl)propyl]piperidine	-134.647492
w/o MS2:NCGC00169960-03!(2E,4E)-12-[(10E,12E)-13-carboxy-3-hydroxy-2-(hydroxymethyl)-8,10,12-trimethyltrideca-10,12-dienoyl]oxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid	-121.849919
w/o MS2:Rhodamine 6G cation	-118.358908
w/o MS2:Scytophycin D	-117.86752

ser\_m1 for dss: up reg by treatment, end up upreg

	convexity



Metabolite Name	
w/o MS2:Calpain Inhibitor II	1335.621483
w/o MS2:Phenol, 5-(1,1-dimethylheptyl)-2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl)cyclohexyl]-, rel-(+)-	825.829974
w/o MS2:(2,4,5-Trichlorophenoxy)acetic acid	751.033579
w/o MS2:7-Benzyl-11,14-dimethyl-16-(2-methylpropyl)-10,13-di(propan-2-yl)-17-oxa-1,5,8,11,14-pentazabicyclo[17.3.0]docosane-2,6,9,12,15,18-hexone	686.437431
w/o MS2:1-(2-Chloroacetyl)-3-isopropylurea	565.549933
w/o MS2:beta-carotene	443.39516
w/o MS2:Methyl 2-[[4-hydroxy-3-(2-methylbut-3-en-2-yl)-5-(3-methylbut-2-enyl)phenyl]methyl]-3-(4-hydroxyphenyl)-4-methoxy-5-oxofuran-2-carboxylate	412.961992
w/o MS2:(3S,4S,6aR,6bS,8R,8aR,12aS,14bR)-8-Hydroxy-4,6a,6b,11,11,14b-hexamethyl-3-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxy-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydronicene-4,8a-dicarboxylic acid	351.015046
w/o MS2:N-(2-Bromobenzyl)acetamide	346.799592
w/o MS2:5-Nitro-2-phenyl-1H-benzimidazole	327.657671
w/o MS2:Trichlorfon	266.183436
w/o MS2:8-Imino-2',5',5',8a'-tetramethyl-3,3',4',4a',5',6,6',7,7',8,8',8a'-dodecahydro-2'H-spiro[furo[2,3-e]isoindole-2,1'-naphthalene]-4,6'-diol	189.473684
w/o MS2:Gliocladic acid_130132	125.348407
w/o MS2:7,8-Dihydro-.alpha.-ionone	112.119512
w/o MS2:1-Methyl-4-[2-(4-piperidinyl)ethyl]piperazine	109.751805

ser\_m1 dss: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-sn-glycerol)	-48533.751926
w/o MS2:5-Heptenoic acid, 7-[(1R,2R,3S,5S)-2-[(1E,3S)-3-(2,3-dihydro-1H-inden-2-yl)-3-hydroxy-1-propen-1-yl]-3-fluoro-5-hydroxycyclopentyl]-, (5Z)-	-704.681795
w/o MS2:C11:db-UHQ aka 2-undecenyl-quinoloin-4(1H)-one position of double bond unknown	-438.000078
w/o MS2:5a,6-Anhydrotetracycline	-369.44577
w/o MS2:2,2,2-Trichloro-N-methylacetamide	-346.159982
w/o MS2:1,2-Dilauroyl-sn-glycero-3-phospho-sn-glycerol	-322.43711
w/o MS2:Kahweol palmitate	-290.359977
w/o MS2:Rosuvastatin	-169.632574
w/o MS2:Phe-Ser-Lys	-143.6108
w/o MS2:Flucythrinate	-141.797493
w/o MS2:Phosphatidylserine 16:0-22:6	-141.3555
w/o MS2:[(3R,4S,8S,8aS)-3-Hydroxy-6,8a-dimethyl-8-[(Z)-2-methylbut-2-enoyl]oxy-3-propan-2-yl-1,2,3a,4,5,8-hexahydroazulen-4-yl] 4-hydroxybenzoate	-134.696219
w/o MS2:4-Amino-4-methylpentanoic acid	-126.81309
w/o MS2:Vinblastine	-121.204627
w/o MS2:3,6,9,12,15-Pentaoxaheptacosan-1-ol, hydrogen sulfate	-95.374579

ser\_m1 for dss: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:Chlorogenic acid	1458.329338
w/o MS2:8Z,14Z-Eicosadienoic acid	734.197752
w/o MS2:NCGC00381205-01_C27H38O6_(5xi,8alpha,9xi,10alpha)-14-Acetoxy-15-[[{(2Z)-2-methyl-2-butenoyl]oxy}kaur-16-en-18-oic acid	637.272042
w/o MS2:Tunicamycin X	530.012605
w/o MS2:p-tert-Octylphenol	472.188055
w/o MS2:Oligomycin B	437.876262

w/o MS2:MLS001332637-01!Tiamulin	409.787864
w/o MS2:Phosphatidylethanolamine alkenyl 16:0-20:0	281.496243
w/o MS2:N-(9-(Butan-2-yl)-21-(4-methoxybenzyl)-18,22-dimethyl-5,8,11,16,20,23-hexaoxo-6-(propan-2-yl)icosahydro-5H,16H-dipyrrolo[2,1-f:2',1'-o][1,4,7,10,13,16]oxapentaazacyclononadecin-17-yl)acetamide	278.942001
w/o MS2:NCGC00380724-01_C28H47NO8_(3R,5R,6S,7S,9R,11E,13S,14R)-14-Ethyl-13-hydroxy-3,5,7,9,13-pentamethyl-2,4,10-trioxooxacyclotetradec-11-en-6-yl 3,4,6-trideoxy-3-(dimethylamino)-D-xylo-hexopyranoside	268.290154
w/o MS2:NCGC00385282-01_C18H28O4_(3E,5R,6E,8S,9E,13S,14R)-5-Hydroxy-8-methoxy-5,9,13,14-tetramethyloxacyclotetradeca-3,6,9-trien-2-one	219.015616
w/o MS2:Cyclo[3-(2-naphthalenyl)-L-alanylglycyl-D-tyrosyl-L-arginyl-L-arginyl]	205.514821
w/o MS2:Phosphatidylcholine alkenyl 16:0-16:0	194.508357
w/o MS2:2(1H)-Pyridinone, 3-[(2S,4S,5R)-5,6-dichloro-2,4-dimethyl-1-oxohexyl]-4-hydroxy-5,6-dimethoxy-	169.468872
w/o MS2:YPFPGPI/1	156.105386

ser\_m1 dss: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:NCGC00381071-01!1,12-dihydroxy-1,6,12,17,23,28-hexazacyclotritriacontane-2,5,13,16,24,27-hexone	-414.451245
w/o MS2:NCGC00380745-01!(5E)-2-heptyl-3,4,7-trihydroxy-2,3,4,7,8,9-hexahydrooxecicin-10-one	-407.722598
w/o MS2:5',6',7',8'-Tetrahydro-1'H-spiro[cyclohexane-1,4'-quinazoline]-2'(3'H)-thione	-325.342696
w/o MS2:2-(Tribromomethylsulfonyl)pyridine	-263.878241
w/o MS2:.beta.-Alanine, N-[2-[(3-hexylphenyl)amino]-2-oxoethyl]-	-251.542299
w/o MS2:D-Glucosamine, 6-sulfate	-186.065105
w/o MS2:NCGC00385080-01!4-[(E)-3-[(2R,3R,4S,5S,6R)-3-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	-163.881565
w/o MS2:cis-Nerolidol	-154.598834
w/o MS2:17-Epioxandrolone	-151.924396
w/o MS2:Destruxin A	-142.215377
w/o MS2:Buprenorphine-d4	-138.956659
w/o MS2:1-O-Hexadecyl-2-O-ethyl-sn-glycero-3-phosphocholine	-131.554898
w/o MS2:NCGC00180529-03!(3S,6R,9S,12R,15S,18R)-4,10,16-trimethyl-3,6,9,12,15,18-hexa(propan-2-yl)-1,7,13-trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone	-99.578759
w/o MS2:MLS002222329-01!26305-03-3	-90.037832
w/o MS2:[(4-Bromophenyl)sulfanyl]acetic acid	-84.643711

ser\_m1 for ab: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:2-(4-tert-Butylphenyl)-4(1H)-quinazolinone	22851.911508
w/o MS2:Gossypol	602.741542
w/o MS2:1-(4-Bromo-1H-pyrrol-2-yl)-2,2,2-trichloroethan-1-one	598.65465
w/o MS2:NCGC00381059-01!5-[5-(3,5-dihydroxydecanoyloxy)-3-hydroxydecanoyl]oxy-3-hydroxydecanoic acid	396.025823
w/o MS2:Cyclo(glycyltryptophylprolylglycylvalylglycyl-.beta.-hydroxytyrosyl)	395.887876
w/o MS2:Tunicamycin X	183.307109
w/o MS2:Amastatin	160.836959
w/o MS2:Dodecanedioic acid	155.464884
w/o MS2:2-Hydroxy-2',3',4',5'-tetrachlorobiphenyl	140.2082
w/o MS2:Benzoic acid, 3-[[[(3-carboxycyclohexyl)amino]carbonyl]-4-[3-[4-[4-(cyclohexyloxy)butoxy]phenyl]propoxyl]-	122.27138
w/o MS2:Decahydrogambogic Acid	120.647105
w/o MS2:NCGC00385003-01!4-[3-methyl-5-(5,6,7-trihydroxy-1,2,4a,5-tetramethyl-3,4,6,7,8,8a-hexahydro-2H-naphthalen-1-yl)pentoxyl]-4-oxobutanoic acid	119.746181

w/o MS2:3-(5,5-Dimethyl-5,6-dihydro[1,2,4]triazolo[3,4-a]isoquinolin-3-yl)phenol	107.945458
w/o MS2:Phosphatidylinositol 18:0-20:4	101.502297
w/o MS2:1-O-Hexadecyl-2-deoxy-2-thio-S-acetyl-sn-glycerol-3-phosphorylcholine	90.031233

ser\_m1 ab: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:5-Heptenoic acid, 7-[(1R,2R,3S,5S)-2-[(1E,3S)-3-(2,3-dihydro-1H-inden-2-yl)-3-hydroxy-1-propen-1-yl]-3-fluoro-5-hydroxycyclopentyl]-, (5Z)-	-703.49755
w/o MS2:NCGC00381071-01!1,12-dihydroxy-1,6,12,17,23,28-hexazacyclotritriacontane-2,5,13,16,24,27-hexone	-505.529913
w/o MS2:C11:db-UHQ aka 2-undecenyl-quinoloin-4(1H)-one position of double bond unknown	-438.670728
w/o MS2:Vinblastine	-264.246807
w/o MS2:2-(Tribromomethylsulfonyl)pyridine	-263.871431
w/o MS2:D-Glucosamine, 6-sulfate	-203.385196
w/o MS2:Rosuvastatin	-173.882131
w/o MS2:(3S,4S,6aR,6bS,8R,8aR,12aS,14bR)-8-Hydroxy-4,6a,6b,11,11,14b-hexamethyl-3-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxy-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydronicene-4,8a-dicarboxylic acid	-167.649868
w/o MS2:NCGC00385080-01!4-[(E)-3-[(2R,3R,4S,5S,6R)-3-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	-165.481236
w/o MS2:17-Epioxandrolone	-149.146144
w/o MS2:Buprenorphine-d4	-147.359724
w/o MS2:Phosphatidylserine 16:0-22:6	-141.38473
w/o MS2:NCGC00180529-03!(3S,6R,9S,12R,15S,18R)-4,10,16-trimethyl-3,6,9,12,15,18-hexa(propan-2-yl)-1,7,13-trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone	-107.957356
w/o MS2:3,6,9,12,15-Pentaoxaheptacosan-1-ol, hydrogen sulfate	-98.575573
w/o MS2:MLS00222329-01!26305-03-3	-89.965442

ser\_m1 for ab: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:N.epsilon.-Acetyl-L-lysine	4922.050439
w/o MS2:Dimefox	4070.249612
w/o MS2:N-Cyclohexyl-1-pyrrolidinecarboxamide	353.129099
w/o MS2:2-(Hexopyranosyloxy)-1,20,25-trihydroxy-9,10,14-trimethyl-22-oxo-4,9-cyclo-9,10-secocholest-5-en-16-yl acetate	328.345085
w/o MS2:NCGC00385919-01_C20H34O_2-Penten-1-ol, 5-[(1S,4aS,8aS)-decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-3-methyl-, (2E)-	301.737127
w/o MS2:4,5-Dibromo-2-furoic acid	221.643704
w/o MS2:NCGC00160181-01!MAHANIMBINE	202.71749
w/o MS2:NCGC00381240-01!1,3,4-trihydroxy-5-[(E)-3-[2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoyl]oxycyclohexane-1-carboxylic acid	198.364457
w/o MS2:Cholest-5-ene-3.beta.,4.beta.-diol	187.479816
w/o MS2:RGDS/-1	181.760057
w/o MS2:2,7-Dichlorodihydrofluorescein diacetate	173.52114
w/o MS2:Tetradecylamine	169.393986
w/o MS2:Finasteride	149.737819
w/o MS2:NG-Amino-L-arginine	146.685453
w/o MS2:Ethanone, 1-[1-(2-cyclohexylethyl)-1H-indol-3-yl]-2-(2-methoxyphenyl)-	99.432652

ser\_m1 ab: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-sn-glycerol)	-48604.036637



w/o MS2:NCGC00380745-01!(5E)-2-heptyl-3,4,7-trihydroxy-2,3,4,7,8,9-hexahydrooxecin-10-one	-407.363111
w/o MS2:5a,6-Anhydrotetracycline	-362.470909
w/o MS2:2,2,2-Trichloro-N-methylacetamide	-330.942213
w/o MS2:5',6',7',8'-Tetrahydro-1'H-spiro[cyclohexane-1,4'-quinazoline]-2'(3'H)-thione	-325.808702
w/o MS2:1,2-Dilauroyl-sn-glycero-3-phospho-sn-glycerol	-317.724744
w/o MS2:Kahweol palmitate	-300.617906
w/o MS2:.beta.-Alanine, N-[2-[(3-hexylphenyl)amino]-2-oxoethyl]-	-254.922856
w/o MS2:[(3R,4S,8S,8aS)-3-Hydroxy-6,8a-dimethyl-8-[(Z)-2-methylbut-2-enoyl]oxy-3-propan-2-yl-1,2,3a,4,5,8-hexahydroazulen-4-yl] 4-hydroxybenzoate	-192.5404
w/o MS2:Flucythrinate	-145.782469
w/o MS2:Destruxin A	-144.26839
w/o MS2:Phe-Ser-Lys	-142.958606
w/o MS2:cis-Nerolidol	-138.169538
w/o MS2:1-O-Hexadecyl-2-O-ethyl-sn-glycero-3-phosphocholine	-133.691119
w/o MS2:4-Amino-4-methylpentanoic acid	-129.595914

ser\_m1 for dab: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Diisooctyl phthalate	477.105187
w/o MS2:NCGC00381159-01!2-[[3,21-dihydroxy-20-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxydocosan-2-yl]amino]acetic acid	294.345068
w/o MS2:Octanediamide, N1-hydroxy-N8-[4-[4-[(1-oxo-5-hexyn-1-yl)amino]benzoyl]phenyl]-	213.143534
w/o MS2:3-(5,5-Dimethyl-5,6-dihydro[1,2,4]triazolo[3,4-a]isoquinolin-3-yl)phenol	199.858225
w/o MS2:VRKRTLRL/2	149.443683
w/o MS2:Phosphatidylethanolamine alkyl 20:0-22:6	130.835165
w/o MS2:Phosphoric acid	121.956565
w/o MS2:Nelfinavir	75.167459
w/o MS2:Phosphatidylcholine 18:1-22:6	70.66618
w/o MS2:Withanolide B	68.606247
w/o MS2:Orlistat	62.131983
w/o MS2:1-palmitoyl-2-linoleoyl-sn-glycero-3-phospho-(1'-rac-glycerol)	52.362714
w/o MS2:Leukotriene C4	47.931007
w/o MS2:5-Heptenamide, 7-[(1R,2R,3S,5S)-2-[(3R)-3-(2,3-dihydro-1H-inden-2-yl)-3-hydroxy-1-propen-1-yl]-3-fluoro-5-hydroxycyclopentyl]-N-ethyl-, (5Z)-	46.775694
w/o MS2:1-Methyl-L-histidine	40.748736

ser\_m1 dab: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-sn-glycerol)	-48614.075814
w/o MS2:NCGC00381071-01!1,12-dihydroxy-1,6,12,17,23,28-hexazacyclotritriacontane-2,5,13,16,24,27-hexone	-511.912624
w/o MS2:C11:db-UHQ aka 2-undecenyl-quinoloin-4(1H)-one position of double bond unknown	-438.350601
w/o MS2:5a,6-Anhydrotetracycline	-370.247944
w/o MS2:2,2,2-Trichloro-N-methylacetamide	-345.05902
w/o MS2:5',6',7',8'-Tetrahydro-1'H-spiro[cyclohexane-1,4'-quinazoline]-2'(3'H)-thione	-325.80004
w/o MS2:1,2-Dilauroyl-sn-glycero-3-phospho-sn-glycerol	-308.685466
w/o MS2:Kahweol palmitate	-303.540147
w/o MS2:2-(Tribromomethylsulfonyl)pyridine	-264.247564
w/o MS2:.beta.-Alanine, N-[2-[(3-hexylphenyl)amino]-2-oxoethyl]-	-256.667347
w/o MS2:Rosuvastatin	-171.970957

<b>w/o MS2:(3S,4S,6aR,6bS,8R,8aR,12aS,14bR)-8-Hydroxy-4,6a,6b,11,11,14b-hexamethyl-3-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxy-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydronicene-4,8a-dicarboxylic acid</b>	-169.860496
<b>w/o MS2:Phe-Ser-Lys</b>	-144.274154
<b>w/o MS2:Phosphatidylserine 16:0-22:6</b>	-142.511427
<b>w/o MS2:1-O-Hexadecyl-2-O-ethyl-sn-glycero-3-phosphocholine</b>	-133.169261

ser\_m1 for dab: up reg, end up down reg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:KILDK/10</b>	287.758755
<b>w/o MS2:L-beta-Homomethionine</b>	242.96421
<b>w/o MS2:2-(Dicyclohexylphosphino)-2'-methylbiphenyl</b>	228.508304
<b>w/o MS2:NCGC00347652-02_C35H53N5O7_12-Benzyl-3-isobutyl-6,9-diisopropyl-5,8-dimethyldodecahydro-1H,3H-pyrrolo[1,2-q][1,4,7,10,13,17]oxapentaazacyclononadecine-1,4,7,10,13,17(14H)-hexone</b>	215.19955
<b>w/o MS2:Myriocin</b>	206.633892
<b>w/o MS2:Sodium chlorate</b>	153.454425
<b>w/o MS2:.beta.-D-Glucopyranosyl 6-O-(8-methylnonanoyl)-.beta.-D-glucopyranoside</b>	151.205276
<b>w/o MS2:1,2-Dipentadecanoyl-sn-glycero-3-phosphoethanolamine</b>	118.120242
<b>w/o MS2:o-Tolidine</b>	108.246643
<b>w/o MS2:Dichlorvos</b>	107.483995
<b>w/o MS2:1,2-Dipalmitoyl-rac-glycero-3-phospho-L-serine</b>	105.458354
<b>w/o MS2:4-Methyl-2-[4-(trifluoromethyl)phenyl]-1,3-thiazole-5-carboxylic acid</b>	103.864559
<b>w/o MS2:1H-Indole-1-pentanoic acid, 3-[[[1-(aminocarbonyl)-2,2-dimethylpropyl]amino]carbonyl]-</b>	77.822727
<b>w/o MS2:Phytic acid</b>	67.990547
<b>w/o MS2:5-Butyl-8,8-dimethyl-3,6,8,9-tetrahydropyrazolo[3,4-b]thiopyrano[4,3-d]pyridin-1-amine</b>	66.528498

ser\_m1 dab: down reg, end up down reg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:5-Heptenoic acid, 7-[(1R,2R,3S,5S)-2-[(1E,3S)-3-(2,3-dihydro-1H-inden-2-yl)-3-hydroxy-1-propen-1-yl]-3-fluoro-5-hydroxycyclopentyl]-, (5Z)-</b>	-702.622404
<b>w/o MS2:NCGC00380745-01!(5E)-2-heptyl-3,4,7-trihydroxy-2,3,4,7,8,9-hexahydrooxecin-10-one</b>	-404.868089
<b>w/o MS2:Vinblastine</b>	-269.366302
<b>w/o MS2:D-Glucosamine, 6-sulfate</b>	-202.920262
<b>w/o MS2:[(3R,4S,8S,8aS)-3-Hydroxy-6,8a-dimethyl-8-[(Z)-2-methylbut-2-enoyl]oxy-3-propan-2-yl-1,2,3a,4,5,8-hexahydroazulen-4-yl] 4-hydroxybenzoate</b>	-193.136202
<b>w/o MS2:NCGC00385080-01!4-[(E)-3-[(2R,3R,4S,5S,6R)-3-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one</b>	-162.524912
<b>w/o MS2:cis-Nerolidol</b>	-155.164679
<b>w/o MS2:17-Epioxandrolone</b>	-144.093736
<b>w/o MS2:Destruxin A</b>	-143.19074
<b>w/o MS2:Flucythrinate</b>	-142.727588
<b>w/o MS2:4-Amino-4-methylpentanoic acid</b>	-128.950767
<b>w/o MS2:NCGC00180529-03!(3S,6R,9S,12R,15S,18R)-4,10,16-trimethyl-3,6,9,12,15,18-hexa(propan-2-yl)-1,7,13-trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone</b>	-107.564517
<b>w/o MS2:3,6,9,12,15-Pentaoxaheptacosan-1-ol, hydrogen sulfate</b>	-98.870952
<b>w/o MS2:Buprenorphine-d4</b>	-91.950524
<b>w/o MS2:MLS00222329-01!26305-03-3</b>	-89.453526

cec\_m2 for dss: up reg by treatment, end up upreg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:Met-Val-Lys</b>	5991.319409

w/o MS2:(Z)-Dimethylvinphos	665.327473
w/o MS2:SLPEAGPGRTLVSSKPQAHGAPAPPSGSAPHFL/5	516.920137
w/o MS2:Pheophorbide a	410.626533
w/o MS2:2-[(2E,6E,10E)-14,15-Dihydroxy-3,7,11,15-tetramethylhexadeca-2,6,10-trienyl]-2,4,6,9-tetrahydroxy-5,7-dimethylphenalene-1,3-dione	319.9354
w/o MS2:Leukotriene D4 methyl ester	285.484615
w/o MS2:Arg-Gln	221.237292
w/o MS2:(3S)-1-Azabicyclo[2.2.2]octan-3-amine	207.253698
w/o MS2:Neoruscogenin	170.752439
w/o MS2:Mononervonin (15c)	160.473342
w/o MS2:DL-2,4-Diaminobutyric acid	156.081164
w/o MS2:NCGC00169462-02!17-(2,6-dihydroxy-6-methyl-3-oxoheptan-2-yl)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,2,3,7,8,10,12,15,16,17-decahydrocyclopenta[a]phenanthren-11-one	135.502567
w/o MS2:2-[[4-(Dipentylamino)-2-hydroxyphenyl]carbonyl]benzoic acid	130.618682
w/o MS2:Iromycin A	124.479563
w/o MS2:9-Nitrooleic acid	101.206245

cec\_m2 dss: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Pimecrolimus	-74498.18412
w/o MS2:1-Piperidinecarboxylic acid, 4-(aminomethyl)-4-fluoro-, 1,1-dimethylethyl ester	-1607.503832
w/o MS2:N-(Phenylacetyl)urea	-460.471644
w/o MS2:2-Methoxy-4-((1R,2S,4R,6S)-5,5,6-trimethylbicyclo[2.2.1]heptan-2-yl)phenol	-417.313379
w/o MS2:Jasplakinolide	-409.379716
w/o MS2:Benzenemethanaminium, N-cyclopentyl-N,N-dimethyl-3,4-bis(tetradecyloxy)-	-333.192173
w/o MS2:Tocainide	-313.375208
w/o MS2:1-Palmitoyl-2-(4-ketododec-3-enedioyl)phosphatidylcholine	-288.515325
w/o MS2:Flecainide	-215.470377
w/o MS2:1-(4-Bromophenyl)-5-oxo-3-pyrrolidinecarboxylic acid	-214.085072
w/o MS2:NCGC00384824-01!methyl 3-hydroxy-2-[[3-hydroxy-2-[[2-[(3-hydroxy-2,4-dimethyltetradecanoyl)amino]-3-methylbutanoyl]amino]butanoyl]amino]propanoate	-167.60698
w/o MS2:NCGC00380884-01!(2S,3R,10R,13R,14S)-2,3,14-trihydroxy-10,13-dimethyl-17-[(2R,3R,5R)-2,3,5-trihydroxy-5,6-dimethylheptan-2-yl]-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	-165.095503
w/o MS2:Vaccinoside	-153.903559
w/o MS2:13-(Dodecan-2-yl)-6-(1-hydroxyethyl)-3-(hydroxymethyl)-12-methyl-9-(propan-2-yl)-1-oxa-4,7,10-triazacyclotridecane-2,5,8,11-tetrone	-129.514724
w/o MS2:Mildronate	-125.496385

cec\_m2 for dss: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:3-(.alpha.-L-Arabinofuranosyloxy)pimara-8(14),15-dien-12-yl 6-deoxy-.beta.-D-galactopyranoside	4149.888498
w/o MS2:Finasteridecarboxylic acid	2571.298343
w/o MS2:Inosine 5'-triphosphate	2448.760647
w/o MS2:Digoxigenin monodigitoxoside	1956.841144
w/o MS2:L-Arachidonoylcarnitine	587.01978
w/o MS2:8,14-Epoxy-3-hydroxycarda-16,20(22)-dienolide triglycoside	455.557495
w/o MS2:Lansoprazole	425.398895
w/o MS2:2-(4-Chlorobenzenesulfinyl)acetic acid	264.800371
w/o MS2:N-(2-Adamantyl)-N'-butylthiourea	254.542248

w/o MS2:Minaprine	202.377253
w/o MS2:Eugenol gentiobioside	193.526624
w/o MS2:(1S)-1,5-Anhydro-6-O-(6-deoxy-.alpha.-L-mannopyranosyl)-1-((2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-6-yl)-D-glucitol	192.922191
w/o MS2:Dovitinib	188.218113
w/o MS2:N-(Cyclopropylmethyl)-1-(5-fluoropentyl)-1H-indole-3-carboxamide	140.329068
w/o MS2:Cabergoline	115.010201

cec\_m2 dss: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:NCGC00384803-01!2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	-40624.124004
w/o MS2:(3.beta.,5.Xi.,8.alpha.,9.beta.,10.alpha.,16.beta.)-16-Hydroxykauran-3-yl .beta.-D-glucopyranoside	-1167.238241
w/o MS2:Bazedoxifene	-650.937658
w/o MS2:2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphoserine	-592.677544
w/o MS2:NCGC00380113-01!2,3,14-trihydroxy-10,13-dimethyl-17-(2,3,6,7-tetrahydroxy-5,6-dimethylheptan-2-yl)-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	-485.519343
w/o MS2:Tyr-Tyr-Tyr	-443.990548
w/o MS2:1,1,3-Tris(2-methyl-4-hydroxy-5-tert-butylphenyl)butane	-310.153569
w/o MS2:NCGC00385651-01_C23H32O7_	-281.954448
w/o MS2:1-Oleoyl-sn-glycero-3-phosphocholine	-260.228993
w/o MS2:13-Acetyl-9-dihydrobaccatin III	-243.135921
w/o MS2:G0-3Ac a	-219.931706
w/o MS2:2-Methylbutyryl-L-carnitine	-167.575472
w/o MS2:GB 1a	-165.655282
w/o MS2:[(1S)-1-[[[(7-Bromo-1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny]methyl]amino]ethyl]phosphonic acid	-143.437024
w/o MS2:N1-Acetylspermine	-116.852987

cec\_m2 for ab: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Specnuezhenide	1005.157487
w/o MS2:Pinoxaden	476.719758
w/o MS2:NCGC00380734-01_C39H65NO10_2-{6-[5-Hydroxy-3-(2-hydroxy-2-propanyl)-6a,9b-dimethyldodecahydrocyclopenta[f]chromen-7-yl]-4a-methyl-3,4,4a,7,8,8a-hexahydro-2H-chromen-2-yl}-2-propanyl 2-acetamido-2-deoxy-6-O-methylhexopyranoside	429.964264
w/o MS2:Phosphatidylethanolamine alkenyl 18:0-20:0	371.4594
w/o MS2:N-(6-Amino-1-butyl-2,4-dioxo-1,2,3,4-tetrahydro-5-pyrimidinyl)-N-methylbenzamide	367.437459
w/o MS2:2-[[[4-(Dipentylamino)-2-hydroxyphenyl]carbonyl]benzoic acid	206.70939
w/o MS2:Atovaquone	204.354603
w/o MS2:Octanoic acid, 4-[(1-oxo-7-phenylheptyl)amino]-, (4R)-	192.441438
w/o MS2:(3.beta.,8.xi.,9.xi.,12.beta.,14.beta.)-11,12,14-Trihydroxy-20-oxopregn-5-en-3-yl 6-deoxyhexopyranosyl-(1->4)-2,6-dideoxy-3-O-methylhexopyranosyl-(1->4)-2,6-dideoxy-3-O-methylhexopyranoside	177.898126
w/o MS2:Bisphenol M	175.539574
w/o MS2:Timosaponin B II	171.301991
w/o MS2:Curine	158.096032
w/o MS2:EADPTGHSY/-2	153.570317
w/o MS2:Sodium 2,2'-methylene bis(4,6-di-tert-butylphenyl) phosphate	129.69979
w/o MS2:Glycyl-L-norleucine	125.259156

cec\_m2 ab: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Pimecrolimus	-74498.45279
w/o MS2:(3.beta.,5.Xi.,8.alpha.,9.beta.,10.alpha.,16.beta.)-16-Hydroxykauran-3-yl .beta.-D-glucopyranoside	-1178.852456
w/o MS2:Bazedoxifene	-654.699967
w/o MS2:2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphoserine	-592.055971
w/o MS2:NCGC00380113-01!2,3,14-trihydroxy-10,13-dimethyl-17-(2,3,6,7-tetrahydroxy-5,6-dimethylheptan-2-yl)-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	-486.824187
w/o MS2:2-Methoxy-4-((1R,2S,4R,6S)-5,5,6-trimethylbicyclo[2.2.1]heptan-2-yl)phenol	-415.760879
w/o MS2:Benzenemethanaminium, N-cyclopentyl-N,N-dimethyl-3,4-bis(tetradecyloxy)-	-331.274812
w/o MS2:Tocainide	-316.90667
w/o MS2:1,1,3-Tris(2-methyl-4-hydroxy-5-tert-butylphenyl)butane	-315.602531
w/o MS2:1-Palmitoyl-2-(4-ketododec-3-enedioyl)phosphatidylcholine	-281.095405
w/o MS2:NCGC00385651-01_C23H32O7_	-278.295671
w/o MS2:1-Oleoyl-sn-glycero-3-phosphocholine	-249.606409
w/o MS2:13-Acetyl-9-dihydrobaccatin III	-241.984731
w/o MS2:G0-3Ac a	-219.537784
w/o MS2:1-(4-Bromophenyl)-5-oxo-3-pyrrolidinecarboxylic acid	-216.29644

cec\_m2 for ab: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:NOSCAPINE	9426.411783
w/o MS2:Undecapropylene glycol monobutyl ether	8683.741087
w/o MS2:9-Deoxy-9-methylene-16,16-dimethylprostaglandin E2	4524.823042
w/o MS2:1H-Indazole-3-carboxamide, N-[(1S)-1-(aminocarbonyl)-2-methylpropyl]-1-pentyl-	3318.489744
w/o MS2:Perfluorooctanoic acid	741.534743
w/o MS2:Benzoylecgonine-d3	433.176551
w/o MS2:Gossypetin 3,3',8-trimethylether	383.588342
w/o MS2:1H-Indazole-3-carboxamide, N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-(4-hydroxypentyl)-	323.778867
w/o MS2:PNTCEICAYAACTGC/2	303.158515
w/o MS2:3,6,8-Tribromo-7-hydroxy-4-methyl-2H-chromen-2-one	267.213536
w/o MS2:Phosphatidylcholine alkyl 16:0-16:0	250.137168
w/o MS2:LVFFAEDVGSNK/1	217.41558
w/o MS2:Ile-Ile	183.885332
w/o MS2:Acarbose	148.24263
w/o MS2:Sphingomyelin d18:1-C22:1	145.555603

cec\_m2 ab: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:NCGC00384803-01!2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	-40627.53753
w/o MS2:1-Piperidinecarboxylic acid, 4-(aminomethyl)-4-fluoro-, 1,1-dimethylethyl ester	-1597.401787
w/o MS2:N-(Phenylacetyl)urea	-461.994149
w/o MS2:Tyr-Tyr-Tyr	-439.408845
w/o MS2:Jasplakinolide	-410.45643
w/o MS2:NCGC00384824-01!methyl 3-hydroxy-2-[[3-hydroxy-2-[[2-[(3-hydroxy-2,4-dimethyltetradecanoyl)amino]-3-methylbutanoyl]amino]butanoyl]amino]propanoate	-170.725797
w/o MS2:2-Methylbutyryl-L-carnitine	-167.627615
w/o MS2:GB 1a	-165.014896



<b>w/o MS2:[(1S)-1-[[[(7-Bromo-1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny)methyl]amino]ethyl]phosphonic acid</b>	-158.168909
<b>w/o MS2:Vaccinoside</b>	-153.962064
<b>w/o MS2:13-(Dodecan-2-yl)-6-(1-hydroxyethyl)-3-(hydroxymethyl)-12-methyl-9-(propan-2-yl)-1-oxa-4,7,10-triazacyclotridecane-2,5,8,11-tetrone</b>	-127.774454
<b>w/o MS2:Mildronate</b>	-124.797699
<b>w/o MS2:6-Sialylgalactose</b>	-107.077863
<b>w/o MS2:N1-Acetylspermine</b>	-103.446774
<b>w/o MS2:Butalamine</b>	-93.339519

cec\_m2 for dab: up reg by treatment, end up upreg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:3,7,13,17-O-Tetraacetyl-5-O-(2-methylbutyryl)-14-oxopremyrsinol</b>	1618.451418
<b>w/o MS2:Specnuezhenide</b>	1209.933257
<b>w/o MS2:Nicotine N-.beta.-D-glucuronide</b>	542.389133
<b>w/o MS2:Okaramine B</b>	287.789491
<b>w/o MS2:Phosphatidylcholine 16:1-20:5</b>	278.129247
<b>w/o MS2:n-Octylpentaoxyethylene</b>	277.340316
<b>w/o MS2:NCGC00381019-01_C33H40O10_1H-Cyclopentacyclododecene-4,10(2H,5H)-dione, 3a,9,13-tris(acetyloxy)-1-(benzoyloxy)-3,3a,8,9,13,13a-hexahydro-2,5,8,8,12-pentamethyl-, (6E,11E)-</b>	263.269971
<b>w/o MS2:Phosphatidylcholine lyso 18:1</b>	243.987145
<b>w/o MS2:Rhaponticin</b>	242.809331
<b>w/o MS2:WTVPTA/1</b>	230.447376
<b>w/o MS2:Myriocin</b>	218.825029
<b>w/o MS2:YGGFLRRIRPKLKWDNQ/3</b>	205.010401
<b>w/o MS2:Scillaren A</b>	191.010411
<b>w/o MS2:13,14-Dihydro-15-ketotetranorprostaglandin D2</b>	177.249127
<b>w/o MS2:Curine</b>	144.705224

cec\_m2 dab: down reg by treatment, end up upreg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:1-Piperidinecarboxylic acid, 4-(aminomethyl)-4-fluoro-, 1,1-dimethylethyl ester</b>	-1607.975054
<b>w/o MS2:(3.beta.,5.Xi.,8.alpha.,9.beta.,10.alpha.,16.beta.)-16-Hydroxykauran-3-yl .beta.-D-glucopyranoside</b>	-1179.435968
<b>w/o MS2:Bazedoxifene</b>	-653.800857
<b>w/o MS2:NCGC00380113-0112,3,14-trihydroxy-10,13-dimethyl-17-(2,3,6,7-tetrahydroxy-5,6-dimethylheptan-2-yl)-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one</b>	-486.724539
<b>w/o MS2:N-(Phenylacetyl)urea</b>	-450.883151
<b>w/o MS2:1,1,3-Tris(2-methyl-4-hydroxy-5-tert-butylphenyl)butane</b>	-316.817085
<b>w/o MS2:1-Palmitoyl-2-(4-ketododec-3-enedioyl)phosphatidylcholine</b>	-287.913155
<b>w/o MS2:Tocainide</b>	-277.096203
<b>w/o MS2:1-Oleoyle-sn-glycero-3-phosphocholine</b>	-261.104966
<b>w/o MS2:13-Acetyl-9-dihydrobaccatin III</b>	-243.034982
<b>w/o MS2:2-Methylbutyryl-L-carnitine</b>	-166.977549
<b>w/o MS2:NCGC00380884-01!(2S,3R,10R,13R,14S)-2,3,14-trihydroxy-10,13-dimethyl-17-[(2R,3R,5R)-2,3,5-trihydroxy-5,6-dimethylheptan-2-yl]-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one</b>	-166.707713
<b>w/o MS2:[(1S)-1-[[[(7-Bromo-1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny)methyl]amino]ethyl]phosphonic acid</b>	-145.844598
<b>w/o MS2:Sodium nitrate</b>	-130.149643
<b>w/o MS2:13-(Dodecan-2-yl)-6-(1-hydroxyethyl)-3-(hydroxymethyl)-12-methyl-9-(propan-2-yl)-1-oxa-4,7,10-triazacyclotridecane-2,5,8,11-tetrone</b>	-126.268347

cec\_m2 for dab: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:pGlu-Glu-Pro-amide	34479.060124
w/o MS2:Geraniol	7256.076018
w/o MS2:6-[(3,5-Dimethyl-1-piperidinyl)methyl]-N2,N2-dimethyl-1,3,5-triazine-2,4-diamine	7208.810303
w/o MS2:3-[(4-Bromo-2-chlorophenoxy)methyl]-4-methoxybenzaldehyde	3686.765194
w/o MS2:KRPPGFSPFR/3	1930.444467
w/o MS2:4-(Bromomethyl)-2(1H)-quinolinone	1788.287644
w/o MS2:Methanol	795.760535
w/o MS2:1-Piperidinecarboxylic acid, 4-[6-[4-[(methoxycarbonyl)amino]phenyl]-4-(4-morpholinyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-, methyl ester	728.714015
w/o MS2:Benzeneacetamide, N-[(1S)-2-[[[(3S)-2,3-dihydro-1-methyl-2-oxo-5-phenyl-1H-1,4-benzodiazepin-3-yl]amino]-1-methyl-2-oxoethyl]-3,5-difluoro-	544.108441
w/o MS2:15-Deoxy-.DELTA.12,14-prostaglandin J2 glutathione	535.398551
w/o MS2:NCGC00380799-01!5-[5-[5-(3,5-dihydroxydecanoyloxy)-3-hydroxydecanoyl]oxy-3-hydroxydecanoyl]oxy-3-hydroxydecanoic acid	485.575505
w/o MS2:Tuberonic acid glucoside	346.003152
w/o MS2:3-[(3-Nitroanilino)carbonyl]-2-naphthyl dihydrogen phosphate	327.889189
w/o MS2:5-Bromo-2-[[[(2,4-dichlorophenoxy)acetyl]amino]benzoic acid	243.536997
w/o MS2:N-Acetylphenylalanyl-2-methylalanyl-2-methylalanyl-2-methylalanylvalylglycylleucyl-2-methylalanyl-2-methylalanyl-4-hydroxyprolylglutaminy-2-methylalanyl-4-hydroxyprolyl-N-(1-hydroxy-3-phenylpropan-2-yl)-2-methylalaninamide	194.977029

cec\_m2 dab: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:Pimecrolimus	-74489.71903
w/o MS2:NCGC00384803-01!2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	-40627.061946
w/o MS2:2-Oleo-1-palmitoyl-sn-glycero-3-phosphoserine	-591.936825
w/o MS2:Tyr-Tyr-Tyr	-421.984654
w/o MS2:2-Methoxy-4-((1R,2S,4R,6S)-5,5,6-trimethylbicyclo[2.2.1]heptan-2-yl)phenol	-418.651931
w/o MS2:Jasplakinolide	-409.453812
w/o MS2:Benzenemethanaminium, N-cyclopentyl-N,N-dimethyl-3,4-bis(tetradecyloxy)-	-324.923662
w/o MS2:NCGC00385651-01_C23H32O7_	-281.783232
w/o MS2:Flecainide	-215.148701
w/o MS2:1-(4-Bromophenyl)-5-oxo-3-pyrrolidinecarboxylic acid	-213.797485
w/o MS2:NCGC00384824-01!methyl 3-hydroxy-2-[[3-hydroxy-2-[[2-[(3-hydroxy-2,4-dimethyltetradecanoyl)amino]-3-methylbutanoyl]amino]butanoyl]amino]propanoate	-163.829459
w/o MS2:G0-3Ac a	-151.230516
w/o MS2:Vaccinoside	-141.842812
w/o MS2:GB 1a	-139.363727
w/o MS2:Mildronate	-126.257599

ser\_m2 for dss: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Gly-Pro-Arg-Pro-amide	912.796463
w/o MS2:N-Cyclohexyl-1-pyrrolidinecarboxamide	540.93536
w/o MS2:Neoandrographolide	416.180958
w/o MS2:Benamide, N-(5Z,8Z,11Z,14Z)-5,8,11,14-eicosatetraen-1-yl-4-hydroxy-	327.65645
w/o MS2:4-Quinolinol, 6-bromo-2-(trifluoromethyl)-	266.728019

w/o MS2:Oleamide	228.8319
w/o MS2:Butanoic acid, 4-(2,4-dichlorophenoxy)-	214.331487
w/o MS2:1-Butanol, 2-[[9-(1-methylethyl)-6-[[[4-(2-pyridinyl)phenyl]methyl]amino]-9H-purin-2-yl]amino]-, (2R)-	210.040203
w/o MS2:N-Isovaleroylglycine	191.643186
w/o MS2:Cholesteryl acetate	185.273573
w/o MS2:Man3F	172.151415
w/o MS2:cis-5-Dodecenoic acid	160.001545
w/o MS2:(17E)-3-((2-O-Hexopyranosylhexopyranosyl)oxy)-14-hydroxycard-17-enolide	134.467135
w/o MS2:Estrone	131.407092
w/o MS2:TFLLR/2	126.737729

ser\_m2 dss: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Oligomycin A	-38709.641107
w/o MS2:Carbamic acid, [3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-, 2-[[[(5Z,8Z,11Z,14Z)-1-oxo-5,8,11,14-eicosatetraenyl]amino]ethyl ester	-3315.525127
w/o MS2:Phytic acid	-2071.344514
w/o MS2:Glycocholic acid	-1358.739088
w/o MS2:5-Bromo-2-hydroxynicotinic acid	-772.253093
w/o MS2:Pimecrolimus	-404.240614
w/o MS2:Allantoic acid	-391.715282
w/o MS2:Benzoic acid, 4-hydroxy-3-[[[2-(4-tricyclo[3.3.1.1(3,7)]dec-1-ylphenoxy)acetyl]amino]-, methyl ester	-264.548817
w/o MS2:FAHFA 32:1	-227.573324
w/o MS2:Peimisine	-199.445349
w/o MS2:5-(N-Ethyl-N-isopropyl)amiloride	-183.139757
w/o MS2:cis-5,8,11,14-Eicosatetraenoic acid	-176.212
w/o MS2:D-myo-Inositol-1,2,6-triphosphate	-160.870907
w/o MS2:Thromboxane B2	-149.332125
w/o MS2:Cinnarizine	-136.311406

ser\_m2 for dss: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:Ile-Trp-Lys	2106.946004
w/o MS2:1-Oleoyl-2-acetyl-sn-glycerol	1085.697034
w/o MS2:1-Palmitoyl-sn-glycero-3-phosphocholine	559.719698
w/o MS2:Methyl 3-(acetyloxy)-16-hydroxy-4,4,8,12,16-pentamethyl-15,17-dioxoandrost-11-ene-14-carboxylate	506.112556
w/o MS2:Antibiotic JM 971B	435.145397
w/o MS2:2,4,6-Tribromo-3-(trifluoromethyl)phenol	264.465011
w/o MS2:2,4,6-Trihydroxy-5-[1-(4-hydroxy-1,1,4,7-tetramethyl-1a,2,3,4a,5,6,7a,7b-octahydrocyclopropa[h]azulen-7-yl)-3-methylbutyl]benzene-1,3-dicarbaldehyde	140.941795
w/o MS2:3'S diLN	140.327353
w/o MS2:(3.beta.,5.Xi.,9.Xi.,16.beta.)-28-(.beta.-D-Glucopyranosyloxy)-16-hydroxyolean-12-en-3-yl .beta.-D-xylopyranosyl-(1->6)-.beta.-D-glucopyranosyl-(1->6)-.beta.-D-glucopyranoside	135.369316
w/o MS2:L-Cysteine S-sulfate	128.928681
w/o MS2:Desferrioxamine E	124.642862
w/o MS2:RKDVY/1	118.442313
w/o MS2:2-(1-Piperazinyl)quinoline	112.175588
w/o MS2:Halosulfuron-methyl	106.266171
w/o MS2:Arg-Arg	99.823294

ser\_m2 dss: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:1H-Indazole-3-carboxamide, N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl-	-16448.713231
w/o MS2:N-(Cyclohexylmethyl)-3-(4-morpholinyl)-1-propanamine	-706.727316
w/o MS2:Hematoporphyrin	-353.316369
w/o MS2:6-Deoxy-2-O-((3.Xi.)-6-deoxy-3-O-((2S,3R,4R)-3-(.beta.-D-glucopyranosyloxy)-4-hydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.alpha.-L-arabino-hexopyranosyl)-1-O-(3-(.beta.-D-glucopyranuronosyloxy)-2,22,23-trihydroxy-23,28-dioxolean-12-en-28-yl)-.beta.-D-glucopyranose	-274.86092
w/o MS2:L-Lysine	-262.223226
w/o MS2:Virginiamycin component a	-250.866019
w/o MS2:Geranyl pyrophosphate	-194.718482
w/o MS2:N-(2-Chloro-4-nitrophenyl)acetamide	-177.563199
w/o MS2:Sclareolide	-134.627618
w/o MS2:1,2-Dilinolenoyl-sn-glycero-3-phosphoethanolamine	-128.61367
w/o MS2:Tolytoxin	-84.593572
w/o MS2:Caylin-1	-61.788081
w/o MS2:Aniline	-58.846709
w/o MS2:Benzenesulfonamide, 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]-	-48.929033
w/o MS2:Phosphatidylcholine 16:0-22:6	-43.946961

ser\_m2 for ab: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Taurocholic acid	736.46746
w/o MS2:4-(3-Bromo-4-methoxyphenyl)-1,3-thiazol-2-ylamine	245.726279
w/o MS2:Dichlorphenamide	229.852226
w/o MS2:4-Bromo-2,6-dinitrobenzoic Acid	225.278334
w/o MS2:Bis(1,2,2,6,6-pentamethyl-4-piperidyl)sebacate	208.399877
w/o MS2:3-Hydroxy-2',3',5',6'-tetrachlorobiphenyl	167.792508
w/o MS2:6-Aminosaccharin	133.275302
w/o MS2:Benzoic acid, 3-[(3-methoxybenzoyl)amino]-4-(4-methyl-1-piperazinyl)-, methyl ester	108.583614
w/o MS2:Trp(Dioxidation)-Trp(Dioxidation)-Arg	103.796815
w/o MS2:Glu-Pro-Arg	71.695257
w/o MS2:Gln-Gln	71.375393
w/o MS2:Psychosine	65.491253
w/o MS2:Fasciculic acid D	64.807785
w/o MS2:3,5-Diiodo-L-thyronine	60.486974
w/o MS2:NCGC00384608-01_C41H66O12_4,13,22,31,37,38,39,40-Octaoxapentacyclo[32.2.1.1~7,10~.1~16,19~.1~25,28~]tetracontane-3,12,21,30-tetrone, 5-ethyl-2,11,14,20,23,29,32-heptamethyl-, (1R,2R,5R,7R,10S,11S,14S,16S,19R,20R,23R,25R,28S,29S,32S,34S)-	56.229436

ser\_m2 ab: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Carbamic acid, [3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-, 2-[[[(5Z,8Z,11Z,14Z)-1-oxo-5,8,11,14-eicosatetraenyl]amino]ethyl ester	-3316.611687
w/o MS2:Phytic acid	-2069.589299
w/o MS2:Glycocholic acid	-1358.628243
w/o MS2:Hematoporphyrin	-348.609412
w/o MS2:L-Lysine	-263.494824

w/o MS2:Virginiamycin component a	-254.482974
w/o MS2:Geranyl pyrophosphate	-195.684417
w/o MS2:Gly-Pro-Arg-Pro-amide	-194.530638
w/o MS2:D-myo-Inositol-1,2,6-triphosphate	-162.730454
w/o MS2:Thromboxane B2	-149.153299
w/o MS2:Cinnarizine	-134.565729
w/o MS2:1,2-Dilinolenoyl-sn-glycero-3-phosphoethanolamine	-126.215101
w/o MS2:Norfloxacin	-105.576067
w/o MS2:1,2-Dimyristoyl-sn-glycero-3-phosphate	-94.637971
w/o MS2:Glu-Lys-Lys	-81.467903

ser\_m2 for ab: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:13S-Hydroxy-9Z,11E-octadecadiene-(2-biotinyl)hydrazide	712.901341
w/o MS2:Spiculisporic acid	493.729346
w/o MS2:N-(Octadecanoyl)sphing-4-enine-1-phosphocholine	393.179004
w/o MS2:N-Cyclohexyl-N'-cyclooctylurea	333.025524
w/o MS2:6,12-Dimethoxy-7a-(2-methylbut-3-en-2-yl)-3-(propan-2-yl)-7a,12-dihydro-1H,5H-imidazo[1',2':1,2]pyrido[2,3-b]indole-2,5(3H)-dione	304.462812
w/o MS2:Strophantidin	232.782851
w/o MS2:p-tert-Octylphenol nonaglycol ether	199.191027
w/o MS2:2-(5-Oxovaleryl)phosphatidylcholine	195.833912
w/o MS2:Veratroylzygadenin	186.224347
w/o MS2:Progesterone 3-PEG11-biotin	173.495543
w/o MS2:Phosphoric acid	163.146636
w/o MS2:INLKALAALAKKIL/3	161.308508
w/o MS2:2,6-Di-tert-butyl-4-methoxyphenol	132.42187
w/o MS2:3-(4-Bromophenyl)-.beta.-alanine	98.442714
w/o MS2:p-tert-Octylphenol decaglycol ether	96.547381

ser\_m2 ab: down reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:Oligomycin A	-38720.080237
w/o MS2:1H-Indazole-3-carboxamide, N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl-	-16475.392586
w/o MS2:N-(Cyclohexylmethyl)-3-(4-morpholinyl)-1-propanamine	-1509.428677
w/o MS2:5-Bromo-2-hydroxynicotinic acid	-751.954382
w/o MS2:Pimecrolimus	-402.273834
w/o MS2:Allantoic acid	-392.097865
w/o MS2:6-Deoxy-2-O-((3.Xi.)-6-deoxy-3-O-((2S,3R,4R)-3-(.beta.-D-glucopyranosyloxy)-4-hydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.alpha.-L-arabino-hexopyranosyl)-1-O-(3-(.beta.-D-glucopyranuronosyloxy)-2,22,23-trihydroxy-23,28-dioxoolean-12-en-28-yl)-.beta.-D-glucopyranose	-279.534897
w/o MS2:Benzoic acid, 4-hydroxy-3-[[2-(4-(tricyclo[3.3.1.1(3,7)]dec-1-ylphenoxy)acetyl]amino]-, methyl ester	-264.735962
w/o MS2:FAHFA 32:1	-227.537132
w/o MS2:Peimisine	-200.504479
w/o MS2:5-(N-Ethyl-N-isopropyl)amiloride	-183.105556
w/o MS2:N-(2-Chloro-4-nitrophenyl)acetamide	-176.472557
w/o MS2:Sclareolide	-162.226972
w/o MS2:cis-5,8,11,14-Eicosatetraenoic acid	-159.756824
w/o MS2:FAHFA 37:1	-102.1519



ser\_m2 for dab: up reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Bohemine	3511.932337
w/o MS2:1H-Indole-3-carboxylic acid, 1-(4-hydroxypentyl)-, 8-quinolinyl ester	1387.230274
w/o MS2:Etodolac	1047.058265
w/o MS2:Yohimbic acid	221.57716
w/o MS2:4,5-Dihydroxynaphthalene-2,7-disulfonic acid	193.887633
w/o MS2:NCGC00380213-01_C19H32O8_2-Butanone, 4-[3-(beta-D-glucopyranosyloxy)-4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-	155.023743
w/o MS2:Hepcinat	146.231721
w/o MS2:Erythromycin, 12-deoxy-	139.156585
w/o MS2:Hymeglusin	131.357502
w/o MS2:13-(Dodecan-2-yl)-6-(1-hydroxyethyl)-3-(hydroxymethyl)-12-methyl-9-(propan-2-yl)-1-oxa-4,7,10-triazacyclotridecane-2,5,8,11-tetrone	131.236257
w/o MS2:Geldanamycin, 17-demethoxy-17-[[2-(dimethylamino)ethyl]amino]-	93.151165
w/o MS2:2,4-Bis(1,1-dimethylethyl)phenol phosphate	83.24853
w/o MS2:1-Stearoyl-2-arachidonyl-sn-glycero-3-phosphocholine	74.339199
w/o MS2:5-Sulfosalicylic acid	72.612338
w/o MS2:Methanone, [1-(hexahydro-1-methyl-1H-azepin-3-yl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)-	55.831801

ser\_m2 dab: down reg by treatment, end up upreg

	convexity
Metabolite Name	
w/o MS2:Oligomycin A	-38712.021123
w/o MS2:Carbamic acid, [3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-, 2-[[[(5Z,8Z,11Z,14Z)-1-oxo-5,8,11,14-eicosatetraenyl]amino]ethyl ester	-3310.15202
w/o MS2:Phytic acid	-2071.923864
w/o MS2:Glycocholic acid	-1352.342731
w/o MS2:5-Bromo-2-hydroxynicotinic acid	-772.408531
w/o MS2:Pimecrolimus	-405.105522
w/o MS2:Allantoic acid	-391.716562
w/o MS2:6-Deoxy-2-O-((3.Xi.)-6-deoxy-3-O-((2S,3R,4R)-3-(.beta.-D-glucopyranosyloxy)-4-hydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.alpha.-L-arabino-hexopyranosyl)-1-O-(3-(.beta.-D-glucopyranuronosyloxy)-2,22,23-trihydroxy-23,28-dioxoolean-12-en-28-yl)-.beta.-D-glucopyranose	-278.070455
w/o MS2:Virginiamycin component a	-253.182647
w/o MS2:FAHFA 32:1	-226.790118
w/o MS2:Peimisine	-200.5196
w/o MS2:N-(2-Chloro-4-nitrophenyl)acetamide	-177.404063
w/o MS2:cis-5,8,11,14-Eicosatetraenoic acid	-177.208927
w/o MS2:Sclareolide	-160.222063
w/o MS2:D-myo-Inositol-1,2,6-triphosphate	-159.895017

ser\_m2 for dab: up reg, end up down reg

	convexity
Metabolite Name	
w/o MS2:NCGC00384618-01_C33H50O10_(1beta,3beta,9xi,11alpha,14xi)-1,3,11-Trihydroxyfurosta-5,20(22),25-trien-27-yl beta-D-glucopyranoside	274.476519
w/o MS2:Estrone	265.956179
w/o MS2:[(2-Bromobenzoyl)amino]acetic acid	163.773252
w/o MS2:1-Oleoyl-2-acetyl-sn-glycerol	127.997515
w/o MS2:Suramin	93.952243

<b>w/o MS2:(2E)-3-(4-Bromothiophen-2-yl)prop-2-enoic acid</b>	93.06021
<b>w/o MS2:.alpha.-Paxitriol</b>	89.580593
<b>w/o MS2:Dimepiperate</b>	77.709349
<b>w/o MS2:Irganox 1135</b>	73.126114
<b>w/o MS2:NCGC00380973-01_C21H30O6_</b>	65.991447
<b>w/o MS2:1-Tetrahydro-2H-pyran-4-yl-4-piperidinamine</b>	52.734139
<b>w/o MS2:INLKALAALAKKIL/3</b>	51.229236
<b>w/o MS2:Piperidine, 1-[3-[4-(1-piperidinylmethyl)phenoxy]propyl]-</b>	48.807469
<b>w/o MS2:Dronedarone</b>	38.563861
<b>w/o MS2:echinulin</b>	38.16222

ser\_m2 dab: down reg, end up down reg

	<b>convexity</b>
<b>Metabolite Name</b>	
<b>w/o MS2:1H-Indazole-3-carboxamide, N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl-</b>	-16494.508812
<b>w/o MS2:N-(Cyclohexylmethyl)-3-(4-morpholinyl)-1-propanamine</b>	-1510.624365
<b>w/o MS2:Hematoporphyrin</b>	-351.076206
<b>w/o MS2:Benzoic acid, 4-hydroxy-3-[[2-(4-tricyclo[3.3.1.1(3,7)]dec-1-ylphenoxy)acetyl]amino]-, methyl ester</b>	-264.386213
<b>w/o MS2:L-Lysine</b>	-236.513732
<b>w/o MS2:Gly-Pro-Arg-Pro-amide</b>	-199.614665
<b>w/o MS2:Geranyl pyrophosphate</b>	-194.770389
<b>w/o MS2:5-(N-Ethyl-N-isopropyl)amiloride</b>	-183.579415
<b>w/o MS2:3,5-di-tert-butyl-4-hydroxyacetophenone</b>	-85.887798
<b>w/o MS2:Glu-Lys-Lys</b>	-81.801064
<b>w/o MS2:Ethyl N-Boc-5-hydroxypiperidine-3-carboxylate</b>	-76.281759
<b>w/o MS2:8-Bromoadenosine-cyclic-monophosphate</b>	-73.506286
<b>w/o MS2:2-Amino-3,4,5,6-tetrachlorobenzoic acid</b>	-68.837185
<b>w/o MS2:Adonitol</b>	-63.495577
<b>w/o MS2:Caylin-1</b>	-60.548468