

Cluster 1.2 METLIN										Cluster 1.2 IMPaLA Enrichment			
All m/z values	m/z values	metlin ID	m/z	adduct	mass	ppm	name	chemical formula	pathway name	pathway source	number of overlapping	number of p value	
508.4023	508.4023	76663	802.5837	[M+H]	801.5884	14	PS(O)-16:0/22:4:4H8ANOPP		Insulin Metabolism Pathway	SMDB	1 51146-55-5	12 (13)	0.0025
802.5837	802.5837	76682	802.5837	[M+H]	801.5884	14	PS(O)-18:0/21:4:4H8ANOPP		Glucocorticoid & Mineralocorticoid Metabolism Pathway	Wikipedia	1 85-92-2	13 (13)	0.0035
218.918	218.918	78700	802.5837	[M+H]	801.5884	14	PS(O)-20:0/16:0:4H8ANOPP		alpha-Linolenic acid metabolism - H KEGG		1 6402-36-4	16 (42)	0.0066
88.52177	88.52177	78765	802.5837	[M+H]	801.5884	14	PS(P)-16:0/22:4:4H8ANOPP		Insulin Action Pathway	SMDB	1 51146-55-5	68 (79)	0.0693
218.9283	218.9283	78787	802.5837	[M+H]	801.5884	14	PS(P)-18:0/20:4:4H8ANOPP		Steroid hormone biosynthesis - H KEGG		1 85-92-2	85 (99)	0.0661
209.145	209.145	78808	802.5837	[M+H]	801.5884	14	PS(P)-20:0/18:0:4H8ANOPP		Biochemical Pathways Part I	Wikipedia	1 85-92-2	437 (467)	0.39
223.1317	223.1317	60999	802.5837	[M+H]	779.5829	14	FE(22:4/7Z,1C4)H8NO7P						
784.5483	784.5483	62195	802.5837	[M+H]	779.5829	14	FE(18:0/22:4)H8NO7P						
223.1629	223.1629	77563	802.5837	[M+H]	779.5829	14	FE(20:0/20:4)H8NO7P						
536.3304	536.3304	77663	802.5837	[M+H]	779.5829	14	FE(20:0/20:4)H8NO7P						
782.5333	782.5333	66568	218.9283	[M+Na]	217.9224	5	delta-1,4,5,6-C6H6O4						
91.9755	91.9755	691	223.1317	[M+H]	222.1256	5	Hydroxybutyrate C11H20O3				51146-55-5		
403.2775	403.2775	53571	223.1317	[M+H]	222.1256	5	(5S)-dehydro C11H20O3						
264.8452	264.8452	82704	223.1317	[M+H]	222.1256	5	Atenazone C11H20O3				211183-73-2		
403.2914	403.2914	91833	223.1317	[M+H]	222.1256	5	Dihydroxybutyrate C11H20O3				15764-81-5		
403.3054	403.3054	93513	223.1317	[M+H]	222.1256	5	Isomethyl pantoic C11H20O3				27739-29-3		
404.2908	404.2908	35681	223.1317	[M+H]	200.1412	5	2R-hydroxybutyrate C11H20O3						
256.825	256.825	35682	223.1317	[M+H]	200.1412	5	2S-hydroxybutyrate C11H20O3						
403.3194	403.3194	35728	223.1317	[M+H]	200.1412	5	Pelargonic acid C11H20O3						
404.3047	404.3047	35729	223.1317	[M+H]	200.1412	5	3-oxopentanoic acid C11H20O3						
680.5313	680.5313	35730	223.1317	[M+H]	200.1412	5	4-heptanoic acid C11H20O3				NA		
128.0661	128.0661	35731	223.1317	[M+H]	200.1412	5	8-pentenoic acid C11H20O3						
229.1405	229.1405	35732	223.1317	[M+H]	200.1412	5	9-oxopentanoic acid C11H20O3				NA		
560.3276	560.3276	74542	223.1317	[M+H]	200.1412	5	3-hydroxybutyrate C11H20O3						
172.9654	172.9654	74688	223.1317	[M+H]	200.1412	5	10-hydroxybutyrate C11H20O3						
138.9166	138.9166	74689	223.1317	[M+H]	200.1412	5	10-hydroxybutyrate C11H20O3						
206.8879	206.8879	74725	223.1317	[M+H]	200.1412	5	2-oxoundecanoic acid C11H20O3						
256.8138	256.8138	88603	223.1317	[M+H]	200.1412	5	(5S)-9-hydroxybutyrate C11H20O3						
245.1837	245.1837	91207	223.1317	[M+H]	200.1412	5	Claycit C11H20O3				131766-73-9		
572.361	572.361	92147	223.1317	[M+H]	200.1412	5	3-Nonanoic acid C11H20O3				7779-54-6		
115.0944	115.0944	97330	223.1317	[M+H]	200.1412	5	3Z-Hexenoic acid C11H20O3						
231.177	231.177	97381	223.1317	[M+H]	200.1412	5	5R-hydroxybutyrate C11H20O3						
825.5734	825.5734	97382	223.1317	[M+H]	200.1412	5	5S-hydroxybutyrate C11H20O3						
824.5645	824.5645	97388	223.1317	[M+H]	200.1412	5	6-hydroxybutyrate C11H20O3						
798.5494	798.5494	102868	223.1317	[M+H]	200.1412	5	3-hydroxy-2-oxobutanoic acid C11H20O3						
799.5549	799.5549	98185	223.1317	[M+H]	200.1412	5	5-hydroxy-2-oxobutanoic acid C11H20O3						
520.3833	520.3833	82382	784.5483	[M+H]	783.5414	0	FE(18:0/20:4)H8NO7P						
520.3991	520.3991	82383	784.5483	[M+H]	783.5414	0	FE(18:0/20:4)H8NO7P						
520.3512	520.3512	78658	784.5483	[M+H]	761.5571	2	PS(O)-16:0/16:0:4H8NO7P						
520.3357	520.3357	78672	784.5483	[M+H]	761.5571	2	PS(O)-18:0/17:0:4H8NO7P						
520.3198	520.3198	78693	784.5483	[M+H]	761.5571	2	PS(O)-20:0/17:0:4H8NO7P						
877.5573	877.5573	78756	784.5483	[M+H]	761.5571	2	PS(P)-16:0/19:0:4H8NO7P						
524.6884	524.6884	78776	784.5483	[M+H]	761.5571	2	PS(P)-18:0/17:0:4H8NO7P						
214.1393	214.1393	78800	784.5483	[M+H]	761.5571	2	PS(P)-20:0/15:0:4H8NO7P						
550.3785	550.3785	39434	536.3304	[M+Na]	535.3274	7	PC(16:1/6Z)C26H50NO4						
823.5562	823.5562	78773	782.5333	[M+Na]	759.5414	3	PS(O)-18:0/17:0:4H8NO7P						
510.3864	510.3864	78757	782.5333	[M+Na]	759.5414	3	PS(P)-16:0/17:0:4H8NO7P						
496.9255	496.9255	78777	782.5333	[M+Na]	759.5414	3	PS(P)-18:0/17:0:4H8NO7P						
496.3752	496.3752	78801	782.5333	[M+Na]	759.5414	3	PS(P)-20:0/15:0:4H8NO7P						
496.3907	496.3907	71064	97.9755	[M+H]	74.9876	13	Chlortetracycline C21H24ClN2O8				107-14-2		
496.6297	496.6297	36469	403.2775	[M+Na]	380.2926	10	Perin C23H40O4						
130.0573	130.0573	43154	403.2775	[M+Na]	380.2926	10	24-Nor-SF-d C23H40O4						
496.507	496.507	43155	403.2775	[M+Na]	380.2926	10	24-Nor-SF-d C23H40O4						
496.4597	496.4597	43156	403.2775	[M+Na]	380.2926	10	24-Nor-SF-d C23H40O4						
496.693	496.693	43157	403.2775	[M+Na]	380.2926	10	24-Nor-SF-d C23H40O4						
510.3333	510.3333	62329	403.2775	[M+Na]	380.2927	10	MG(0:0/20:5)C23H40O4						
496.7424	496.7424	62330	403.2775	[M+Na]	380.2927	10	MG(0:0/20:5)C23H40O4						
496.8007	496.8007	62331	403.2775	[M+Na]	380.2927	10	MG(0:0/20:5)C23H40O4						
498.3996	498.3996	62357	403.2775	[M+Na]	380.2927	10	MG(20:3/11)C23H40O4						
144.1	144.1	62358	403.2775	[M+Na]	380.2927	10	MG(20:3/15Z)C23H40O4						
315.1425	315.1425	62359	403.2775	[M+Na]	380.2927	10	MG(20:3/19Z)C23H40O4						
511.3525	511.3525	64008	403.2775	[M+Na]	380.2927	10	24-Nor-Sterea C23H40O4						
496.8683	496.8683	64009	403.2775	[M+Na]	380.2927	10	24-Nor-Sterea C23H40O4						
702.4879	702.4879	64910	403.2775	[M+Na]	380.2927	10	24-Nor-Sterea C23H40O4						
208.1504	208.1504	64911	403.2775	[M+Na]	380.2927	10	24-Nor-Sterea C23H40O4						
341.271	341.271	88663	403.2775	[M+Na]	380.2927	10	Isopren C23H40O4						
176.0518	176.0518	93979	403.2775	[M+Na]	380.2927	10	2-hydroxy-4-C23H40O4						
822.5514	822.5514	86566	403.3054	[M+Na]	402.2981	0	Sorbitan palmitate C22H42O6				26266-57-9		
523.3664	523.3664	71191	404.2908	[M+Na]	403.2795	0	Itanoyl CoA C18H37NO2						
523.3545	523.3545	84398	404.2908	[M+Na]	381.2991	6	Cannabidiol C21H30O2				57682-64-1		
523.3704	523.3704	41985	403.3194	[M+H]	402.3134	3	11a-hydroxy-C26H42O3						
520.3674	520.3674	41986	403.3194	[M+H]	402.3134	3	28-hydroxy-C26H42O3						
528.433	528.433	41987	403.3194	[M+H]	402.3134	3	11a,25-dihydro-C26H42O3						
991.689	991.689	41988	403.3194	[M+H]	402.3134	3	11a,25-dihydro-C26H42O3						
526.3981	526.3981	41989	403.3194	[M+H]	402.3134	3	11a,25-dihydro-C26H42O3						
991.6561	991.6561	42192	403.3194	[M+H]	402.3134	3	22-ethyl-11a, C26H42O3						
525.4171	525.4171	73560	403.3194	[M+H]	402.3134	3	Androstene C26H42O3				NA		
524.4564	524.4564	83935	403.3194	[M+H]	402.3134	3	27-oxo-22R-C26H42O3						
992.6639	992.6639	86283	403.3194	[M+H]	402.3134	3	Oryzanol C26H42O3						
518.3306	518.3306	74786	403.3194	[M+H]	380.329	2	15-oxo-18Z-C26H42O3						
524.4291	524.4291	5862	229.1405	[M+H]	228.1362	12	Transmaleic acid C12H20O4				6402-36-4		
524.4132	524.4132	35963	229.1405	[M+H]	228.1362	12	Transmaleic acid C12H20O4						
524.3973	524.3973	45942	229.1405	[M+H]	228.1362	12	(-)-11-hydroxyl C12H20O4						
524.3813	524.3813	45945	229.1405	[M+H]	228.1362	12	(-)-12-hydroxyl C12H20O4						
510.349	510.349	74730	229.1405	[M+H]	228.1362	12	8,12-dioxo-d C12H20O4						
523.3533	523.3533	74918	229.1405	[M+H]	228.1362	12	2Z-Dodecenoic acid C12H20O4						
523.4012	523.4012	87338	229.1405	[M+H]	228.1362	12	5-hydroxybutyrate C12H20O4						
523.3852	523.3852	98532	229.1405	[M+H]	228.1362	12	Acetone P, 3 C12H20O4						
523.3693	523.3693	68215	560.3276	[M+H]	559.3145	10	Auricline C31H45NO8				22595-00-2		
524.5654	524.5654	39354	560.3276	[M+H]	537.3431	8	PC(16:0/2:0)C26H52NO4						
548.5474	548.5474	39355	560.3276	[M+H]	537.3431	8	PC(16:0/2:0)C26H52NO4						
570.5403	570.5403	39356	560.3276	[M+H]	537.3431	8	PC(16:0/2:0)C26H52NO4						
547.5477													

4137	126.0317	[M-H]	125.0242	1 2-Aminothiazine C2H8N2S	2041-14-7	Metabolism of nitric oxide	Wkpathways	1 74-79-3	31 (38)	0.103
66044	126.0317	[M-H]	125.0242	1 D-(1-Amino) C2H8N2S	60687-36-7	Amino compound SLC transporters	Reactome	1 74-79-3	31 (35)	0.103
67952	126.0317	[M-H]	103.0422	2 Benzothiazine C7H5N	100-47-0	eNOS activation and regulation	Reactome	1 74-79-3	32 (38)	0.106
69883	251.0339	[M-H]	250.0235	13 4,4'-Sulfenyl C12H10O4S	80-09-1	VEGFA-VEGFR2 Pathway	Reactome	1 74-79-3	32 (38)	0.106
91160	251.0339	[M-H]	250.0235	12 (S)-Spinobol C11H18O2S2	128722-96-3	<O>-S<-O>-methyl-5-oxo-4-oxo-1-phosphate degradation	HumanCyc	1 74-79-3	32 (35)	0.106
93241	251.0339	[M-H]	250.0235	12 Cyclobutane C11H18O2S2	128722-96-3	Signaling by VEGF	Reactome	1 74-79-3	32 (38)	0.106
64103	251.0339	[M-H]	228.0423	9 Eucarbonyl C13H20O4	529-61-3	Vitamin B3 (nicotinate and nicotinamide) metabolism	EIMN	1 74-79-3	32 (36)	0.106
85253	251.0339	[M-H]	228.0423	9 Urethrin A C13H20O4	1143-70-0	Metabolism of nitric oxide	Reactome	1 74-79-3	32 (38)	0.106
96301	251.0339	[M-H]	228.047	9 1-phenyl-1H-C11H8N4S		Class I MHC mediated antigen processing & presentation	Wkpathways	1 74-79-3	33 (35)	0.109
72335	251.045	[M-H]	228.0553	1 2-Methyl-4-c C11H15CO2	94-81-5	Hypocretin/leptin	SMPOB	1 74-79-3	34 (34)	0.112
1210	251.056	[M-H]	250.0477	3 2H-1-Benzox C12H10O6	71942-06-8	Aspartate Metabolism	SMPOB	1 74-79-3	34 (34)	0.112
2434	251.056	[M-H]	250.0524	14 Sulfadiazine C10H10N4O	68-35-9	Central carbon metabolism in cancer - Homo sapiens (human)	SMPOB	1 74-79-3	34 (34)	0.112
66735	251.056	[M-H]	250.0477	3 2-Hydroxy-6 C12H10O6		One carbon metabolism and related pathways	KEGG	1 74-79-3	34 (37)	0.112
66438	251.056	[M-H]	228.0634	13 2-Hydroxy-3 C10H12O6		Pyrimidine metabolism	Wkpathways	1 636-58-8	36 (37)	0.119
68770	251.056	[M-H]	228.0666	0 Measurone C10H12O6	19937-59-8	Pyrimidine metabolism	Reactome	1 636-58-8	37 (39)	0.122
50505	251.0229	[M-H]	250.0147	3 3,4-Dihydro C8H10O7S	3415-68-7	Alanine Aspartate Asparagine metabolism	INOI	1 74-79-3	39 (45)	0.128
72466	251.0229	[M-H]	250.0162	2 Heptanophos C8H12O4S2	21560-59-0	Transmembrane transport of small molecules	Reactome	2 558-09-8, 74-185 (212)		0.132
89902	251.0229	[M-H]	250.0156	0 2-Propenyl 3 C8H14O2S3	118990-71-9	G alpha (q) signalling events	Reactome	1 74-79-3	42 (47)	0.137
89031	127.0331	[M-H]	126.0252	5 2-C-Methyl C8H14N2S	21948-70-9	Amino acid and oligopeptide SLC transporters	Reactome	1 74-79-3	42 (49)	0.137
91335	127.0331	[M-H]	126.0252	5 Pyrazinone C8H14N2S	59021-02-2	Protein digestion and absorption - Homo sapiens (human)	KEGG	1 74-79-3	45 (47)	0.146
91293	251.0341	[M-H]	230.0514	9 6-Methoxy-3 C12H18O2S2	135531-87-2	2-Hydroxyglutamic Aciduria (D And L Form)	SMPOB	1 636-58-8	46 (49)	0.149
66443	251.0227	[M-H]	252.0189	3 2-Hydroxy-6 C12H18O2S2		Hemocyaninosis	SMPOB	1 636-58-8	46 (49)	0.149
72468	251.0227	[M-H]	252.0221	9 3,3'-Dichloro C12H10Cl2S2	91-94-1	Hyperuricemia-Hyperuricemia Syndrome	SMPOB	1 636-58-8	46 (49)	0.149
72170	251.0227	[M-H]	230.0361	6 Axiolam C8H10N2O4	3337-71-1	Succinate semialdehyde dehydrogenase deficiency	SMPOB	1 636-58-8	46 (49)	0.149
3379	251.067	[M-H]	250.0623	10 1-Glu-Cys C8H14N2O5	636-58-8	4-Hydroxybutyric Aciduria/Succinyl Semialdehyde Dehydrogenase	SMPOB	1 636-58-8	46 (49)	0.149
35884	251.067	[M-H]	250.0668	11 10-bromo-deo C10H18BrO2NA		Glutamate Metabolism	SMPOB	1 636-58-8	46 (49)	0.149
35885	251.067	[M-H]	250.0668	11 2-bromo-deo C10H18BrO2NA		Transport of inorganic cations/anions and amino acids/oligopeptides	Reactome	1 74-79-3	48 (55)	0.155
34822	251.067	[M-H]	250.0668	11 9-bromo-deo C10H18BrO2		Hyperhomocysteinemia with gyrate atrophy (HOGA)	SMPOB	1 74-79-3	49 (52)	0.158
85167	251.067	[M-H]	250.0668	3 TCEP C8H15O4P	51805-43-9	Creatine deficiency, guanidinosuccinate methyltransferase deficiency	SMPOB	1 74-79-3	49 (52)	0.158
91	251.067	[M-H]	228.0746	12 2-Deoxyuridine C8H12N2O5	951-78-0	L-arginine:glycine amidotransferase deficiency	SMPOB	1 74-79-3	49 (52)	0.158
1678	251.067	[M-H]	228.0786	3 4-Hydroxy-4 C14H12O3	51350-23-3	Hyperhomocysteinemia-hyperhomocysteinemia-homocystinuria (HHC-sy)	SMPOB	1 74-79-3	49 (52)	0.158
6979	251.067	[M-H]	228.0786	3 trans-Raven C14H12O3	501-36-0	Guanidinosuccinate Methyltransferase Deficiency (GAMT Deficiency)	SMPOB	1 74-79-3	49 (52)	0.158
41779	251.067	[M-H]	228.0786	3 XANTHYLL C14H12O3	553-19-5	Proline Type II	SMPOB	1 74-79-3	49 (52)	0.158
44878	251.067	[M-H]	228.0786	3 cis-Raven C14H12O3	61434-67-1	Proline Deficiency (PD)	SMPOB	1 74-79-3	49 (52)	0.158
67596	251.067	[M-H]	228.0786	3 Sacin C14H12O3	523-99-1	Arginine and Proline Metabolism	SMPOB	1 74-79-3	49 (52)	0.158
64015	251.067	[M-H]	228.0786	3 5,6-Dihydro C14H12O3	1952-41-6	15 Hyperprolinemia Type I	SMPOB	1 74-79-3	49 (52)	0.158
70024	251.067	[M-H]	228.0786	3 Benzylparab C14H12O3	94-18-8	Hyperprolinemia Type II	SMPOB	1 74-79-3	49 (52)	0.158
70684	251.067	[M-H]	228.0786	3 3,4-Dihydro C14H12O3		Oxalate Aminoaciduria Deficiency (OAT Deficiency)	SMPOB	1 74-79-3	49 (52)	0.158
73215	251.067	[M-H]	228.0786	3 4,6,8-Trimethyl C14H12O3	90370-29-9	Arginine: Glycine Amidotransferase Deficiency (AGAT Deficiency)	SMPOB	1 74-79-3	49 (52)	0.158
85441	251.067	[M-H]	228.0786	7 Pemisul C10H18NO	100299-08-9	Metabolism of polyamines	Wkpathways	1 74-79-3	49 (57)	0.158
86523	251.067	[M-H]	228.0786	3 Benzyl salicy C14H12O3	118-58-1	Metabolism of polyamines	Reactome	1 74-79-3	50 (60)	0.161
88268	251.067	[M-H]	228.0786	3 2,4-Difuryl C14H12O3	64280-32-6	Gastrin-CREB signaling pathway via PKC and MAPK	Reactome	1 74-79-3	50 (56)	0.161
92502	251.067	[M-H]	228.0786	3 o-Tolyl salicy C14H12O3	617-01-6	Transport of inorganic cations/anions and amino acids-oligopeptides	Wkpathways	1 74-79-3	50 (51)	0.161
96475	251.067	[M-H]	228.0746	12 Zebulone C8H12N2O5	10763690	Class C3 (Metabotropic glutamate) receptors	Reactome	1 74-79-3	50 (54)	0.161
96744	251.067	[M-H]	228.0786	3 trans-Raven C14H12O3	NA	Amino Acid interconversion	Wkpathways	1 74-79-3	51 (51)	0.164
69173	241.149	[M-H]	240.1393	9 Minisul C13H21ClN2	2519-75-7	Glycine Serine metabolism	INOI	1 74-79-3	52 (68)	0.167
71173	170.0279	[M-H]	169.0197	5 Thiosemicarbazide C7H7N2OS		Sulfur amino acid metabolism	Reactome	1 636-58-8	53 (65)	0.17
70187	170.0279	[M-H]	147.0392	3 N-Methyl-N'-C2H4S2N3O3	76-25-7	Hemostasis	Reactome	1 74-79-3	53 (68)	0.17
63393	185.0283	[M-H]	184.0233	12 5-Hydroxy C8H14NO4		Non Ketotic Hyperglycemia	SMPOB	1 74-79-3	54 (55)	0.173
70568	169.0679	[M-H]	168.0387	11 3-Fluoro-1-C8H9F6O2		3-Phosphoglycerate dehydrogenase deficiency	SMPOB	1 74-79-3	54 (55)	0.173
92463	169.0679	[M-H]	164.0765	12 4-Methyl-4-C7H14O5	23550-40-5	Glycine and Serine Metabolism	SMPOB	1 74-79-3	54 (55)	0.173
94037	169.0679	[M-H]	164.0765	12 5-Methyl-4-C7H14O5	2432-77-1	Dihydroxyglycine Dehydrogenase Deficiency	SMPOB	1 74-79-3	54 (55)	0.173
94040	169.0679	[M-H]	164.0765	12 5-Methyl-4-C7H14O5	61122-71-2	Hyperglycemia, non-ketotic	SMPOB	1 74-79-3	54 (55)	0.173
94721	169.0679	[M-H]	164.0765	12 3-Methyl-4-C7H14O5	38433-74-8	Dihydroxyglycine Dehydrogenase Deficiency	SMPOB	1 74-79-3	54 (55)	0.173
73569	175.1585	[M-H]	174.1494	10 gamma-Buty C8H12NO2	51963-62-3	Sarcosinemia	SMPOB	1 74-79-3	54 (55)	0.173
85236	175.1585	[M-H]	174.1494	10 Butyrylchol C8H12NO2	3922-86-9	Dihydroxyphenylalanine Dehydrogenase Deficiency (DHDP)	SMPOB	1 74-79-3	54 (55)	0.173
86601	175.1585	[M-H]	174.1494	10 (2S,4R,5S)-3 C8H12NO2	300-54-9	Arginine and proline metabolism - Homo sapiens (human)	KEGG	1 74-79-3	54 (76)	0.173
						Pyrimidine nucleotides nucleosides metabolism	INOI	1 951-78-0	55 (56)	0.176
						Phenylalanine metabolism - Homo sapiens (human)	KEGG	1 122-78-1	55 (72)	0.176
						Folate Metabolism	Wkpathways	1 74-79-3	55 (67)	0.176
						Sulfur amino acid metabolism	Wkpathways	1 636-58-8	55 (63)	0.176
						Ben Uridopropionate Deficiency	SMPOB	1 951-78-0	56 (57)	0.179
						UMP Synthase Deficiency (Orotic Aciduria)	SMPOB	1 951-78-0	56 (57)	0.179
						Pyrimidine Metabolism	SMPOB	1 951-78-0	56 (57)	0.179
						MNGIE (Mitochondrial Neurogastrointestinal Encephalopathy)	SMPOB	1 951-78-0	56 (57)	0.179
						Dihydropyrimidine Deficiency	SMPOB	1 951-78-0	56 (57)	0.179
						Pyrimidine metabolism	Reactome	1 951-78-0	58 (60)	0.185
						Biochemical Pathways Part I	Wkpathways	3 636-58-8, 3931-437 (467)		0.185
						Transport of vitamins, nucleosides, and related molecules	Wkpathways	1 958-09-8	59 (60)	0.188
						Parine metabolism	Reactome	1 958-09-8	62 (67)	0.196
						Transport of vitamins, nucleosides, and related molecules	Reactome	1 958-09-8	62 (64)	0.196
						Parine Nucleotide Phosphorylase Deficiency	SMPOB	1 958-09-8	69 (73)	0.216
						Xanthine Dehydrogenase Deficiency (Xanthinuria)	SMPOB	1 958-09-8	69 (73)	0.216
						Adenylosuccinate Lyase Deficiency	SMPOB	1 958-09-8	69 (73)	0.216
						AlCA-Ribosiduria	SMPOB	1 958-09-8	69 (73)	0.216
						Adenine phosphoribosyltransferase deficiency (APRT)	SMPOB	1 958-09-8	69 (73)	0.216
						Mitochondrial DNA depletion syndrome	SMPOB	1 958-09-8	69 (73)	0.216
						Myoadenylate deaminase deficiency	SMPOB	1 958-09-8	69 (73)	0.216
						Parine Metabolism	SMPOB	1 958-09-8	69 (73)	0.216
						Methylglutamate Co-factor Deficiency	SMPOB	1 958-09-8	69 (73)	0.216
						Adenosine Deaminase Deficiency	SMPOB	1 958-09-8	69 (73)	0.216
						Gout or Kelley-Seegmiller Syndrome	SMPOB	1 958-09-8	69 (73)	0.216
						Lesch-Nyhan Syndrome (LNS)	SMPOB	1 958-09-8	69 (73)	0.216
						Xanthinuria type I	SMPOB	1 958-09-8	69 (73)	0.216
						Xanthinuria type II	SMPOB	1 958-09-8	69 (73)	0.216
						Glycine, serine, alanine and threonine metabolism	EIMN	1 74-79-3	70 (88)	0.219
						Human metabolism overview	Wkpathways	1 74-79-3	71 (113)	0.222
						Pyrimidine metabolism	EIMN	1 951-78-0	71 (77)	0.222
						Metabolism of water-soluble vitamins and cofactors	Wkpathways	1 4754-39-6	73 (94)	0.227
						Innate Immune System	Reactome	1 74-79-3	74 (116)	0.23
						Parine metabolism - Homo sapiens (human)	KEGG	1 958-09-8	74 (92)	0.23
						Parine nucleotides nucleosides metabolism	INOI	1 958-09-8	75 (80)	0.233
						Transport of glucose and other sugars, bile salts and organic acids	Reactome	1 74-79-3	76 (83)	0.235
						Transport of glucose and other sugars, bile salts and organic acids	Wkpathways	1 74-79-3	76 (83)	0.235
						Mercaptopurine Action Pathway	SMPOB	1 958-09-8	77 (84)	0.238
						Thioguanine Action Pathway	SMPOB	1 958-09-8	78 (85)	0.241
						Azathioprine Action Pathway	SMPOB	1 958-09-8	79 (86)	0.244
						Parine metabolism	EIMN	1 958-09-8	82 (94)	0.252
						Metabolism of water-soluble vitamins and cofactors	Reactome	1 4754-39-6	88 (120)	0.268
						Immune System	Reactome	1 74-79-3	91 (149)	0.275
						Tyrosine metabolism	EIMN	1 122-78-1	94 (105)	0.283
						Metabolism of vitamins and cofactors	Reactome	1 4754-39-6	112 (155)	0.328
						Metabolism of proteins	Reactome	1 74-79-3	113 (227)	0.331
						GPCR downstream signaling	Reactome	1 74-79-3	115 (127)	0.336
						Phase II conjugation	Reactome	1 636-58-8	125 (147)	0.359
						GPCR ligand binding	Reactome	1 74-79-3	127 (135)	0.364
						Signaling by GPCR	Reactome	1 74-79-3	147 (163)	0.409
						Phase I - Functionalization of compounds	Wkpathways	1 122-78-1	154 (189)	0.424
						Signal Transduction	Reactome	1 74-79-3	215 (254)	0.541

61897	825.5734	[M-H]	824.5567	11	PG(18:1)(11Z,C46H81O10P
61912	825.5734	[M-H]	824.5567	11	PG(18:1)(9Z,C46H81O10P
79219	825.5734	[M-H]	824.5567	11	PG(18:3)(6Z,C46H81O10P
79247	825.5734	[M-H]	824.5567	11	PG(18:3)(9Z,C46H81O10P
79277	825.5734	[M-H]	824.5567	11	PG(18:4)(6Z,C46H81O10P
79348	825.5734	[M-H]	824.5567	11	PG(20:9)(20:5,C46H81O10P
79375	825.5734	[M-H]	824.5567	11	PG(20:1)(11Z,C46H81O10P
79405	825.5734	[M-H]	824.5567	11	PG(20:2)(11Z,C46H81O10P
79435	825.5734	[M-H]	824.5567	11	PG(20:3)(8Z,C46H81O10P
79464	825.5734	[M-H]	824.5567	11	PG(20:4)(5Z,C46H81O10P
79491	825.5734	[M-H]	824.5567	11	PG(20:5)(5Z,C46H81O10P
79566	825.5734	[M-H]	824.5567	11	PG(22:1)(11Z,C46H81O10P
79595	825.5734	[M-H]	824.5567	11	PG(22:2)(13Z,C46H81O10P
79596	825.5734	[M-H]	824.5567	11	PG(22:2)(13Z,C46H81O10P
79624	825.5734	[M-H]	824.5567	11	PG(22:4)(7Z,C46H81O10P
81028	825.5734	[M-H]	824.5779	14	PHO-20:0(14,C43H85O12P
81058	825.5734	[M-H]	824.5779	14	PHO-18:0(14,C43H85O12P
81065	825.5734	[M-H]	824.5779	14	PHO-16:0(14,C43H85O12P
79025	825.5734	[M-H]	802.5724	14	PG(14:0)(22:2,C44H83O10P
79048	825.5734	[M-H]	802.5724	14	PG(14:1)(9Z,C44H83O10P
79127	825.5734	[M-H]	802.5724	14	PG(17:2)(9Z,C44H83O10P
79181	825.5734	[M-H]	802.5724	14	PG(18:2)(9Z,C44H83O10P
79323	825.5734	[M-H]	802.5724	14	PG(19:1)(9Z,C44H83O10P
79365	825.5734	[M-H]	802.5724	14	PG(20:1)(11Z,C44H83O10P
79394	825.5734	[M-H]	802.5724	14	PG(20:2)(11Z,C44H83O10P
79509	825.5734	[M-H]	802.5724	14	PG(21:0)(17:2,C44H83O10P
79557	825.5734	[M-H]	802.5724	14	PG(22:1)(11Z,C44H83O10P
79587	825.5734	[M-H]	802.5724	14	PG(22:2)(13Z,C44H83O10P
79776	825.5734	[M-H]	802.5724	14	PG(20:9)(18:2,C44H83O10P
79783	825.5734	[M-H]	802.5724	14	PG(18:1)(9Z,C44H83O10P
79788	825.5734	[M-H]	802.5724	14	PG(18:0)(20:2,C44H83O10P
41625	824.5645	[M-H]	823.5479	11	C18-OH, 5a/7 C42H81NO12S
103141	798.5494	[M-H]	797.5418	0	PS-Cer(18:0,C40H80NO12P
103159	798.5494	[M-H]	797.5418	0	PS-Cer(18:0,C40H80NO12P
46708	798.5494	[M-H]	775.5516	10	PE(P-18:0)(22:C45H78NO7P
61033	798.5494	[M-H]	775.5516	10	PE(22:5)(4Z,C45H78NO7P
61034	798.5494	[M-H]	775.5516	10	PE(22:5)(4Z,C45H78NO7P
61066	798.5494	[M-H]	775.5516	10	PE(22:5)(7Z,C45H78NO7P
61067	798.5494	[M-H]	775.5516	10	PE(22:5)(7Z,C45H78NO7P
61097	798.5494	[M-H]	775.5516	10	PE(22:4)(6Z,C45H78NO7P
62224	798.5494	[M-H]	775.5516	10	PE(P-18:1)(11:C45H78NO7P
62225	798.5494	[M-H]	775.5516	10	PE(P-18:1)(11:C45H78NO7P
62253	798.5494	[M-H]	775.5516	10	PE(P-18:1)(9Z,C45H78NO7P
62254	798.5494	[M-H]	775.5516	10	PE(P-18:1)(9Z,C45H78NO7P
40870	799.5549	[M-H]	798.5411	8	PG(18:0)(20:4,C44H79O10P
61856	799.5549	[M-H]	798.5411	8	PG(16:0)(22:4,C44H79O10P
61894	799.5549	[M-H]	798.5411	8	PG(18:1)(11Z,C44H79O10P
61895	799.5549	[M-H]	798.5411	8	PG(18:1)(11Z,C44H79O10P
61899	799.5549	[M-H]	798.5411	8	PG(18:1)(9Z,C44H79O10P
61910	799.5549	[M-H]	798.5411	8	PG(18:1)(9Z,C44H79O10P
79183	799.5549	[M-H]	798.5411	8	PG(18:2)(9Z,C44H79O10P
79211	799.5549	[M-H]	798.5411	8	PG(18:3)(6Z,C44H79O10P
79239	799.5549	[M-H]	798.5411	8	PG(18:3)(9Z,C44H79O10P
79269	799.5549	[M-H]	798.5411	8	PG(18:4)(6Z,C44H79O10P
79367	799.5549	[M-H]	798.5411	8	PG(20:1)(11Z,C44H79O10P
79368	799.5549	[M-H]	798.5411	8	PG(20:1)(11Z,C44H79O10P
79396	799.5549	[M-H]	798.5411	8	PG(20:2)(11Z,C44H79O10P
79426	799.5549	[M-H]	798.5411	8	PG(20:3)(8Z,C44H79O10P
79455	799.5549	[M-H]	798.5411	8	PG(20:4)(5Z,C44H79O10P
79618	799.5549	[M-H]	798.5411	8	PG(22:4)(7Z,C44H79O10P
79775	799.5549	[M-H]	798.5411	8	PG(20:9)(18:4,C44H79O10P
40860	799.5549	[M-H]	776.5567	11	PG(18:0)(18:1,C42H81O10P
40868	799.5549	[M-H]	776.5567	11	PG(18:0)(18:1,C42H81O10P
43206	799.5549	[M-H]	776.5567	11	1-Stranoyl-2-C42H81O10P
61877	799.5549	[M-H]	776.5567	11	PG(18:0)(18:1,C42H81O10P
61888	799.5549	[M-H]	776.5567	11	PG(18:1)(11Z,C42H81O10P
61903	799.5549	[M-H]	776.5567	11	PG(18:1)(9Z,C42H81O10P
78931	799.5549	[M-H]	776.5567	11	PG(14:0)(22:1,C42H81O10P
78959	799.5549	[M-H]	776.5567	11	PG(14:1)(9Z,C42H81O10P
79011	799.5549	[M-H]	776.5567	11	PG(15:1)(9Z,C42H81O10P
79041	799.5549	[M-H]	776.5567	11	PG(16:1)(9Z,C42H81O10P
79063	799.5549	[M-H]	776.5567	11	PG(17:0)(19:1,C42H81O10P
79089	799.5549	[M-H]	776.5567	11	PG(17:1)(9Z,C42H81O10P
79285	799.5549	[M-H]	776.5567	11	PG(19:0)(17:1,C42H81O10P
79313	799.5549	[M-H]	776.5567	11	PG(19:1)(9Z,C42H81O10P
79339	799.5549	[M-H]	776.5567	11	PG(20:0)(16:1,C42H81O10P
79359	799.5549	[M-H]	776.5567	11	PG(20:1)(11Z,C42H81O10P
79504	799.5549	[M-H]	776.5567	11	PG(21:0)(15:1,C42H81O10P
79527	799.5549	[M-H]	776.5567	11	PG(22:0)(14:1,C42H81O10P
79552	799.5549	[M-H]	776.5567	11	PG(22:1)(11Z,C42H81O10P
79795	799.5549	[M-H]	776.5567	11	PG(16:0)(20:1,C42H81O10P
46692	520.3357	[M-H]	519.3325	13	PC(19:1)(11:C28H56NO7P
1	520.3357	[M-H]	519.3325	7	1-Linolenyl-PC(28H56NO7) 15895-41-7
40300	520.3357	[M-H]	519.3325	7	PC(18:2)(24:C28H56NO7P
40301	520.3357	[M-H]	519.3325	7	PC(18:2)(9Z,C28H56NO7P
40302	520.3357	[M-H]	519.3325	7	PC(18:2)(9Z,C28H56NO7P
61696	520.3357	[M-H]	519.3325	7	Lysyl-PC(18:2,C28H56NO7P
65437	520.3198	[M-H]	497.3353	8	Tumanoic Ac C47H74NO7
40990	877.5573	[M-H]	876.5559	6	Megalomicin C40H80NO2O15
102977	524.4684	[M-H]	523.4601	2	Cer(14:2)(4E,C32H61NO4
102997	524.4684	[M-H]	523.4601	2	Cer(14:1)(4E,C32H61NO4
40011	550.3785	[M-H]	549.3794	14	PC(O-18:1)(19:C28H56NO7P
40012	550.3785	[M-H]	549.3794	14	PC(O-18:1)(9:C28H56NO7P
40013	550.3785	[M-H]	549.3794	14	PC(O-18:1)(9:C28H56NO7P
40016	550.3785	[M-H]	549.3794	14	PC(O-18:1)(9:C28H56NO7P
40017	550.3785	[M-H]	549.3794	14	PC(O-18:1)(9:C28H56NO7P
40021	550.3785	[M-H]	549.3794	14	PC(2:0)(0-18:C28H56NO7P
40022	550.3785	[M-H]	549.3794	14	PC(2:0)(0-18:C28H56NO7P
40176	550.3785	[M-H]	549.3794	14	PC(7:18)(0-2:C28H56NO7P
40313	550.3785	[M-H]	549.3794	14	PC(20:1)(9Z,C28H56NO7P
43412	550.3785	[M-H]	549.3794	14	1-O-(6is-9-O-C28H56NO7) 86288-90-1
61701	550.3785	[M-H]	549.3794	14	Lysyl-PC(20:1,C28H56NO7P
62930	550.3785	[M-H]	549.3794	14	Pymolidino F C28H56NO7 91021-63-5
62941	550.3785	[M-H]	549.3794	14	Brainyl-1-PA(C28H56NO7) NA
76573	550.3785	[M-H]	549.3794	14	PC(20:1)(11Z,C28H56NO7P
96561	550.3785	[M-H]	527.3889	0	PAF C-16-d6 C26H50D4N NA
40871	823.5562	[M-H]	822.5411	9	PG(18:0)(22:4,C46H79O10P
43205	823.5562	[M-H]	822.5411	9	1-Stranoyl-2-C46H79O10P
61898	823.5562	[M-H]	822.5411	9	PG(18:1)(11Z,C46H79O10P
61899	823.5562	[M-H]	822.5411	9	PG(18:1)(11Z,C46H79O10P
61913	823.5562	[M-H]	822.5411	9	PG(18:1)(9Z,C46H79O10P
61914	823.5562	[M-H]	822.5411	9	PG(18:1)(9Z,C46H79O10P
61927	823.5562	[M-H]	822.5411	9	PG(18:2)(9Z,C46H79O10P
64718	823.5562	[M-H]	822.5507	2	NBD-Stranoyl C47H74N4O NA
79278	823.5562	[M-H]	822.5411	9	PG(18:4)(6Z,C46H79O10P
79376	823.5562	[M-H]	822.5411	9	PG(20:1)(11Z,C46H79O10P
79406	823.5562	[M-H]	822.5411	9	PG(20:2)(11Z,C46H79O10P
79436	823.5562	[M-H]	822.5411	9	PG(20:3)(8Z,C46H79O10P
79465	823.5562	[M-H]	822.5411	9	PG(20:4)(5Z,C46H79O10P
79492	823.5562	[M-H]	822.5411	9	PG(20:5)(5Z,C46H79O10P
79597	823.5562	[M-H]	822.5411	9	PG(22:2)(13Z,C46H79O10P
79625	823.5562	[M-H]	822.5411	9	PG(22:4)(7Z,C46H79O10P
79652	823.5562	[M-H]	822.5411	9	PG(22:4)(4Z,C46H79O10P
61881	823.5562	[M-H]	800.5567	12	PG(18:0)(20:3,C44H81O10P

61882	823.5562	[M-H] ⁺	800.5567	12	PG(18:0/20:3/C44H81O10P
79049	823.5562	[M-H] ⁺	800.5567	12	PG(16:1(9Z)/C44H81O10P
79159	823.5562	[M-H] ⁺	800.5567	12	PG(18:1(9Z)/C44H81O10P
79182	823.5562	[M-H] ⁺	800.5567	12	PG(18:2(9Z)/C44H81O10P
79210	823.5562	[M-H] ⁺	800.5567	12	PG(18:3(9Z)/C44H81O10P
79238	823.5562	[M-H] ⁺	800.5567	12	PG(18:3(9Z)/C44H81O10P
79343	823.5562	[M-H] ⁺	800.5567	12	PG(20:0/18:3/C44H81O10P
79344	823.5562	[M-H] ⁺	800.5567	12	PG(20:0/18:3/C44H81O10P
79366	823.5562	[M-H] ⁺	800.5567	12	PG(20:1(11Z)/C44H81O10P
79395	823.5562	[M-H] ⁺	800.5567	12	PG(20:2(11Z)/C44H81O10P
79425	823.5562	[M-H] ⁺	800.5567	12	PG(20:3(12Z)/C44H81O10P
79588	823.5562	[M-H] ⁺	800.5567	12	PG(22:0/18:3/C44H81O10P
96443	510.3804	[M-H] ⁺	509.373	0	UNC638 C30H47N5O 125556-76-7
40178	496.3752	[M-H] ⁺	495.3689	1	PCIO-1:0:0-C25H54NO6P
40203	496.3752	[M-H] ⁺	495.3689	1	PCIO-16:0:0-C25H54NO6P
40204	496.3752	[M-H] ⁺	495.3689	1	PCIO-16:0:0-C25H54NO6P
40205	496.3752	[M-H] ⁺	495.3689	1	PCIO-16:0:0-C25H54NO6P
40387	496.3752	[M-H] ⁺	495.3689	1	PCIO-17:0:0-C25H54NO6P
43417	496.3752	[M-H] ⁺	495.3689	1	2-O-urethyl 7 C25H54NO6 78858-44-3
77700	496.3752	[M-H] ⁺	495.3689	1	HEU-20:0:0-C25H54NO6P
70769	496.3907	[M-H] ⁺	473.4022	1	N-Methylind C34H51N
6589	144.1	[M-H] ⁺	143.0946	13	1-Aminoethyl C7H11NO2
7089	144.1	[M-H] ⁺	143.0946	13	Proline beta C7H11NO2
66118	144.1	[M-H] ⁺	143.0946	13	4-Trimethyl C7H11NO2
16954	144.1	[M-H] ⁺	143.0946	13	L-2-Amino-3 C7H11NO2 29784-96-1
93560	144.1	[M-H] ⁺	143.0946	13	Beta-Ala C7H11NO2
88591	315.1425	[M-H] ⁺	314.1392	12	L-Alanine C18H28NO4 172924-24-2
64338	315.1425	[M-H] ⁺	292.1576	13	16-Epivellon C19H28NO2
64339	315.1425	[M-H] ⁺	292.1576	13	Vellonine C19H28NO2 6874-98-2
71300	315.1425	[M-H] ⁺	292.1576	13	Cinchonine C19H28NO2
71382	315.1425	[M-H] ⁺	292.1576	13	Cinchonidine C19H28NO2
42577	511.3525	[M-Na] ⁺	488.3686	10	11,25-Dihydro C30H52O3S
70250	511.3525	[M-Na] ⁺	488.3686	4	Cholesta-5,7-C34H66O2 1182-06-5
33561	341.271	[M-H] ⁺	340.2613	6	15(S)-HqD C20H36O4 145373-41-3
36124	341.271	[M-H] ⁺	340.2613	6	PGH1 Alkox C20H36O4 21562-57-2
36139	341.271	[M-H] ⁺	340.2613	6	11-deoxy-PG C20H36O4 37785-98-1
36141	341.271	[M-H] ⁺	340.2613	6	11-deoxy-PG C20H36O4 37785-98-2
36172	341.271	[M-H] ⁺	340.2613	6	PGH2 Alkox C20H36O4 13261-27-3
45415	341.271	[M-H] ⁺	340.2614	6	Protogasterin C20H36O4 NA
45967	341.271	[M-H] ⁺	340.2614	6	Therobutan C20H36O4
85390	341.271	[M-H] ⁺	318.2797	6	Tridhexethyl C21H36NO 60-49-1
78683	822.5514	[M-Na] ⁺	799.5727	12	PSO-18:0:2(C44H82NO8P
78701	822.5514	[M-Na] ⁺	799.5727	12	PSO-20:0:1(C44H82NO8P
78702	822.5514	[M-Na] ⁺	799.5727	12	PSO-20:0:1(C44H82NO8P
78766	822.5514	[M-Na] ⁺	799.5727	12	PSO-16:0:2(C44H82NO8P
78788	822.5514	[M-Na] ⁺	799.5727	12	PSO-18:0:2(C44H82NO8P
78809	822.5514	[M-Na] ⁺	799.5727	12	PSO-20:0:1(C44H82NO8P
92150	523.3545	[M-Na] ⁺	522.3404	13	Polyorbane 2 C26H50O10 9005-54-5
71023	523.3545	[M-Na] ⁺	500.3614	7	Vicostatin C30H48NO2 150999-65-6
42518	523.3704	[M-H] ⁺	522.3709	14	11,25-dihydro-C34H66O4
45287	523.3704	[M-H] ⁺	522.3604	5	Oleic Acid-b C28H56NO4 NA
44453	523.3704	[M-H] ⁺	500.3866	10	OLEANAN C32H52O4
70849	523.3704	[M-H] ⁺	500.3866	10	Beta-Hydro C32H52O4
95205	525.433	[M-Na] ⁺	524.4229	5	Haridakiol D C33H56O3 156980-40-4
43328	525.433	[M-Na] ⁺	502.4471	6	Hexadec C28H56N8 155146-31-5
56047	591.5561	[M-Na] ⁺	590.6603	11	NeuAalpa C31H58N2O16
40303	518.3306	[M-H] ⁺	517.3168	12	PC18.3(6Z)/C26H48NO7P
40304	518.3306	[M-H] ⁺	517.3168	12	PC18.3(6Z)/C26H48NO7P
40305	518.3306	[M-H] ⁺	517.3168	12	PC18.3(6Z)/C26H48NO7P
61697	518.3306	[M-H] ⁺	517.3168	12	LysePC(18:3) C26H48NO7P
61698	518.3306	[M-H] ⁺	517.3168	12	LysePC(18:3) C26H48NO7P
76570	518.3306	[M-H] ⁺	517.3168	12	PC18.3(6Z)/C26H48NO7P
85482	518.3306	[M-H] ⁺	517.3226	1	Reupamalin C30H47NO4 224452-66-8
40179	524.4132	[M-H] ⁺	523.4002	10	PCIO-1:0:0-C27H58NO6P
40180	524.4132	[M-H] ⁺	523.4002	10	PCIO-1:0:0-C27H58NO6P
40184	524.4132	[M-H] ⁺	523.4002	10	PCIO-10:0:0-C27H58NO6P
40215	524.4132	[M-H] ⁺	523.4002	10	PCIO-16:0:0-C27H58NO6P
40220	524.4132	[M-H] ⁺	523.4002	10	PCIO-18:0:0-C27H58NO6P
40221	524.4132	[M-H] ⁺	523.4002	10	PCIO-18:0:0-C27H58NO6P
40222	524.4132	[M-H] ⁺	523.4002	10	PCIO-18:0:0-C27H58NO6P
40391	524.4132	[M-H] ⁺	523.4002	10	PCIO-19:0:0-C27H58NO6P
43416	524.4132	[M-H] ⁺	523.4002	11	2-O-urethyl 7 C27H58NO6 77286-66-9
3739	524.3813	[M-H] ⁺	501.3852	13	(Z)-2-hexano C28H56NO4S
24068	510.349	[M-H] ⁺	509.3481	12	1-heptadecan C25H52NO7 50930-21-9
40033	510.349	[M-H] ⁺	509.3481	12	PCIO-1:0:16-C25H52NO7P
40053	510.349	[M-H] ⁺	509.3481	12	PCIO-15:0:2-C25H52NO7P
40054	510.349	[M-H] ⁺	509.3481	12	PCIO-15:0:2-C25H52NO7P
40057	510.349	[M-H] ⁺	509.3481	12	PCIO-16:0:1-C25H52NO7P
40158	510.349	[M-H] ⁺	509.3481	12	PC16:0:0-1-C25H52NO7P
40290	510.349	[M-H] ⁺	509.3481	12	PC17:0:0:0-C25H52NO7P
40291	510.349	[M-H] ⁺	509.3481	12	PC17:0:0:0-C25H52NO7P
62269	510.349	[M-H] ⁺	509.3481	12	LysePC(17:0) C25H52NO7P
62296	510.349	[M-H] ⁺	509.3481	12	LysePC(20:0) C25H52NO7P
62785	510.349	[M-H] ⁺	509.3481	12	LysePC(17:0) C25H52NO7P
63707	510.349	[M-H] ⁺	509.3353	12	Narbeneycin C28H47NO7 6056-25-5
76587	510.349	[M-H] ⁺	509.3481	12	PC16:0:0-1-C25H52NO7P
77678	510.349	[M-H] ⁺	509.3481	12	PE(20:0:0:0) C25H52NO7P
80028	525.3533	[M-H] ⁺	524.3478	3	PG(P-20:0:0) C26H52O8P
92593	525.3533	[M-H] ⁺	502.3658	3	Ganoderic acid C31H50O5 114557-49-6
66335	525.4012	[M-H] ⁺	502.4175	10	2-Hexapreny C36H64O
42451	525.3852	[M-Na] ⁺	502.4022	11	11-Hydroxy C32H54O4
42452	525.3852	[M-Na] ⁺	502.4022	11	11,25-dihydro C32H54O4
42453	525.3852	[M-Na] ⁺	502.4022	11	(2S)-11,25-C32H54O4
42454	525.3852	[M-Na] ⁺	502.4022	11	(2S)-11,25-C32H54O4
42455	525.3852	[M-Na] ⁺	502.4022	11	26,27-dihydro C32H54O4
42539	525.3852	[M-Na] ⁺	502.4022	11	11,25-Dihydro C32H54O4
34488	524.3654	[M-H] ⁺	523.3638	10	PAF C-16 C26H54NO7 74389-68-7
40075	524.3654	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40076	524.3654	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40077	524.3654	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40161	524.3654	[M-H] ⁺	523.3638	10	PC2:0:0-16-C26H54NO7P
40292	524.3654	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40293	524.3654	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40294	524.3654	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40342	524.3654	[M-H] ⁺	523.3638	10	PCIO:0:18:0-C26H54NO7P
40343	524.3654	[M-H] ⁺	523.3638	10	PCIO:0:18:0-C26H54NO7P
40344	524.3654	[M-H] ⁺	523.3638	10	PCIO:0:18:0-C26H54NO7P
43413	524.3654	[M-H] ⁺	523.3638	10	LysePC(18:0) C26H54NO7P
61694	524.3654	[M-H] ⁺	523.3638	10	LysePC(18:0) C26H54NO7P
61695	524.3654	[M-H] ⁺	523.3638	10	LysePC(18:0) C26H54NO7P
77692	524.3654	[M-H] ⁺	523.3638	10	PE(21:0:0:0) C26H54NO7P
4075	546.3474	[M-H] ⁺	545.3481	14	1-(RZ)-1,12,14-C28H52NO7P
61703	546.3474	[M-H] ⁺	545.3481	14	LysePC(20:3) C28H52NO7P
61704	546.3474	[M-H] ⁺	545.3481	14	LysePC(20:3) C28H52NO7P
76575	546.3474	[M-H] ⁺	545.3481	14	PC20:3(6Z)/C28H52NO7P
34488	546.3474	[M-H] ⁺	523.3638	10	PAF C-16 C26H54NO7 74389-68-7
40075	546.3474	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40076	546.3474	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40077	546.3474	[M-H] ⁺	523.3638	10	PCIO-16:0:2-C26H54NO7P
40161	546.3474	[M-H] ⁺	523.3638	10	PC2:0:0-16-C26H54NO7P
40292	546.3474	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40293	546.3474	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40294	546.3474	[M-H] ⁺	523.3638	10	PC18:0:0:0-C26H54NO7P
40342	546.3474	[M-H] ⁺	523.3638	10	PCIO:0:18:0-C26H54NO7P

40343	546.3474	[M-H]	523.3638	10	PC(0.0/18.0)/C26H54NO7P
40344	546.3474	[M-H]	523.3638	10	PC(0.0/18.0)/C26H54NO7P
43413	546.3474	[M-H]	523.3638	10	lysine-PAP C26H54NO7 117985-57-6
61694	546.3474	[M-H]	523.3638	10	LysylPC(18:0)/C26H54NO7P
61991	546.3474	[M-H]	523.3638	10	LysylPC(20:0)/C26H54NO7P
77692	546.3474	[M-H]	523.3638	10	PE(21:0/0:0)/C26H54NO7P
61711	570.3493	[M-H]	569.3481	10	LysylPC(22:5)/C30H52NO7P
61712	570.3493	[M-H]	569.3481	10	LysylPC(22:5)/C30H52NO7P
95159	570.3493	[M-H]	569.3505	14	Janthrone C37H47NO4 73561-91-8
40019	570.3493	[M-H]	547.3638	6	PC(O-18:2)/C28H54NO7P
40020	570.3493	[M-H]	547.3638	6	PC(O-18:2)/C28H54NO7P
61702	570.3493	[M-H]	547.3638	6	LysylPC(20:2)/C28H54NO7P
76574	570.3493	[M-H]	547.3638	6	PC(20:2)/C28H54NO7P
63709	547.3477	[M-H]	546.3404	0	3-O-Mycaric C28H50O10 34698-88-9
40019	548.3661	[M-H]	547.3638	9	PC(O-18:2)/C28H54NO7P
40020	548.3661	[M-H]	547.3638	9	PC(O-18:2)/C28H54NO7P
61702	548.3661	[M-H]	547.3638	9	LysylPC(20:2)/C28H54NO7P
76574	548.3661	[M-H]	547.3638	9	PC(20:2)/C28H54NO7P
40373	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
40375	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
40376	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
40404	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
40405	508.3711	[M-H]	507.3689	9	PC(P-18:0)/C26H54NO6P
76582	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
76583	508.3711	[M-H]	507.3689	9	PC(O-18:1)/C26H54NO6P
96524	508.3711	[M-H]	485.3783	6	Lysyl-PAP C C24H48N4NA
24070	482.3663	[M-H]	481.3532	12	Lysyl-PAP C C24H48N4NA 52691-62-0
40201	482.3663	[M-H]	481.3532	12	PC(O-15:0)/C24H52NO6P
40256	482.3663	[M-H]	481.3532	12	PC(O-8:0)/C24H52NO6P
40257	482.3663	[M-H]	481.3532	12	PC(O-8:0)/C24H52NO6P
40384	482.3663	[M-H]	481.3532	12	PC(O-16:0)/C24H52NO6P
40385	482.3663	[M-H]	481.3532	12	PC(O-16:0)/C24H52NO6P
40386	482.3663	[M-H]	481.3532	12	PC(O-16:0)/C24H52NO6P
90486	509.3753	[M-Na]	508.3705	4	2'-Apo-beta-c C37H68O 5525-46-2
78660	774.557	[M-H]	773.5571	9	PS(O-16:0)/C42H80NO9P
78675	774.557	[M-H]	773.5571	9	PS(O-18:0)/C42H80NO9P
78759	774.557	[M-H]	773.5571	9	PS(P-16:0)/C42H80NO9P
78803	774.557	[M-H]	773.5571	9	PS(P-20:0)/C42H80NO9P
78831	774.557	[M-H]	773.5571	9	PS(P-18:0)/C42H80NO9P
61000	800.5652	[M-Na]	777.5672	10	PE(22:4/22:1)/C45H80NO7P
61001	800.5652	[M-Na]	777.5672	10	PE(22:4/22:1)/C45H80NO7P
61032	800.5652	[M-Na]	777.5672	10	PE(22:5/22:2)/C45H80NO7P
61065	800.5652	[M-Na]	777.5672	10	PE(22:5/22:2)/C45H80NO7P
62196	800.5652	[M-Na]	777.5672	10	PE(P-18:0)/C45H80NO7P
62197	800.5652	[M-Na]	777.5672	10	PE(P-18:0)/C45H80NO7P
62223	800.5652	[M-Na]	777.5672	10	PE(P-18:1)/C45H80NO7P
62252	800.5652	[M-Na]	777.5672	10	PE(P-18:1)/C45H80NO7P
76406	800.5652	[M-Na]	777.5672	10	PE(O-18:0)/C45H80NO7P
77664	800.5652	[M-Na]	777.5672	10	PE(P-20:0)/C45H80NO7P
103142	826.5829	[M-H]	825.5731	3	PI-Cor(18:0)/C42H84NO12P
103147	826.5829	[M-H]	825.5731	3	PI-Cor(20:0)/C42H84NO12P
103160	826.5829	[M-H]	825.5731	3	PI-Cor(18:0)/C42H84NO12P
103177	826.5829	[M-H]	825.5731	3	PI-Cor(20:0)/C42H84NO12P
77670	826.5829	[M-H]	803.5829	13	PE(P-20:0)/C47H82NO7P
78662	826.5829	[M-H]	803.604	12	PS(O-16:0)/C44H86NO9P
78681	826.5829	[M-H]	803.604	12	PS(O-18:0)/C44H86NO9P
78699	826.5829	[M-H]	803.604	12	PS(O-20:0)/C44H86NO9P
78764	826.5829	[M-H]	803.604	12	PS(P-16:0)/C44H86NO9P
78786	826.5829	[M-H]	803.604	12	PS(P-18:0)/C44H86NO9P
78807	826.5829	[M-H]	803.604	12	PS(P-20:0)/C44H86NO9P
66426	184.9432	[M-H]	183.9353	3	Arachidonic acid C20H34O5 107-38-0
44843	343.259	[M-H]	342.2559	12	Camphor C15H24O 1242-67-7
44958	343.259	[M-H]	342.2559	12	Dodecylacetate C21H42O2 2566-96-7
74389	343.259	[M-H]	342.2559	12	TriHA C23H46O2
44939	343.259	[M-H]	320.2715	5	Dihomo-P-Li C21H40O2 21061-10-9
57885	343.259	[M-H]	320.2715	5	3a,20b-Preg C21H40O2
58339	343.259	[M-H]	320.2715	5	7a,17-dimeth C21H40O2 13611-10-4
63335	343.259	[M-H]	320.2715	5	Pregnenediol C21H40O2 80-92-2
63356	343.259	[M-H]	320.2715	5	5-Si-Pregnane C21H40O2 566-58-5
65503	343.259	[M-H]	320.2715	5	5-(Z,Z,Z,Z,Z) C21H40O2 NA
68597	343.259	[M-H]	320.2715	5	5-Pentadecyl C21H40O2 3158-56-3
70381	343.259	[M-H]	320.2715	5	6a,17-Di C21H40O2
70481	343.259	[M-H]	320.2715	5	6aeta,17-Di C21H40O2
70541	343.259	[M-H]	320.2715	5	11,17-Dimeth C21H40O2
70686	343.259	[M-H]	320.2715	5	3-Ethyl-5a,8 C21H40O2
74400	343.259	[M-H]	320.2715	5	21,3,5Z,14Z C21H40O2
91768	343.259	[M-H]	320.2715	5	1-Hydroxy-2 C21H40O2
97251	343.259	[M-H]	320.2715	5	(E,E)-3,7,11 C21H40O2
98205	343.259	[M-H]	320.2715	5	7E,9E-4,6,10 C21H40O2

Supplementary Table I. Pathway enrichment of co-regulated metabolites.

Metabolic pathways altered in RA synovial fluid. Metabolites in clusters 1.1 and 1.2 of Figure 1A were identified via METLIN and enriched for relevant pathways via IMPaLA.

[illegible]

[illegible]

76382	508.3711	[M-H]	507.3689	9	PC(10-18:1)(12:0,0)	C20H54NO6P
76383	508.3711	[M-H]	507.3689	9	PC(10-18:1)(0:0,0)	C20H54NO6P
96234	508.3711	[M-H]	485.3783	6	Lys-PAP C-16-44	C34H48N4O11NA
24070	482.3663	[M-H]	481.3532	12	Lys-PAP C-16	C24H32N2O10NA
40201	482.3663	[M-H]	481.3532	12	PC(10-15:0)-1:0[U]	C24H32NO6P
40256	482.3663	[M-H]	481.3532	12	PC(10-8:0)-8:0	C24H32NO6P
40257	482.3663	[M-H]	481.3532	12	PC(10-8:0)-8:0[U]	C24H32NO6P
40384	482.3663	[M-H]	481.3532	12	PC(10-16:0)-0:0	C24H32NO6P
40385	482.3663	[M-H]	481.3532	12	PC(10-16:0)-0:0[U]	C24H32NO6P
40386	482.3663	[M-H]	481.3532	12	PC(10-16:0)-0:0[U]	C24H32NO6P
90486	509.3751	[M-Na]	508.3705	4	2'-Apobeta-cristatal	C37H48O3
78660	774.5571	[M-H]	773.5571	9	PhQ-16:0(20:1)(2,14Z)	C42H80NO6P
78675	774.5571	[M-H]	773.5571	9	PhQ-18:0(18:2)(9Z,12Z)	C42H80NO6P
78739	774.5571	[M-H]	773.5571	9	PhQ-16:0(20:1)(12Z)	C42H80NO6P
78803	774.5571	[M-H]	773.5571	9	PhQ-20:0(16:1)(9Z)	C42H80NO6P
78831	774.5571	[M-H]	773.5571	9	PhQ-18:0(18:1)(9Z)	C42H80NO6P
61000	800.5652	[M-Na]	777.5672	10	PE(22-4:7Z,10Z,13Z,16Z)P-18:1(11Z)	C45H88NO7P
61001	800.5652	[M-Na]	777.5672	10	PE(22-4:7Z,10Z,13Z,16Z)P-18:1(9Z)	C45H88NO7P
61052	800.5652	[M-Na]	777.5672	10	PE(25-5:4Z,7Z,10Z,13Z,16Z)aa(18:0)	C45H88NO7P
61065	800.5652	[M-Na]	777.5672	10	PE(22-5:7Z,10Z,13Z,16Z,19Z)P-18:0	C45H88NO7P
62196	800.5652	[M-Na]	777.5672	10	PE(18-18:0)-22-5:4Z,7Z,10Z,13Z,16Z)	C45H88NO7P
62197	800.5652	[M-Na]	777.5672	10	PE(18-18:0)-22-5:7Z,10Z,13Z,16Z,19Z)	C45H88NO7P
62223	800.5652	[M-Na]	777.5672	10	PE(18-18:1)(11Z)-22-4:7Z,10Z,13Z,16Z)	C45H88NO7P
62252	800.5652	[M-Na]	777.5672	10	PE(18-18:1)(9Z)-22-4:7Z,10Z,13Z,16Z)	C45H88NO7P
76406	800.5652	[M-Na]	777.5672	10	PE(10-18:0)-22-4:4Z,7Z,10Z,13Z,16Z,19Z)	C45H88NO7P
77664	800.5652	[M-Na]	777.5672	10	PE(18-20:20-5:5Z,8Z,11Z,14Z,17Z)	C45H88NO7P
103142	826.5829	[M-H]	825.5731	3	PE-Car(18:0)(18:0)	C42H84NO12P
103147	826.5829	[M-H]	825.5731	3	PE-Car(20:0)(16:0)	C42H84NO12P
103160	826.5829	[M-H]	825.5731	3	PE-Car(18:0)(18:0C20H)	C42H84NO12P
103177	826.5829	[M-H]	825.5731	3	PE-Car(20:0)(16:0C20H)	C42H84NO12P
77670	826.5829	[M-H]	803.604	13	PEP-20:0(22-6:4Z,7Z,10Z,13Z,16Z,19Z)	C47H82NO7P
78662	826.5829	[M-H]	803.604	12	PhQ-16:0(22:1)(12Z)	C44H86NO6P
78681	826.5829	[M-H]	803.604	12	PhQ-18:0(20:1)(12Z)	C44H86NO6P
78689	826.5829	[M-H]	803.604	12	PhQ-20:0(18:1)(9Z)	C44H86NO6P
78764	826.5829	[M-H]	803.604	12	PhQ-16:0(22:0)	C44H86NO6P
78786	826.5829	[M-H]	803.604	12	PhQ-18:0(20:0)	C44H86NO6P
78807	826.5829	[M-H]	803.604	12	PhQ-20:0(18:0)	C44H86NO6P
66426	184.9432	[M-H]	183.9333	3	Aromatocaine	C20H34N6P
44843	343.259	[M-H]	342.2559	12	Canabidiol dimethyl ether	C21H34O2
44958	343.259	[M-H]	342.2559	12	Decanoicacetic Acid methyl ester	C21H34O2
54389	343.259	[M-H]	342.2559	12	TdH4	C21H34O2
44939	343.259	[M-H]	320.2715	5	Dihomo-P-Limonene Acid methyl ester	C21H36O2
57885	343.259	[M-H]	320.2715	5	26-28-Pregnenediol	C21H36O2
58339	343.259	[M-H]	320.2715	5	7a,17-dimethyl-28-Androstane-3a,17b-diol	C21H36O2
63335	343.259	[M-H]	320.2715	5	Pregnenediol	C21H36O2
63336	343.259	[M-H]	320.2715	5	St-Pregnen-3L-20b-diol	C21H36O2
65093	343.259	[M-H]	320.2715	5	5Z,Z(R,Z,L11(Z)-Eicosatrienoic Acid methyl ester	C21H36O2
68097	343.259	[M-H]	320.2715	5	5-Pentamethylisovalinal	C21H36O2
70381	343.259	[M-H]	320.2715	5	6alpha,17-Dimethyl-Sulpha-androstane-3beta,17beta-C21H36O2	C21H36O2
70481	343.259	[M-H]	320.2715	5	6beta,17-Dimethyl-Sulpha-androstane-3beta,17beta-C21H36O2	C21H36O2
70541	343.259	[M-H]	320.2715	5	11,17-Dimethyl-Sulpha-androstane-11beta,17beta-diolC21H36O2	C21H36O2
70686	343.259	[M-H]	320.2715	5	3-Ethyl-Sulpha-androstane-3alpha,17beta-diol	C21H36O2
74400	343.259	[M-H]	320.2715	5	31-35Z,14Z,17Z)	C21H36O2
91768	343.259	[M-H]	320.2715	5	1-Hydroxy-2,12,15-hexacosatriene-4-one	C21H36O2
97251	343.259	[M-H]	320.2715	5	(R,R)-3,7,11-Triethyl-2,6,10-tetradecatrienyl hexanoateC21H36O2	C21H36O2
96205	343.259	[M-H]	320.2715	5	7E,9E-Hexacosadiene-6,11-one	C21H36O2

Supplementary Table II Volcano plot enrichment of significantly upregulated and downregulated metabolites in diseased synovial fluid. Global metabolic profiling revealed significantly

Upregulated in RA		Downregulated in RA	
Log2 fold change	p-value	Log2 fold change	p-value
431.0161	1.16	548.3661	0.03
547.3477	6.31	61.702	0.0122
570.3609	6.33	76.754	0.0166
351.728	5.05	67.709	0.0155
296.8079	4.72	67.171	0.0175
236.8118	2.55	67.712	0.0208
546.3474	4.31	546.3474	0.0297
158.0799	4.47	40.019	0.0403
523.3784	17.8	40.020	0.0403
523.3561	16.01	76.754	0.0403
341.239	3.35	40.020	0.0403

Metabolic pathway	Metabolic pathway
Glucosylated & Methylated Metabolites	Glucosylated & Methylated Metabolites
Glucosylated & Methylated Metabolites	Glucosylated & Methylated Metabolites
Glucosylated & Methylated Metabolites	Glucosylated & Methylated Metabolites

unregulated or downregulated metabolites. Significant metabolites with a p-value<0.05 and greater than two-fold change in the upper right and left quadrants of Figure 1D were matched to metabolite identities

Upregulated in RA		Downregulated in RA	
Log2 fold change	p-value	Log2 fold change	p-value
431.0161	1.16	548.3661	0.03
547.3477	6.31	61.702	0.0122
570.3609	6.33	76.754	0.0166
351.728	5.05	67.709	0.0155
296.8079	4.72	67.171	0.0175
236.8118	2.55	67.712	0.0208
546.3474	4.31	546.3474	0.0297
158.0799	4.47	40.019	0.0403
523.3784	17.8	40.020	0.0403
523.3561	16.01	76.754	0.0403
341.239	3.35	40.020	0.0403

Figure 1D were matched to metabolite identities

Upregulated in RA		Downregulated in RA	
Log2 fold change	p-value	Log2 fold change	p-value
431.0161	1.16	548.3661	0.03
547.3477	6.31	61.702	0.0122
570.3609	6.33	76.754	0.0166
351.728	5.05	67.709	0.0155
296.8079	4.72	67.171	0.0175
236.8118	2.55	67.712	0.0208
546.3474	4.31	546.3474	0.0297
158.0799	4.47	40.019	0.0403
523.3784	17.8	40.020	0.0403
523.3561	16.01	76.754	0.0403
341.239	3.35	40.020	0.0403

Supplementary Table III. METLIN identification of potential RA biomarkers. ROC analysis identified 30 putative biomarkers of RA in human synovial fluid (AUC >0.9). 15 metabolites did not match to any known metabolite identities. The remaining 15 metabolites matched to 119 potential metabolite identities (m/z $\pm$ 15 ppm).

m/z >0.9	m/z	adduct	mass	ppm	name
89.519249	184.94318	[M+Na]	183.9353	3	Arsonoacetate
90.020088		[M+H]	342.2559	12	Cannabidiol dimethyl ether
90.033287		[M+H]	342.2559	12	Docosahexaenoic Acid methyl ester
138.90434		[M+H]	342.2559	12	TrHA
138.91664		[M+H]	320.2715	4	Dihomo- γ -Linolenic Acid methyl ester
184.94318		[M+H]	320.2715	4	3a,20b-Pregnanediol
198.85887		[M+H]	320.2715	4	7a,17-dimethyl-5b-Androstane-3a,17b-diol
245.1837		[M+H]	320.2715	4	Pregnanediol
256.81381		[M+H]	320.2715	4	5 β -Pregnane-3a,20a-diol
343.25903		[M+H]	320.2715	4	5(Z),8(Z),11(Z)-Eicosatrienoic Acid methyl ester
351.758		[M+H]	320.2715	4	6a,17-Dimethyl-5a-androstane-3 β ,17 β -diol
482.35104		[M+H]	320.2715	4	6 β ,17-Dimethyl-5a-androstane-3 β ,17 β -diol
482.3663		[M+H]	320.2715	4	11,17-Dimethyl-5a-androstane-11 β ,17 β -diol
496.414		[M+H]	320.2715	4	3-Ethyl-5a-androstane-3a,17 β -diol
497.32098		[M+H]	320.2715	4	21:3(5Z,14Z,17Z)
497.33649		[M+H]	320.2715	4	1-Hydroxy-2,12,15-heneicosatrien-4-one
497.35199		[M+H]	320.2715	4	(E,E)-3,7,11-Trimethyl-2,6,10-dodecatrienyl hexanoate
497.36749		[M+H]	320.2715	4	7E,9E-Heneicosadien-6,11-one
497.38303		[M+H]	496.3122	3	Postin
497.39853		[M+H]	496.3165	5	PG(P-18:0/0:0)
498.33746		[M+H]	474.3345	5	18-acetoxy- α ,25-dihydroxyvitamin D3 / 18-acetoxy-1 α ,25-dihydroxycholecalciferol
498.35297		[M+H]	474.3345	5	11-acetoxy-3 β ,6a-dihydroxy-24-methyl-27-nor-9,11-seco-5a-cholesta-7,22E-dien-9-one
498.3685		[M+H]	474.3345	5	(3 β ,17 α ,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one
508.37112		[M+H]	474.3345	5	(3 β ,17 α ,23S)-17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one
510.349	509.37527	[M+Na]	508.3705	4	2'-Apo-beta-carotenal
520.31982	520.31982	[M+H]	497.3353	8	Tumonoic Acid I
520.33569		[M+H]	519.3325	7	1-Linoleoylglycerophosphocholine
520.3512		[M+H]	519.3325	7	PC(18:2(2E,4E)/0:0)
520.36743		[M+H]	519.3325	7	PC(18:2(9Z,12Z)/0:0)
520.3833		[M+H]	519.3325	7	PC(18:2(9Z,12Z)/0:0)[U]
520.39911		[M+H]	519.3325	7	LysoPC(18:2(9Z,12Z))
523.35449	520.3833	[M+Na]	519.3689	13	PC(P-19:1(12Z)/0:0)
523.37042		[M+H]	522.3709	14	1 α -hydroxy-18-[m-(1-hydroxy-1-ethylpropyl)-benzyloxy]-23,24,25,26,27-pentanorvitamin
523.38635		[M+H]	522.3604	5	Oleic Acid-biotin
524.34949		[M+H]	500.3866	10	Oleananoic acid acetate
524.36542		[M+H]	500.3866	10	3 β -Hydroxylanostane-7,11-dione acetate
524.38135		[M+H]	773.5571	9	PS(O-16:0/20:2(11Z,14Z))
524.39728		[M+H]	773.5571	9	PS(O-18:0/18:2(9Z,12Z))
524.41321		[M+H]	773.5571	9	PS(P-16:0/20:1(11Z))
524.42914		[M+H]	773.5571	9	PS(P-20:0/16:1(9Z))
525.35333		[M+H]	773.5571	9	PS(P-18:0/18:1(9Z))
525.36926		[M+H]	797.5418	0	PI-Cer(t18:0/16:0)
525.38519		[M+H]	797.5418	0	PI-Cer(d18:0/16:0(2OH))
525.40118		[M+H]	775.5516	10	PE(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
546.34735		[M+H]	775.5516	10	PE(22:5(4Z,7Z,10Z,13Z,16Z)/P-18:1(11Z))
547.34766		[M+H]	775.5516	10	PE(22:5(4Z,7Z,10Z,13Z,16Z)/P-18:1(9Z))
548.36608		[M+H]	775.5516	10	PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-18:1(11Z))
570.3493		[M+H]	775.5516	10	PE(22:5(7Z,10Z,13Z,16Z,19Z)/dm18:1(9Z))
176.06178		[M+H]	775.5516	10	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:0)
351.74496		[M+H]	775.5516	10	PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))
508.35544		[M+H]	775.5516	10	PE(P-18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))
508.38681		[M+H]	775.5516	10	PE(P-18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))
509.37527		[M+H]	775.5516	10	PE(P-18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))
774.55701		[M+H]	798.541	8	PG(18:0/20:4(5Z,8Z,11Z,14Z))
798.54938		[M+H]	798.5411	8	PG(16:0/22:4(7Z,10Z,13Z,16Z))
799.55487		[M+H]	798.5411	8	PG(18:1(11Z)/20:3(5Z,8Z,11Z))
800.56525		[M+H]	798.5411	8	PG(18:1(11Z)/20:3(8Z,11Z,14Z))
822.55143		[M+H]	798.5411	8	PG(18:1(9Z)/20:3(5Z,8Z,11Z))
824.56451		[M+H]	798.5411	8	PG(18:1(9Z)/20:3(8Z,11Z,14Z))
826.58295		[M+H]	798.5411	8	PG(18:2(9Z,12Z)/20:2(11Z,14Z))
		[M+H]	798.5411	8	PG(18:3(6Z,9Z,12Z)/20:1(11Z))
		[M+H]	798.5411	8	PG(18:3(9Z,12Z,15Z)/20:1(11Z))
		[M+H]	798.5411	8	PG(18:4(6Z,9Z,12Z,15Z)/20:0)
		[M+H]	798.5411	8	PG(20:1(11Z)/18:3(6Z,9Z,12Z))
		[M+H]	798.5411	8	PG(20:1(11Z)/18:3(9Z,12Z,15Z))
		[M+H]	798.5411	8	PG(20:2(11Z,14Z)/18:2(9Z,12Z))
		[M+H]	798.5411	8	PG(20:3(8Z,11Z,14Z)/18:1(9Z))
		[M+H]	798.5411	8	PG(20:4(5Z,8Z,11Z,14Z)/18:0)
		[M+H]	798.5411	8	PG(22:4(7Z,10Z,13Z,16Z)/16:0)
		[M+H]	798.5411	8	PG(20:0/18:4(6Z,9Z,12Z,15Z))
		[M+H]	776.5567	11	PG(18:0/18:1(9Z))[U]
	799.55487	[M+H]	776.5567	11	PG(18:0/18:1(9Z))

		[M+H]	776.5567	11	1-Stearoyl-2-Oleoyl-sn-Glycero-3-[Phospho-rac-(1-glycerol)]
		[M+H]	776.5567	11	PG(18:0/18:1(11Z))
		[M+H]	776.5567	11	PG(18:1(11Z)/18:0)
		[M+H]	776.5567	11	PG(18:1(9Z)/18:0)
		[M+H]	776.5567	11	PG(14:0/22:1(11Z))
		[M+H]	776.5567	11	PG(14:1(9Z)/22:0)
		[M+H]	776.5567	11	PG(15:1(9Z)/21:0)
		[M+H]	776.5567	11	PG(16:1(9Z)/20:0)
		[M+H]	776.5567	11	PG(17:0/19:1(9Z))
		[M+H]	776.5567	11	PG(17:1(9Z)/19:0)
		[M+H]	776.5567	11	PG(19:0/17:1(9Z))
		[M+H]	776.5567	11	PG(19:1(9Z)/17:0)
		[M+H]	776.5567	11	PG(20:0/16:1(9Z))
		[M+H]	776.5567	11	PG(20:1(11Z)/16:0)
		[M+H]	776.5567	11	PG(21:0/15:1(9Z))
		[M+H]	776.5567	11	PG(22:0/14:1(9Z))
		[M+H]	776.5567	11	PG(22:1(11Z)/14:0)
		[M+H]	776.5567	11	PG(16:0/20:1(11Z))
	800.56525	[M+Na]	777.5672	10	PE(22:4(7Z,10Z,13Z,16Z)/P-18:1(11Z))
		[M+Na]	777.5672	10	PE(22:4(7Z,10Z,13Z,16Z)/P-18:1(9Z))
		[M+Na]	777.5672	10	PE(22:5(4Z,7Z,10Z,13Z,16Z)/dm18:0)
		[M+Na]	777.5672	10	PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-18:0)
		[M+Na]	777.5672	10	PE(P-18:0/22:5(4Z,7Z,10Z,13Z,16Z))
		[M+Na]	777.5672	10	PE(P-18:0/22:5(7Z,10Z,13Z,16Z,19Z))
		[M+Na]	777.5672	10	PE(P-18:1(11Z)/22:4(7Z,10Z,13Z,16Z))
		[M+Na]	777.5672	10	PE(P-18:1(9Z)/22:4(7Z,10Z,13Z,16Z))
	822.55143	[M+Na]	777.5672	10	PE(O-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
		[M+Na]	777.5672	10	PE(P-20:0/20:5(5Z,8Z,11Z,14Z,17Z))
		[M+Na]	799.5727	12	PS(O-18:0/20:3(8Z,11Z,14Z))
		[M+Na]	799.5727	12	PS(O-20:0/18:3(6Z,9Z,12Z))
		[M+Na]	799.5727	12	PS(O-20:0/18:3(9Z,12Z,15Z))
	824.56451	[M+Na]	799.5727	12	PS(P-16:0/22:2(13Z,16Z))
		[M+Na]	799.5727	12	PS(P-18:0/20:2(11Z,14Z))
		[M+Na]	799.5727	12	PS(P-20:0/18:2(9Z,12Z))
		[M+Na]	823.5479	11	C18-OH Sulfatide
	826.58295	[M+H]	825.5731	3	PI-Cer(t18:0/18:0)
		[M+H]	825.5731	3	PI-Cer(t20:0/16:0)
		[M+H]	825.5731	3	PI-Cer(d18:0/18:0(2OH))
		[M+H]	825.5731	3	PI-Cer(d20:0/16:0(2OH))
		[M+H]	803.5829	13	PE(P-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
		[M+H]	803.604	12	PS(O-16:0/22:1(11Z))
		[M+H]	803.604	12	PS(O-18:0/20:1(11Z))
		[M+H]	803.604	12	PS(O-20:0/18:1(9Z))
		[M+H]	803.604	12	PS(P-16:0/22:0)
		[M+H]	803.604	12	PS(P-18:0/20:0)
		[M+H]	803.604	12	PS(P-20:0/18:0)

Supplementary Table IV. Metabolomics data. LC-MS based metabolomic profiling of RA and healthy (H) synovial fluid detected a large multivariate dataset with over a thousand metabolite features and corresponding peak intensities.

m/z	H1	H2	H3	H4	H5	RA1	RA2	RA3
60.042408	12454	16752	10550	15593	15962	6418	0	12982
60.053188	3557	4258	2895	4020	4151	0	2930	3271
61.038174	260446	267141	210479	229631	403390	201525	180529	230244
61.049042	67898	66960	57027	57289	159785	53356	45753	58031
64.013374	33683	0	0	38189	34597	15807	30718	0
64.024506	10027	0	0	10737	9754	0	8987	0
64.035637	2047	0	0	2303	2099	0	1793	0
68.992561	12125	8686	12862	17932	13983	16784	11837	17990
69.00412	2918	0	3238	4109	3142	3959	2740	4159
70.062584	70398	0	89122	106434	91631	52311	58024	0
70.074226	20360	0	26983	30620	26072	15680	16851	0
72.041245	22591	0	0	0	19799	0	25742	14148
72.07962	154493	0	100721	0	117708	99375	55601	0
72.935432	7377	16338	7439	16460	16983	13598	6762	14958
72.947311	0	3488	1728	3449	3684	3028	0	3273
73.045364	0	0	8349	8256	9296	8119	9245	9007
74.059425	0	0	12844	23033	17578	18269	15968	0
74.095345	2580	0	0	0	0	0	2207	2416
81.51992	0	26510	5095	6902	0	5008	8437	25873
81.934921	4091	9118	4622	11356	10315	8372	3895	7574
84.041656	9420	0	10387	13300	14207	0	5310	0
84.959145	11006	11373	0	0	11156	6211	11128	10131
84.97197	2795	2998	0	0	3570	0	2051	2509
88.508682	0	0	6566	0	5057	8384	8533	0
89.506088	123121	68281	111205	151022	107470	149811	119790	154670
89.519249	41056	21356	34133	41757	26288	44120	42672	44702
89.532417	17406	5439	13821	15287	8840	16581	18305	16854
89.545578	11293	3235	9186	9572	5143	10271	12007	10796
89.562035	6243	0	5256	5061	0	5895	6812	6049
89.575195	2490	0	2104	0	0	1913	2744	2483
90.006889	20789	11524	18241	23284	15440	22984	20886	22784
90.020088	5231	2500	4540	5564	3547	5921	5855	5607
90.033287	1779	0	0	1846	0	1876	2017	1901
90.053085	86243	0	88012	0	73423	21374	23387	4236
90.505783	6713	6259	0	7327	6166	0	6179	6457
90.899918	7573	11922	7718	16787	18185	12926	6910	12515
90.976196	0	0	42648	0	0	32824	52635	0

90.989464	0	0	7982	0	0	6144	17746	0
91.002731	0	0	2062	0	0	1412	3180	0
92.896851	2460	4146	2703	5690	6949	4233	2434	3624
96.918144	4184	0	5839	5905	4812	2190	0	0
97.965179	5165	7417	5022	9391	9834	5005	4884	8512
97.975502	2111	3087	0	3854	4182	0	0	3401
99.076668	5836	0	9090	0	9662	4314	9115	0
102.0514	6516	0	9075	16631	12314	11144	9759	0
109.02067	4882	0	4368	3419	0	3962	4803	4502
110.01788	63730	0	53685	48350	27872	55250	64977	55421
110.02882	31857	0	24430	20296	11021	23737	30613	23872
110.03976	12789	0	9434	7360	3652	8637	12411	9026
110.0507	6112	0	4086	3052	0	3690	5607	3901
110.06165	4517	0	0	0	0	2495	4314	0
110.06895	10316	13674	12665	13276	14518	9419	7943	0
110.51818	11222	0	9875	6739	3932	8758	12225	9266
110.52914	4802	0	4248	3002	0	3839	5366	3910
113.95925	15647	21845	14357	26847	21647	0	15294	27043
113.97039	7218	9694	6982	11791	9353	0	7109	11975
113.98153	2112	2686	0	3478	2802	0	2101	3688
114.07066	22345	0	0	0	0	22656	11133	0
114.08923	98491	271254	57810	129703	127605	66252	86150	121399
115.95409	5070	6293	0	5033	5609	4260	6597	4219
115.96532	2150	2408	0	2086	2546	1836	2778	1928
116.06645	563078	0	682910	317437	718176	406986	396045	0
116.0777	312088	0	296932	0	319831	221750	218270	0
116.08894	118803	0	110755	120569	119953	80550	78655	0
116.10393	19964	49483	9041	0	0	10778	13440	25239
117.07272	36964	0	43991	51248	46915	26581	27912	0
117.95111	0	2065	0	1897	1993	0	2408	0
118.08334	0	0	352309	0	0	319026	321477	0
118.09468	0	17813	0	288163	0	176101	187096	0
118.10602	0	5207	75903	109059	0	62959	66556	0
118.12113	0	0	32884	34688	14502	26828	29492	0
119.08692	0	3310	29646	39855	21599	25066	25234	0
119.0983	9310	0	11205	14700	7829	9473	9406	0
120.06425	40059	0	76020	144224	92976	92325	91792	0
121.06854	38420	0	33915	34543	96126	33390	27909	37219
122.09238	68401	61418	54898	64506	68817	52171	65696	56963
122.10391	28718	25223	24065	26579	28696	22938	28072	23678
122.11544	8648	7643	7021	7922	8671	6966	8520	7049

122.12697	2867	2466	2368	2610	2859	2289	2787	2280
122.96238	12382	14959	11677	22775	19603	19446	11775	19435
122.97395	4382	4964	3914	7583	6632	6633	3857	6523
123.09738	6637	0	20580	42619	20523	9259	0	0
123.10896	2315	2352	2217	2748	2514	2062	0	2150
124.08326	54145	89535	34215	81444	75928	52361	50368	90516
124.09488	21603	35801	14002	32442	30061	21723	20650	36830
125.98483	28296	30752	0	34574	33995	16648	29681	29067
125.99654	9713	10481	0	13716	11519	5667	10129	9681
126.00825	2525	2713	0	3755	3051	1665	2663	2517
126.01996	102610	256080	168467	208657	255462	40025	17681	87221
126.03167	37365	96915	63540	78922	97254	14296	6120	31147
126.09024	14671	0	12062	0	0	9973	13086	0
126.10195	6323	0	4192	0	6764	3472	5073	0
128.06609	0	0	0	0	0	5016	3854	0
129.9304	7559	8979	6204	13920	14412	10141	6532	10224
129.94231	2775	0	2575	5427	5953	4514	0	4104
130.04539	110846	0	127552	152700	169475	0	58741	0
130.0573	48888	0	59030	66425	75106	0	25998	0
130.06918	15833	0	18894	21421	24737	0	7916	0
131.92801	103758	0	88857	201561	77170	146773	0	147285
131.94	37282	0	31836	74186	0	54114	33984	53361
131.95198	10979	0	9397	23332	23950	16621	9904	0
131.96396	4215	5165	3503	9317	9671	6327	3695	6364
131.97595	2916	0	2444	6625	6895	4564	2452	4416
132.06386	0	0	295435	289434	237081	106914	130702	0
132.07585	90913	0	0	0	0	38225	47477	0
132.09982	694988	0	0	0	0	617027	239164	0
132.92851	5717	6324	5211	10209	11095	7460	4635	7309
132.94055	2035	0	1963	3872	4247	3030	1880	2660
132.98065	4905	4953	0	0	5028	0	6054	4120
132.99268	1901	1878	0	1705	1934	0	2097	0
133.05685	31687	0	32065	31990	71560	14282	0	0
133.92476	35113	0	30116	62972	65505	46764	31590	47100
133.93683	12322	0	10669	21827	23117	16842	10916	16020
133.9489	3374	3485	2876	6111	6370	4804	2909	0
135.92433	4100	3366	0	3333	4689	2880	4811	3870
136.07033	11285	0	16748	0	23674	14556	4684	0
137.04161	326447	1159581	344980	598278	317225	165713	150124	206033
138.90434	5306	0	0	3976	4312	6139	6237	4516
138.91664	0	0	1540	0	0	2208	2019	1465

139.95972	2773	3653	0	4098	4612	2666	2328	3134
140.89934	0	2239	3456	2791	2925	4189	3884	2922
141.00255	2099	2644	0	3109	2449	0	2487	0
141.95395	32791	44196	0	22063	56783	0	30062	48468
141.95395	0	0	0	0	0	28734	14678	0
141.96638	13645	18078	12273	6609	0	0	12952	20414
141.99124	0	1651	0	2055	2093	0	0	1883
142.95844	2145	3276	0	3932	3881	2093	2035	3302
143.95395	7031	8405	0	9652	8431	4648	9334	9126
143.96648	3118	3400	0	4086	3670	0	4053	3897
144.10004	579013	0	133393	748192	76516	528327	0	0
144.11256	310045	0	47971	317522	26668	285556	0	0
144.12508	115263	0	14560	116055	0	102196	0	0
144.97804	0	0	0	35808	0	0	41727	48443
145.1037	44777	0	10889	57254	0	40051	0	0
145.95114	3019	3564	0	3778	4619	0	3863	3375
146.11505	25950	0	0	0	131480	11331	7743	11223
146.12766	9178	0	0	0	47939	4103	2719	3862
147.07507	337483	0	388552	0	472241	14140	0	0
147.12148	35182	54581	46756	31061	0	35187	0	46592
148.07632	0	0	27633	36229	36832	0	12846	0
148.9324	4877	0	4806	0	4870	4934	0	0
148.94513	1758	0	0	0	0	1711	2069	0
150.01662	0	3671	0	2556	0	0	3534	5085
150.05495	74001	0	107142	0	116844	43075	0	0
150.08904	8103	0	9099	12874	0	4102	10375	0
150.12312	0	0	0	0	3106	12849	4988	0
150.13591	0	0	0	0	0	5471	2143	0
150.92989	0	57846	0	38611	0	8969	33175	0
151.03209	5181	4905	0	7015	4264	0	2693	5246
152.06815	0	0	0	0	13528	13413	15780	0
152.08101	0	0	0	0	4528	4635	5398	0
152.10246	75827	0	59428	115614	97697	42681	105171	0
152.11533	32442	0	25427	49430	40987	18815	45024	0
152.12819	9993	0	0	15196	12571	5447	14274	0
154.05591	16526	58124	36334	23357	44208	2991	4517	0
154.9637	10190	9880	0	8901	0	8019	12517	0
156.07394	230553	325596	283403	270145	312756	222874	188053	260784
156.08699	88848	0	112729	104503	122692	85793	72296	98580
156.10002	96375	0	229077	107868	146749	127246	108562	0
156.11305	33858	0	85351	38428	52487	45760	38713	0

156.97894	4104	5407	0	4588	5202	3243	5505	0
157.07481	18185	23802	21342	19918	24762	16333	14479	20308
157.08789	8258	10109	10203	8314	11109	0	6654	8690
158.11388	74300	197687	61784	110997	106051	37858	84827	96603
158.127	28765	79599	24158	43009	41495	14903	33900	38370
158.97214	7756	0	7209	10236	8414	5899	9341	0
159.073	60887	0	0	0	33213	29083	23740	0
160.09222	120128	0	0	291204	18055	61761	0	0
160.10542	50823	0	0	127863	7052	26539	0	0
160.13184	0	0	35193	0	0	13821	0	81685
160.14503	0	0	0	0	33529	4598	4565	0
162.10945	281129	573454	290298	314076	640344	250340	157841	326489
162.12273	111796	321135	117133	120792	327666	99458	59734	131067
162.13602	37413	112805	39398	41012	116282	33513	18778	44640
162.14929	15158	50257	16000	19814	52525	13071	6924	18701
162.16258	10358	27985	10500	13999	33205	8817	4346	12644
162.18472	5103	15171	5502	9293	18808	4295	0	6412
163.11169	23640	44891	23880	33664	49763	21275	13087	27779
163.12502	9333	17355	9789	13104	20032	8379	5159	10910
163.13834	0	5134	2817	3765	6005	2549	0	3269
163.98784	10480	3132	8391	7774	4107	9172	10655	9183
164.00121	3597	0	2815	2848	0	3212	3817	3260
164.11256	0	4546	2779	4369	5658	2318	0	3226
166.05179	0	0	209858	0	269608	127303	155294	0
166.06495	0	0	78025	103547	99636	44871	55604	0
166.07867	0	0	0	636693	33470	13698	17389	0
166.08316	320945	0	582440	0	1043298	300214	252342	0
166.0966	109146	0	306199	0	347279	122660	0	0
167.00769	15731	14033	0	18514	15091	7408	12016	16954
167.02118	6833	5851	0	7577	6488	0	5026	7058
168.09708	336872	0	270301	321919	324741	201322	290670	0
168.1106	187871	0	126917	147422	176767	91922	136284	0
168.12413	68007	0	43138	52327	62505	30387	46948	0
168.13766	29261	0	17047	20970	25660	0	18273	0
168.15164	17226	0	0	12374	15337	0	10397	0
168.17374	9817	0	4905	6514	8412	3113	5444	0
169.03171	5680	16158	10713	6787	13484	2086	7232	7457
170.08684	70967	280119	117793	128546	197615	31304	27646	163121
170.11406	37096	110192	19871	35889	54875	26846	51148	53074
172.95164	76973	0	129488	0	233472	80776	161007	195790
172.95164	174493	0	57473	262697	101200	181139	0	0

172.96536	0	0	0	115819	0	0	72540	84308
172.96536	0	0	0	0	0	4718	2653	0
172.9928	9822	0	6580	14937	12401	9954	9194	0
173.00653	6014	3383	3641	8803	6892	5853	5247	5995
173.0294	3122	1525	1916	4661	3484	2811	2838	2911
173.9547	12466	9820	10448	17731	16776	12927	12277	13862
174.11069	0	0	0	0	0	21189	11619	0
174.95145	52472	0	43073	80219	70996	59297	48974	60980
174.96526	18600	0	14932	28456	24169	21653	17139	21257
174.97905	5370	0	4176	7847	6458	6059	4840	0
174.99286	1988	0	0	2866	2443	2154	1717	2138
175.11708	320669	393009	245939	306640	295265	65949	144761	240453
175.13089	176576	219964	92141	113879	110880	23288	50558	87742
175.1447	60135	77167	29886	37592	37298	0	15147	28074
175.95105	4539	3516	3205	5937	5886	4649	3659	4892
176.09869	184435	0	30279	0	97832	80991	75126	0
176.11255	75919	0	12232	0	0	34650	30254	0
176.94888	4561	4567	0	5051	4817	3859	5565	5315
182.07886	166243	0	209061	0	299164	161553	132071	0
182.98096	21467	17400	15529	26683	22840	0	19886	9738
182.98096	7945	0	0	10032	0	14715	0	26537
183.98434	2095	0	0	2650	2466	0	2101	2304
184.09285	318976	0	0	0	0	132006	224156	0
184.10701	134367	0	0	0	0	53398	93456	0
184.92899	6737	0	0	6049	0	6154	5563	3868
184.94318	0	0	0	0	0	2429	2007	1532
184.98102	13097	14508	0	16053	15837	8061	15025	18523
184.99519	5042	5319	0	5973	5988	3059	5577	7015
185.12294	20444	73873	73847	118445	51046	0	24378	137351
186.92535	4173	0	0	3303	0	4788	3700	0
186.97766	5908	6014	0	6298	6965	3190	6030	6489
187.13939	12171	0	19577	17292	25525	47174	12755	12014
188.06824	0	0	10642	0	0	27389	18919	0
190.96444	3216	0	0	5049	3591	0	3495	3199
191.95596	14061	53182	0	49190	21581	0	45480	52650
191.97041	0	24235	0	21989	9860	0	21383	24673
193.9559	0	18258	9298	18601	7654	4652	16390	18533
196.86301	0	0	0	2475	3024	0	3498	3055
198.85887	0	2228	3600	2500	2727	3995	4116	2975
200.12614	0	0	0	59529	0	0	26520	30689
203.14835	15023	40414	38671	0	39578	9739	8018	21287

203.92731	4553	6919	2390	12067	7814	3108	4735	0
204.08128	9132	0	6362	29210	0	0	0	0
204.13594	0	0	0	0	71095	12025	8105	0
204.15085	4560	0	0	0	22327	3373	2070	0
205.12094	7023	0	0	0	21825	4411	2593	0
205.92363	7078	5233	3366	8298	7164	7758	5703	0
206.88791	0	0	5499	0	0	5487	5795	4277
207.91965	77549	22156	36290	59152	0	117334	0	39880
207.92967	46440	13307	22584	36388	34153	77709	38184	0
208.13031	11668	0	8430	7164	14217	7933	12435	0
208.14035	5633	0	4089	3586	6908	3916	6275	0
209.12489	24416	0	0	0	0	53581	65894	0
209.13495	12910	0	0	0	0	28226	32992	0
209.92024	43389	0	0	34144	33804	74316	37751	22416
213.98071	3298	0	2482	3772	2895	3299	2933	3032
214.10283	4013	0	0	0	8120	4031	8434	0
214.13846	16256	0	0	0	0	13250	16444	0
216.91072	0	0	4473	0	0	4107	0	4852
218.918	0	0	0	0	0	5597	7372	0
221.08963	0	0	0	0	6602	4112	11688	0
223.10573	15459	0	0	0	53239	72965	59713	0
223.11612	0	0	0	0	25866	36446	29298	0
223.1317	0	0	0	0	0	2502	2786	0
223.14209	5363	0	0	0	7570	10293	11696	0
223.16287	0	0	0	0	0	2098	2175	0
226.13918	30509	0	18096	42183	31778	8401	24822	0
226.14963	16922	0	9686	21993	16422	4688	13139	0
226.1601	7553	0	4217	0	0	2081	5997	0
226.94527	26053	0	21772	0	26783	18103	0	0
226.95575	16003	0	14465	22145	17107	11588	21049	0
226.96622	6976	0	6569	0	7763	5235	0	0
226.9767	3015	0	2569	4001	3334	2088	3850	0
229.14046	0	0	0	0	0	2724	2040	0
229.15099	0	0	0	0	151997	8244	3895	0
229.16151	0	0	0	0	80923	4424	1948	0
235.15973	145856	0	531502	402321	92704	206961	0	0
236.14737	5213	0	3354	0	0	0	5044	7198
238.13959	3982	8454	0	5267	0	0	7227	7120
244.95503	3198	4229	0	6278	4519	0	2867	4787
245.1837	12039	0	8202	0	0	23219	9221	22108
254.24548	3385	3193	4550	3132	3343	4442	3293	3043

254.81697	2074	0	1929	0	0	2665	2275	0
256.81381	2153	0	2049	1485	0	3559	2854	2286
259.10947	23970	65811	8035	27013	17212	0	0	0
261.12866	20794	12621	8464	0	0	8579	4915	8004
264.15518	0	0	0	0	0	2499	5514	0
267.82483	3108	2656	0	4312	5480	4049	2515	3780
268.09808	7948	0	3917	0	4418	0	2922	0
268.25754	3503	3393	4517	2428	3431	4822	3122	3340
268.26895	1917	0	2999	0	0	3113	1917	0
270.96423	0	6076	0	3532	0	0	3418	5529
277.211	4091	4513	3955	3975	3596	2473	3830	4226
279.22968	8371	7975	6660	0	0	6082	7841	8399
279.24127	5472	5334	3287	0	0	2965	4771	4055
281.24399	2954	3070	2687	3208	2816	2627	2444	2753
282.27722	0	0	35858	0	46880	206336	28706	0
282.28933	0	8181	17902	0	14816	107855	14314	0
282.3006	10295	0	6936	0	5993	47616	5418	0
283.27722	15197	2778	7610	3276	10666	40840	6663	3030
283.28894	8417	0	4714	0	5637	23774	0	0
284.29074	16687	0	13767	0	19103	45784	0	5121
284.90677	3449	0	3629	0	3870	2989	0	0
284.91852	2118	0	1823	2020	1894	0	2048	2558
293.20789	10564	9250	7897	9012	9432	7212	9556	11379
293.21982	5255	4582	3812	4563	4511	3419	4643	5738
294.9314	3817	0	3408	6018	4061	2471	5254	0
294.94333	2490	0	2078	3524	2603	0	3284	0
295.21216	4316	4701	3419	0	4495	2458	0	4091
295.22412	13954	16081	12572	14764	13918	9310	13256	15262
295.23605	7007	7757	5965	8743	6819	4659	6950	7366
295.24802	2798	3210	2343	3790	2650	1913	3150	2977
296.22284	3278	3165	2377	4210	3744	0	2932	3976
296.2887	6008	5575	7461	3926	5291	6261	5123	5192
296.30066	3468	3273	4349	0	3158	3943	3083	2841
297.23526	10429	12063	9285	12742	11948	8446	10307	12278
297.24725	6621	7692	6185	7452	7741	5754	6295	7494
297.25925	3011	3393	0	3351	3512	2789	2850	3300
298.81421	3593	0	1928	4973	4639	2914	2895	3144
298.82623	10752	0	6822	14933	16540	10557	9505	10059
298.83826	7117	5275	0	7146	8021	5186	4786	6020
298.85028	3232	0	0	2805	3088	2030	2033	2683
300.81943	11301	7533	6259	13846	15337	10650	9406	9964

300.83148	6245	0	3971	7866	8722	6699	5570	0
300.84357	2550	1770	1676	3447	3896	2956	2296	0
302.79504	3852	1811	0	5520	6071	4180	3795	3884
302.81924	4623	3009	2560	5958	6134	4608	4022	4303
302.83133	0	1672	0	3792	0	2396	2588	2919
304.78925	3590	1797	0	4197	5699	3279	3518	3672
308.85233	8729	5477	6456	10375	13035	7411	7535	8415
308.86456	4574	3201	3739	5426	6876	4326	4099	4500
308.87677	1827	0	1518	2173	2749	1880	1685	1821
310.30252	8877	8798	0	12265	10607	0	9315	8473
310.31476	5892	5941	0	8460	7209	0	6570	5403
310.327	2653	0	0	3807	3235	0	2859	2556
310.79892	0	1992	0	0	2924	0	3071	2076
310.84796	5833	3471	4656	5960	8487	5727	4943	5566
310.86023	3263	1995	0	3405	4912	3305	2828	3033
311.17914	4775	4822	3783	5385	4648	3564	4566	5820
311.19141	2894	3069	2130	2888	2537	0	2656	3268
311.21597	14749	14466	11629	13226	13165	9804	13892	16246
311.22824	8117	0	6607	7058	0	5373	7698	9185
311.24051	3475	3397	2910	2901	3056	2493	3468	3687
311.30798	2513	2037	3802	2624	2711	4245	2724	1900
312.22293	3410	2969	2244	0	0	0	0	0
312.79468	3475	2437	0	3034	3112	0	3400	2415
312.80698	2145	0	1926	1986	2022	0	2178	0
313.23151	3840	3522	3846	3451	3485	3033	3450	3484
314.77213	2223	0	0	0	0	2384	2260	0
315.1301	10671	0	0	0	0	0	18337	17426
324.32062	5346	7170	8038	4206	4530	5379	5298	5536
324.33316	2904	3587	4343	2369	2416	3046	2999	2802
330.25977	7505	6897	5216	6652	7062	4368	6951	7363
330.2724	3774	3552	2682	3271	3408	2428	3419	3687
338.33493	31002	28235	111083	309177	0	240046	0	0
338.34772	8261	0	13647	6997	0	15448	6797	8255
338.3605	8211	6951	0	98506	44046	76766	52947	6891
338.37329	3498	0	25808	49910	21140	37695	24974	0
339.33997	7999	6561	38896	80845	35395	56112	37774	7115
339.35278	3852	0	21654	45390	18605	32058	20771	3818
340.25668	0	0	0	5987	14105	0	22499	23311
340.25668	18522	27373	19826	17096	9046	17321	8389	6581
340.2699	0	7559	10916	0	4521	9906	0	12471
340.29517	2855	3699	2745	0	0	2262	3114	3077

340.75723	9024	0	0	0	6022	8698	10770	0
340.77005	5645	6151	5517	4279	3416	4944	5728	5573
340.7829	0	2641	2674	1865	1423	0	2815	2491
341.25815	2446	2784	2577	2484	0	2349	3583	2643
341.271	0	0	0	0	0	0	2034	1456
343.25903	3284	2535	0	0	0	3519	5359	2830
344.8588	1927	0	2391	2070	0	0	2462	2357
348.27066	3365	2869	3925	2291	2190	2484	3504	2911
349.23184	4024	3103	5254	3193	2741	4928	4637	3378
351.24292	7435	0	0	7372	5684	7383	0	7786
351.25595	0	6092	0	4692	0	5135	0	4948
351.26248	0	0	0	0	3242	3056	0	4249
351.758	0	2352	0	0	0	2364	2373	2383
352.35181	4550	4336	5507	3602	4483	4329	4142	4169
352.36487	2422	2408	3502	0	0	2437	2379	0
352.89383	4851	0	4750	5978	0	3482	6128	0
353.25977	8231	7546	8004	9449	7765	0	8065	7598
353.27283	5139	4991	5270	5731	4961	0	5600	5010
354.26709	0	2299	2658	2362	2226	2347	2158	2212
355.27582	3326	3430	4138	3285	0	3722	3202	2978
356.27289	5037	6988	4600	7391	5271	4269	5135	6470
356.28601	3044	3822	3189	4099	3062	3082	3284	3816
362.23822	2823	0	3276	0	2177	2714	3492	0
362.92029	4481	0	0	0	4766	2929	5915	0
366.36688	5195	5454	7024	5881	5199	6791	5595	4972
366.38019	2861	2893	3854	3075	2874	3781	3081	2883
367.23941	13256	12968	11549	12424	12618	9432	11925	13157
367.25272	9151	8165	8139	7815	8757	6828	7930	8900
367.26605	4224	3619	3736	3460	3721	3162	3827	3803
368.24643	3187	3179	3145	3186	3473	2582	3389	3698
369.25482	6643	6269	7198	6736	6061	6422	7185	7397
369.26819	4280	3937	4992	4143	3982	4311	4720	5084
369.28156	2020	1880	0	1823	1835	0	0	0
380.38391	2504	2805	3685	0	2636	2997	0	2591
385.25511	3678	0	0	0	0	3727	0	2871
391.27917	10420	16850	9128	16683	18041	7119	9194	16518
394.39468	3065	0	0	0	3391	0	2795	3149
399.24402	8398	14932	9585	14802	15391	7466	10015	12137
399.2579	4674	8089	0	7738	8626	0	5757	7080
400.30093	6281	8745	6590	7613	7303	6048	5873	6154
400.82294	1930	0	0	0	1981	2255	2232	0

401.25473	3376	4252	0	4102	0	0	2974	3208
401.26868	2403	2881	0	2504	0	0	2076	2293
402.81668	2125	0	0	0	0	2425	2182	0
408.41284	0	2022	2515	0	1824	2501	0	0
410.86227	1803	0	2246	0	0	1675	2341	0
412.84546	2206	0	2421	2500	2143	2081	2645	0
420.87595	3873	0	0	5716	4278	2800	0	0
422.42628	2415	0	0	0	0	0	1835	1955
426.68912	3401	1752	2170	4377	5104	3111	3299	3004
430.90909	2931	0	2914	5211	3558	1887	4875	0
430.92355	2080	0	0	3445	2265	0	2944	0
432.2746	48979	6169	5109	5521	916517	29459	0	12835
438.66812	3354	0	2586	2306	3123	3093	2738	1667
440.66614	2542	0	2065	1822	2290	2583	2076	0
441.29419	3146	3191	2632	3342	3133	3289	2840	2897
444.32385	8501	0	0	0	8707	13501	7656	7914
444.33853	5296	5592	7026	5781	5277	8427	4460	4605
450.64313	2682	0	1812	0	2111	0	1800	1602
451.01971	0	0	0	0	0	0	1851	4096
468.30197	5762	13259	0	24766	0	4127	19537	67820
468.31705	0	7077	0	13403	0	0	10739	37553
468.80634	0	0	2112	0	0	0	2103	1735
478.83643	2180	0	2475	2945	2500	2345	0	0
480.33676	0	0	0	23085	0	16088	23459	12438
480.35202	0	0	0	13271	0	9077	14303	7299
480.83231	1686	0	0	2165	1547	0	2279	0
482.31573	0	0	0	10382	0	0	12602	20110
482.35104	0	0	0	5085	0	16693	34104	10179
482.3663	0	0	0	3236	0	11172	21342	6599
488.36536	5908	6803	4673	5602	5992	15308	6211	5575
494.31641	9195	21977	3862	77163	0	11466	47033	94249
494.33188	5315	12478	0	44067	0	6542	26668	54934
494.34687	0	0	0	18712	0	0	11003	23783
495.32247	0	6187	0	19586	0	3251	10885	25136
496.31326	11405	17091	0	42482	0	0	101627	138167
496.32877	152593	221992	0	1019587	17216	0	1215171	1203166
496.34427	111478	159138	0	325702	12279	0	826417	787844
496.35977	54134	77173	0	0	5200	0	415578	393505
496.37524	24879	36679	0	0	0	0	321948	309843
496.39075	12080	18472	0	0	0	0	189767	179868
496.39927	0	0	0	107374	0	26458	0	115825

496.414	0	0	0	72275	0	15530	85376	83591
496.42253	0	0	0	66279	0	11486	0	71384
496.49149	0	0	0	15866	0	0	21999	19970
496.50699	0	0	0	0	0	0	15221	14737
496.74238	0	0	0	0	0	0	5649	5319
497.32098	11037	15097	0	70166	0	19169	76776	79072
497.33649	40068	60597	11622	264090	5368	77579	316941	319546
497.35199	21988	34027	6287	155535	0	43583	194288	194072
497.36749	9323	14014	0	75577	0	19497	95923	94879
497.38303	0	6135	0	39268	0	9002	50979	49587
497.39853	0	0	0	22624	0	4481	29691	29047
497.41403	0	0	0	14143	0	0	18534	18067
497.42957	0	0	0	12253	0	0	16214	15826
497.44458	0	0	0	7806	0	0	10519	10508
498.32193	0	0	0	8290	0	0	8877	9778
498.33746	7759	9192	0	43406	0	14008	51265	51986
498.35297	4416	5513	0	26293	0	8706	32073	32136
498.3685	0	0	0	11424	0	3527	14691	15171
498.38403	0	0	0	5210	0	0	6599	6507
499.33942	0	0	0	6321	0	0	7804	7112
499.35498	0	0	0	3946	0	0	4540	4819
502.36697	2327	0	9057	8868	7777	0	15309	0
508.37112	0	0	0	6415	0	15414	24709	9164
510.349	0	0	0	10716	0	5328	24812	26664
510.36472	0	0	0	5642	0	0	13677	14342
517.3493	4307	0	4824	0	2911	4055	0	3110
517.84772	0	0	2533	0	0	2498	2092	0
518.31476	0	6862	0	7844	0	3409	11096	16712
518.33063	0	0	0	0	0	0	6309	9849
520.31982	0	84318	0	0	0	52033	138073	149269
520.33569	0	181039	8613	0	0	128893	303360	326187
520.3512	26770	98679	5739	0	0	70150	169501	263271
520.36743	0	0	0	0	0	30557	79670	136148
520.3833	0	21294	0	0	0	14255	40933	67027
520.39911	0	11125	0	0	0	7113	23151	35658
521.31982	0	11362	0	23834	0	7631	19705	22768
521.33569	11873	50769	0	96354	0	37550	84905	97643
521.35156	6372	28981	0	55837	0	21706	49245	57775
521.36743	0	12101	0	24813	0	9133	22300	25285
521.38336	0	5103	0	11222	0	0	10070	11497
522.32874	4616	6706	0	29967	0	10874	19505	24197

522.3446	44129	60440	16015	305574	0	117098	207950	256187
522.39233	5268	7009	0	53243	0	16953	34499	43544
522.4082	0	0	0	27962	0	7866	17307	22539
522.42413	0	0	0	16408	0	4485	9396	12593
523.33818	0	0	0	34538	0	13625	25338	31245
523.35449	11456	0	5050	0	0	32292	56699	69590
523.37042	7775	0	0	0	0	16423	29989	36624
523.38635	0	0	0	0	0	6539	12320	15110
523.40171	0	0	0	12288	0	0	5674	6975
524.34949	15657	0	3180	65645	0	27291	105762	84266
524.36542	44049	19696	9333	195608	7761	101156	365142	511209
524.38135	23552	10045	5018	110156	3829	58403	302803	322724
524.39728	9362	0	0	50100	0	24735	160169	160325
524.41321	0	0	0	24431	0	11489	77815	87177
524.42914	0	0	0	12635	0	5452	41597	51410
524.44501	0	0	0	6979	0	0	24903	31711
524.4564	0	0	0	0	0	0	17351	27243
524.46836	0	0	0	0	0	0	13041	17055
525.35333	0	0	0	20712	0	8977	38927	54092
525.36926	12317	5577	0	52355	0	27364	100771	148608
525.38519	6523	0	0	27620	0	14551	55310	83172
525.40118	0	0	0	11252	0	6029	24321	37232
525.41711	0	0	0	0	0	0	11496	18391
526.36615	0	0	0	10148	0	0	18663	26095
526.38208	0	0	0	6918	0	0	12044	18326
526.39807	0	0	0	0	0	0	5343	8657
530.36304	2356	0	2400	3041	2353	0	2412	0
532.37518	13610	0	31058	8235	0	39262	0	0
532.39124	8573	10166	18301	0	8047	24894	4688	9107
532.40729	0	0	7828	0	0	10697	0	3638
533.37866	4728	5222	9850	4562	4744	11019	5997	4537
539.35963	2884	2142	3818	0	0	3450	2710	2809
544.33331	13681	61174	0	134932	0	55496	80520	168409
544.35767	0	22191	0	51784	0	21232	29426	67820
544.38196	0	0	0	15323	0	5437	7740	20850
545.33173	0	17859	0	36767	0	16364	23102	49077
545.35614	0	8589	0	17969	0	8071	10945	23905
546.34735	3307	7310	0	18148	0	16261	25626	32500
546.37177	0	0	0	0	0	6452	0	12012
546.82008	2088	0	1984	2866	0	0	2790	0
547.34766	0	0	0	5362	0	4900	7235	8797

548.36608	0	0	0	4787	0	5080	7559	4691
568.33289	0	6726	0	10957	0	5536	7791	10460
570.3493	0	0	0	4541	0	4273	5378	7585
572.36096	0	0	0	0	0	5599	0	4408
576.40326	18863	23216	39127	18748	19334	54894	0	20810
576.42828	6894	8058	14467	6396	6666	21607	10623	7339
577.40558	7242	6980	12882	6713	6904	17645	9097	6491
585.22015	10226	17672	0	24582	0	5311	9606	8713
585.24542	0	6193	0	9104	0	1969	3206	3136
586.22216	0	5577	0	8829	0	3973	5070	3199
587.2181	0	5901	0	8249	0	0	4081	3279
609.21936	0	16553	0	22749	0	3919	8321	11304
611.22654	0	6008	0	9742	0	2839	3477	0
613.25177	0	0	0	15981	0	3152	10286	15209
614.25224	0	0	0	5183	0	0	4797	5747
615.2514	0	0	0	5244	0	0	4596	5408
620.42926	26630	27289	48929	21100	0	59477	32452	24861
620.45526	9988	0	19132	7172	7121	23852	11937	8248
621.43351	9508	8448	17738	7542	7097	20373	11613	9181
654.32507	9691	10056	7375	12688	12398	0	7904	9878
664.45178	31906	30724	59750	25408	23954	65244	34431	33214
664.47801	13208	12647	26312	10104	10327	29833	14499	13612
665.45618	12374	11079	22573	8977	9917	25786	13355	12102
675.53271	4138	0	0	5861	4266	0	2928	0
679.50028	24183	23542	63950	22297	25964	15275	20749	35616
680.50409	11131	19952	27977	10022	10493	6569	9848	14658
680.53131	4414	0	11750	4077	0	0	0	6184
680.53131	2551	2431	1807	0	2072	0	0	0
681.51078	2572	4314	6646	2483	2818	2166	2569	3663
685.51196	4186	4572	6125	1926	2235	0	6605	5159
685.53925	0	0	2172	0	0	0	2165	1852
686.51392	0	1810	0	0	0	0	2491	2492
701.48352	0	21000	21812	8367	14878	0	9806	16455
701.54701	6922	0	4550	11456	7873	3293	5520	0
702.48785	4335	8622	8889	3746	5631	0	0	6985
702.5155	0	3025	3470	0	2110	0	0	0
703.56671	18329	0	10927	0	37121	17222	42180	0
703.59436	6320	0	3882	0	13247	6467	15725	0
704.57251	8439	0	5386	0	16100	7446	17045	0
708.48267	27620	24940	49381	22316	22441	55127	30963	26052
708.51044	9403	7949	17895	11352	7435	20137	10616	8484

709.48273	12211	10455	21088	9563	8904	20556	13121	10757
752.50385	26936	21751	39115	18131	19797	46626	25769	25303
752.53247	10600	8686	16723	6725	7626	20568	10677	10102
753.50586	10468	9224	15966	7416	8761	19546	10528	9954
759.61823	2073	0	0	0	0	3267	5425	0
760.59619	2290	0	0	0	0	3042	4248	0
766.56384	3865	0	0	0	2055	3468	3538	0
780.54022	13066	2318	0	11128	9229	8043	13318	14008
780.5694	5117	0	0	4314	3741	0	5261	5528
781.54132	5992	0	0	5421	5123	0	6929	6597
782.56244	18107	0	6080	0	0	24661	22604	0
783.56482	9672	0	3528	0	0	12132	11380	0
783.59399	4480	0	0	0	0	4193	3929	0
784.54834	0	0	0	0	0	2380	2603	0
784.57758	20920	0	10639	0	10862	22020	22772	0
785.58118	10698	0	4800	0	0	11052	11425	0
786.58063	2885	0	0	0	0	3098	3333	0
796.5285	21451	15794	32836	15322	15266	34924	22066	19436
796.55718	10557	7508	16801	6654	7251	17470	10030	9543
797.53666	9339	7348	14582	6693	6853	14793	9753	8456
806.55902	0	0	2312	10311	6320	2964	5446	16610
806.58862	0	0	0	3951	2358	0	2043	6042
807.55991	0	0	0	5471	3212	0	2803	7486
808.57507	6870	0	0	16984	6543	0	5260	0
808.60474	2377	0	0	0	0	3146	1911	0
809.57416	3304	0	0	0	0	4180	2997	0
840.55927	15442	12437	25294	9638	10089	25182	15980	13733
840.58954	5419	0	9291	0	0	8955	5563	4793
841.55774	7611	5903	11955	4877	5366	11239	8123	6785
884.58386	10034	6955	14563	5721	7175	14948	10452	8400
884.61514	5231	0	7292	0	0	6773	5194	0
885.58592	5736	3497	7274	0	0	8252	5674	4251
907.42566	2180	0	0	5516	3165	0	2565	0
928.60437	5222	3383	7086	2873	3695	7422	5318	4663
929.61139	3068	0	3755	0	0	3888	3048	2617
972.63812	2441	0	3909	0	0	3670	2812	0
59.060177	5238	0	0	0	0	8402	4923	0
59.070869	0	0	0	0	0	1873	0	5392
69.493202	0	0	0	3209	0	3029	0	2535
76.038757	22395	0	14012	0	17270	8821	0	0
80.946327	0	0	0	0	16573	22187	19212	0

81.94751	0	2140	0	2736	2616	2274	0	1956
86.107353	0	0	37296	44953	0	38214	0	2415
88.521767	0	0	0	0	0	2679	3290	0
90.913177	2274	0	2480	0	5062	4108	0	3718
97.930756	0	2190	0	2775	2533	2538	0	2681
97.975502	0	0	0	0	0	2434	2378	0
108.91177	0	2088	0	2919	3218	2427	0	0
110.0799	3870	4740	4617	4762	4969	3513	2936	3809
114.10037	36321	105230	0	0	15744	24576	13454	21867
115.08318	9601	8705	0	0	9536	11911	0	12654
115.09438	0	0	0	0	0	4885	0	4926
116.11517	33675	0	41616	51311	0	21152	19948	0
117.08401	13021	0	15000	18063	16227	9586	9901	0
118.1476	0	0	0	21190	0	9822	10887	0
122.98551	0	0	0	1915	0	1798	0	1840
123.09738	18518	0	7347	15318	7017	3628	12701	0
126.04338	11247	31206	20258	25313	31506	3954	0	8849
132.12381	0	0	53127	80575	0	114331	30784	0
133.105	20541	0	0	0	22148	29909	4810	32929
133.11703	6143	0	0	0	6463	9255	0	9923
134.92471	0	2394	0	3606	3154	2278	0	2445
137.05383	144258	418982	190407	321752	179643	73893	65057	88714
137.06604	51926	0	68974	0	64910	24604	21277	0
141.97882	0	5486	0	0	6751	3946	3816	0
146.97809	0	0	0	5494	0	7544	6401	0
147.10881	88369	138142	0	80782	0	87082	0	116933
147.13412	10390	17325	14595	0	13032	10825	0	14389
147.14677	0	6016	4965	0	0	3603	0	4853
150.06773	28670	0	41267	0	43875	16394	0	0
156.14781	0	6298	5241	4532	5865	3668	0	0
158.07889	0	0	0	12991	0	15697	8030	11095
166.89536	0	2251	0	32628	33706	66157	28900	18843
167.08411	38281	0	50632	0	92600	37022	0	0
169.09955	37550	0	0	33099	38007	21634	26619	0
170.95422	10002	8348	0	15477	4845	12104	10541	12608
170.97241	3503	2780	2802	0	0	4094	3479	0
172.97908	25644	17493	18378	38980	32853	26206	23905	27316
173.96846	4716	0	4086	0	6602	5419	4574	0
173.98222	0	0	0	1934	1775	1541	0	1408
175.00665	1325	0	0	0	1542	1533	0	1540
175.96489	1903	0	0	2470	2451	1882	1600	1907

176.06178	0	0	0	0	0	2985	7679	6632
178.05624	5155	16986	10183	10695	13266	4800	0	9504
183.00919	2265	1749	0	2829	2341	1664	2134	0
186.10904	0	0	13145	0	48934	28859	14251	0
187.15366	0	0	7876	6536	9911	19442	0	0
189.15718	6669	69630	29602	7982	64299	3264	0	5166
198.10924	13708	0	25665	43087	0	9796	0	0
202.10382	0	0	0	10669	0	2751	4253	0
203.16322	4757	14795	12884	0	13151	3323	0	6646
206.89792	3209	0	0	0	2714	3660	3294	0
209.145	0	0	0	0	0	12236	14073	0
210.96455	0	146186	20372	94919	40007	7947	69137	133638
218.9283	0	0	0	0	0	3723	4546	0
220.96555	3400	8790	4988	0	2990	4244	0	4336
231.16641	0	15329	0	0	0	28498	0	36942
231.17699	0	0	0	0	0	15261	0	18792
245.19458	6136	11469	0	9218	12431	11249	0	10940
247.13705	0	0	41327	0	0	9240	20199	0
256.82495	0	0	0	0	0	1957	1669	0
261.13992	0	0	4067	0	0	4292	0	4010
264.84521	0	0	0	0	0	1581	1489	0
267.83621	0	1502	0	2660	3366	2639	1575	2231
269.15826	0	0	0	0	0	5293	0	14293
269.20392	2071	2013	2724	0	2220	2444	2124	2532
274.87671	2908	0	2927	2998	0	3017	0	0
276.87527	2297	0	2082	1594	0	2390	0	0
277.8541	2379	2036	0	2783	3571	2419	2129	2637
304.29767	0	11964	0	0	0	3227	0	9503
304.80139	2286	0	0	2817	3555	2295	2291	2332
310.79892	3279	0	2816	2268	0	2862	0	0
310.81119	1753	0	0	0	1547	1840	1888	0
338.33493	0	0	0	0	0	24961	0	13336
338.34772	18406	0	0	197694	95406	155798	0	27823
338.38608	0	0	13079	27137	0	20032	12725	0
340.24384	0	9135	6442	0	4354	4931	0	0
340.28235	10687	0	3007	0	2894	1591	0	3999
349.24484	2441	1755	3377	0	1689	3381	2686	1969
351.25595	0	0	6535	0	0	5723	3819	0
351.74496	2821	3731	2307	2980	2568	3997	3950	3794
359.22629	3615	2477	5212	2757	0	4579	0	0
370.29135	5383	7362	3442	9063	8181	2645	4733	5875

394.40075	0	2910	4195	2307	0	2965	0	0
400.31485	0	0	3360	4121	0	2965	0	3211
403.2775	0	0	0	0	0	4480	4371	0
403.29144	0	0	0	0	0	13822	12829	0
403.30542	0	0	0	0	0	6941	6290	0
403.3194	0	0	0	0	0	2832	2351	0
404.29077	0	0	0	0	0	4020	3577	0
404.30475	0	0	0	0	0	2622	2154	0
424.6944	2718	0	0	3317	4005	2614	2176	2186
426.70349	2212	0	0	2576	3256	2010	0	0
428.68851	2227	0	0	2772	3085	2268	0	0
443.30548	0	2467	1635	3098	2342	1833	0	2136
476.2981	42416	0	3082	3632	885915	14923	3819	8921
476.31326	24016	0	0	0	486242	9216	0	5221
481.34338	0	0	0	6489	0	4262	6380	0
482.38159	0	0	0	0	0	4716	9393	0
483.35977	0	0	0	0	0	4091	8596	0
488.34998	10493	0	0	10095	0	25400	0	9941
488.38074	0	0	0	0	0	6514	0	2503
506.35013	0	0	0	4925	0	4203	4877	2279
508.35544	0	0	0	0	0	4928	9336	3068
508.38681	0	0	0	3176	0	8006	12740	4540
508.4025	0	0	0	0	0	3174	4874	0
509.37527	0	0	0	0	0	4903	7344	2646
517.36511	2267	0	3223	0	0	2246	2265	0
522.36053	28970	40406	10667	213707	0	83377	148049	182511
522.3764	13025	17565	4602	105835	0	39503	72114	89694
536.33038	0	0	0	0	0	5790	5924	0
560.32764	0	0	0	0	0	5969	4440	0
679.52648	0	6243	0	0	11939	4038	6634	0
680.53131	0	0	0	0	0	2823	2223	0
701.51117	3661	0	0	0	0	4525	3926	0
774.55701	0	0	0	0	0	4701	13159	6188
782.53326	0	0	0	0	0	2833	2776	0
798.54938	0	0	0	0	0	7706	8100	21244
799.55487	0	0	0	0	0	3342	3517	10154
800.56525	0	0	0	0	0	3794	6940	3881
802.58368	0	0	0	0	0	2710	4105	0
822.55143	0	0	0	0	0	2444	4556	5470
824.56451	0	0	0	0	0	3913	3378	7416
825.57343	0	0	0	0	0	2349	0	3313

826.58295	0	0	0	0	0	4484	3942	3681
928.63617	0	0	3327	0	0	3125	2409	0
80.958839	3842	0	4295	0	3197	0	0	0
96.928413	1853	2635	2521	2475	2009	0	0	0
98.917503	1802	2989	0	2444	2691	0	0	0
105.03805	3042	0	0	3706	2710	0	0	0
110.00694	3788	5724	0	7879	0	0	0	0
112.89257	4090	0	5540	4974	5105	0	0	0
114.88927	2046	4406	3107	2413	2616	0	0	0
116.0777	8157	0	0	6069	8617	0	0	12774
126.05509	4380	12462	7774	10458	12767	0	0	3204
126.06681	2847	9040	5664	7267	8950	0	0	2104
127.02136	3772	8517	6031	7816	9597	0	0	3168
128.01492	5142	11693	8267	9393	12211	0	0	4542
128.02673	2660	5664	3769	4670	5530	0	0	2178
129.06372	3605	0	14731	0	10448	0	0	8010
131.05069	7188	0	8870	11959	10046	0	3869	0
133.07692	12756	0	13006	12106	0	0	0	0
137.06604	22309	243787	0	125412	0	0	0	28967
137.09047	16963	0	17440	0	16153	0	0	5824
137.11082	10083	40480	9407	0	0	0	0	0
138.04494	26447	0	24692	48043	23415	0	0	13213
143.04578	2767	3554	3612	4156	5571	0	0	0
148.00017	2181	5396	2851	2822	3218	0	0	2336
148.05518	38377	0	15031	0	20952	0	16167	0
149.07674	2895	0	3899	4642	5145	0	0	0
152.06815	10772	9255	0	23072	0	0	0	0
153.10774	7569	0	5821	10926	9117	0	9831	0
154.06886	5708	20260	13312	8040	15798	0	0	0
167.03467	1811	0	0	2118	1817	0	0	2077
167.05264	13453	0	15714	0	20464	0	0	0
168.95486	6520	5203	0	5033	5370	0	6047	5143
168.96841	2697	2305	0	2271	2538	0	2725	2265
169.06789	15841	0	15445	14085	22628	0	0	0
169.11311	17692	0	0	15491	17971	0	12871	0
169.12668	5481	0	0	4531	5455	0	3900	0
170.02789	6496	8378	7281	5600	15937	0	0	0
170.10045	32400	133849	55531	57115	93183	0	0	75169
171.09067	6689	25397	9806	10913	17903	0	0	12728
175.15851	24609	0	12202	15987	16141	0	0	0
175.17232	13598	18721	0	11870	11454	0	0	0

176.0341	49502	57614	32486	207665	0	0	0	0
176.04794	18021	20679	12307	82173	0	0	0	0
176.11716	24879	33492	18722	25290	0	0	11969	18566
176.13101	10205	13768	8100	10552	9860	0	0	7638
182.09763	6204	4047	0	7410	6022	0	0	3520
184.94318	3314	0	1871	0	1707	0	0	0
185.02832	8655	0	12190	7754	16611	0	0	0
185.04251	3070	0	4648	0	5727	0	0	0
198.13371	3660	0	0	3404	6290	0	0	0
200.09171	1896	0	0	2082	2056	0	0	2599
204.12103	55272	457896	320264	0	0	0	0	0
204.13594	18935	0	123857	114619	20856	0	0	23617
204.15085	5142	91299	41604	38661	0	0	0	6508
205.13588	3150	20581	13887	13836	0	0	0	3239
214.04686	15078	42745	0	0	52232	0	0	24006
215.09627	24904	0	15832	53898	15746	0	0	0
215.10646	16312	0	10914	34776	0	0	0	0
216.93685	5151	0	0	5603	5130	0	0	0
218.13658	5297	13526	12505	28018	0	0	0	3097
218.91286	5845	0	0	6657	5642	0	0	0
220.1134	9148	0	4770	21495	7167	0	0	0
226.17578	15804	0	9342	73270	57714	0	6344	40972
226.18625	8289	0	4794	38863	30708	0	3329	21766
228.19386	25159	0	13804	45863	28347	0	8400	34218
228.204	16217	0	6951	25537	18293	0	4097	0
229.14046	2505	4418	5317	3394	0	0	0	0
229.15099	21608	38518	63343	28886	0	0	0	13017
229.16151	10669	19495	32656	14514	0	0	0	6505
229.17204	4377	8036	13994	6097	0	0	0	2577
229.18257	1924	3579	6466	0	0	0	0	0
230.15233	2653	6260	7986	4102	0	0	0	0
232.15094	7827	31690	17409	13366	0	0	0	0
232.16153	3898	15787	8896	6703	0	0	0	0
241.149	3362	13509	10449	7829	20866	0	0	3570
244.17732	5612	0	0	6418	4671	0	0	0
244.18819	24938	0	3550	27080	18542	0	4723	46578
244.19905	11831	0	1744	13384	8980	0	2391	22974
244.20993	4682	0	0	5139	3402	0	0	0
245.90848	2593	2116	0	2580	2489	0	0	2423
246.16486	2732	6544	6776	7378	0	0	0	0
246.9512	2180	2928	0	4961	3057	0	2214	0

247.13705	4797	2589	0	0	5168	0	0	0
248.14403	2843	90204	7778	14553	0	0	0	0
251.02292	5006	14412	8339	14008	18665	0	0	0
251.03394	22175	70729	43084	62146	88605	0	0	12364
251.04497	11170	35623	21905	31004	45136	0	0	5843
251.05598	4533	14265	9285	12564	18463	0	0	0
253.10446	13625	3072	0	9666	0	0	0	0
253.11552	18447	12870	0	41152	0	0	0	0
253.1266	12899	6423	0	20107	0	0	0	0
253.13766	5548	2674	0	8236	0	0	0	0
255.93959	2341	2125	0	2466	2389	0	0	2440
256.05643	8187	53638	0	10155	6401	0	0	0
256.06757	5611	37382	0	6469	4346	0	0	0
258.10281	259333	665506	0	287075	174326	0	13252	26113
258.11426	188142	319950	0	198970	122907	0	9193	18160
258.12518	94590	275806	0	99487	59768	0	4037	8460
258.13635	45630	144384	0	48155	27387	0	0	0
258.14752	23833	81066	0	24581	13165	0	0	0
258.15869	13986	0	0	14819	7565	0	0	0
259.12067	12790	37898	4415	13670	0	0	0	0
259.13187	5540	20477	0	5729	0	0	0	0
260.11249	4790	10361	0	4457	0	0	0	0
265.11127	130067	13384	10706	39635	232349	0	16393	87091
265.12262	84164	0	0	24809	155156	0	10846	64322
265.13394	39400	4554	3439	11052	0	0	5299	31955
265.14526	18368	0	0	4691	36496	0	2155	13421
266.11447	18376	0	0	6032	33361	0	2950	13564
266.12582	12053	0	0	3999	21827	0	0	9230
266.13718	5681	0	0	1894	9886	0	0	4804
269.08411	57255	0	16382	56564	25875	0	0	0
273.08072	95027	174390	71670	140075	77808	0	0	29739
273.09219	49140	91112	37908	72032	39774	0	0	0
273.1037	21357	40100	15484	31489	16576	0	0	0
274.0816	13575	23912	9030	19319	10918	0	0	0
274.09311	7517	13627	0	10457	6085	0	0	0
282.27136	69906	12319	0	13876	0	0	0	14519
282.28305	49686	0	0	9708	32273	0	0	9546
284.09143	51399	49461	0	100908	32479	0	0	3394
284.10315	33377	32984	0	67217	22267	0	0	0
284.11487	15327	15232	0	32115	0	0	0	0
285.08289	34351	0	87314	108718	24150	0	0	0

285.0939	22459	0	59668	70495	15849	0	0	0
285.10638	10209	0	27632	33492	0	0	0	0
287.0946	9083	0	0	4731	27908	0	0	17634
287.10638	5107	0	0	2690	14039	0	0	9593
293.19598	2964	2495	0	2674	2059	0	0	0
294.12567	4060	0	0	0	0	0	3197	5342
296.8277	1587	0	0	2534	2364	0	0	0
298.24338	2246	2432	0	3105	2376	0	0	0
299.2532	2163	0	0	0	2194	0	2086	2240
304.95271	2025	7614	3663	2632	2805	0	0	2556
310.8725	1409	0	0	1366	2084	0	0	0
311.0994	13091	8234	0	9380	10018	0	0	0
313.24384	2211	1771	0	1953	2019	0	0	2011
325.11023	4600	7478	0	8423	10081	0	0	2129
325.12277	2683	5172	0	5246	0	0	0	0
328.24045	3061	2881	0	3138	2951	0	2461	3611
332.27258	2775	2695	1664	3005	2747	0	2097	2578
340.2695	7713	0	0	0	0	0	15432	3743
346.99329	4975	0	0	8748	7469	0	0	0
347.00626	2516	0	0	4390	3998	0	0	0
358.29092	2868	3179	2080	3528	3087	0	2660	3552
367.15942	4272	14217	0	9939	0	0	0	3822
382.9657	2964	0	0	4201	4739	0	0	0
391.29294	5421	8298	0	8493	9245	0	0	8266
404.29217	2464	2104	0	2248	2260	0	0	0
418.9447	3130	0	0	5396	5222	0	0	0
420.94016	3069	0	0	4758	4953	0	0	0
425.29663	2460	2035	1602	2375	2091	0	0	2008
452.63861	2227	0	0	1622	2169	0	0	0
459.29968	2392	2216	0	0	0	0	2314	2470
520.36082	11967	43946	0	139455	0	0	0	0
523.8479	1748	2046	0	2416	2475	0	0	1988
548.37329	2962	0	4705	0	2622	0	0	0
725.54486	3528	0	0	4282	8578	0	4154	0
102.03032	0	9261	2599	2907	0	0	3566	8113
134.01733	0	8537	3653	8939	0	0	0	4138
144.10004	0	0	0	0	0	0	14942	13662
150.94662	0	19058	0	12878	6402	0	11080	16798
152.03384	0	0	0	5979	0	0	4688	46719
156.99202	0	2324	0	2026	2237	0	2169	0
170.12767	0	17236	5964	0	11116	0	0	0

182.99507	0	6364	0	0	8351	0	7645	2874
184.09285	0	322608	203639	306555	155012	0	0	139952
184.10701	0	133144	85597	125890	61424	0	0	54943
185.13713	0	32004	35733	52850	22263	0	10856	63248
203.9422	0	2347	0	4102	2757	0	0	0
205.12094	0	48959	31491	33412	0	0	0	8068
210.97466	0	75485	0	48107	20652	0	35284	69465
223.12651	0	0	0	0	0	0	11643	27697
244.96593	0	2293	0	3527	2561	0	0	0
271.22189	0	2815	0	2795	2764	0	2446	2812
277.2226	0	2469	0	2014	1928	0	0	0
293.23172	0	1951	0	1802	1826	0	0	0
294.20917	0	2694	0	2070	2073	0	1968	0
311.2037	0	2409	0	2387	2193	0	0	2688
312.21721	0	0	0	2818	2885	0	2791	3146
315.14246	0	0	0	0	0	0	9266	8468
340.75723	0	11725	9433	7698	0	0	2891	9847
430.31012	0	2588	0	2744	2311	0	0	0
444.32385	0	9809	10785	10384	0	0	0	0
496.4597	0	0	0	0	0	0	51711	49900
496.62969	0	0	0	0	0	0	6290	6257
496.69299	0	0	0	0	0	0	5555	5345
496.80071	0	0	0	0	0	0	4565	4282
497.46057	0	0	0	6922	0	0	8870	8614
497.4761	0	0	0	4810	0	0	4255	5686
510.33328	0	0	0	0	0	0	7100	6808
512.33862	0	0	0	5955	0	0	6251	7636
525.43304	0	0	0	0	0	0	6037	10168
991.65607	0	0	0	0	0	0	82884	134159
90.066292	0	1617	20880	3985	0	0	0	0
100.07263	0	43423	23384	58476	0	0	0	0
112.90366	0	3190	2042	1955	1850	0	0	0
123.05109	0	0	27382	109145	59958	0	0	0
127.03312	0	3352	2440	3258	3605	0	0	0
137.07825	0	116821	28944	0	27156	0	0	10552
140.0667	0	0	5103	4681	4888	0	0	0
146.11505	0	10655	55930	21588	0	0	0	0
155.05896	0	3616	2234	0	2576	0	0	0
159.02475	0	47818	25660	39855	35403	0	0	0
170.04149	0	3473	3011	2158	6345	0	0	0
171.10431	0	10362	4721	0	7604	0	0	0

184.92899	0	3683	4746	0	4777	0	0	0
189.17154	0	24086	10478	0	22061	0	0	0
200.0376	0	6971	3460	0	3219	0	0	0
203.13348	0	2334	2920	0	5717	0	0	0
204.16576	0	39334	18167	16441	0	0	0	0
204.18066	0	22876	12534	11993	0	0	0	0
204.20053	0	10958	5585	5423	0	0	0	0
205.15082	0	5866	4252	3695	0	0	0	0
206.12329	0	6099	4458	4508	0	0	0	0
218.14685	0	7417	6152	13572	3244	0	0	0
232.17213	0	6859	3592	2617	0	0	0	0
241.15981	0	7732	5988	4402	11979	0	0	0
241.17061	0	3476	2615	0	5397	0	0	0
246.17577	0	3356	3871	4183	0	0	0	0
248.15498	0	50659	4531	7900	0	0	0	0
251.067	0	6459	4250	5667	8671	0	0	0
253.02701	0	7139	4046	6276	8120	0	0	0
253.03807	0	4698	2967	4098	5120	0	0	0
260.17981	0	16059	3505	5392	0	0	0	0
265.12262	0	13882	13553	0	97472	0	0	0
269.98621	0	5717	1379	7150	0	0	0	3202
273.06921	0	26954	11057	29052	13038	0	0	0
285.12399	0	27237	8182	5025	11986	0	0	0
285.13574	0	13993	4330	0	5940	0	0	0
298.12329	0	0	6187	17039	7237	0	0	0
304.20667	0	4984	2494	2322	0	0	0	0
307.10684	0	7227	2522	0	4958	0	0	0
312.1246	0	16479	22999	23049	52201	0	0	10449
337.13977	0	0	3485	1828	3356	0	0	0
339.36557	0	0	9362	19996	7811	0	8820	0
347.05807	0	0	7249	5891	8183	0	0	0
352.90689	0	0	2624	4086	0	0	3124	3496
385.24896	0	3017	3625	2497	2583	0	3407	0
429.96393	0	7232	4303	2970	2972	0	0	0
501.05832	0	14216	7780	14153	21879	0	0	0
108.00993	0	4712	0	2755	3866	0	0	0
125.09251	0	5760	0	7987	8346	0	6642	0
126.08633	0	22789	0	13388	15105	0	0	0
162.89856	0	3212	0	3998	3292	0	0	0
188.17317	0	3715	0	4948	11591	0	0	0
205.9386	0	1988	0	2998	2921	0	0	0

