Detailed instructions for submitting Metabolon data to the Metabolomics Workbench (NMDR)

Please read the main NMDR tutorial first!!

https://www.metabolomicsworkbench.org/data/ds_tutorial.pdf

Page 7 of NMDR tutorial

(b): Begin the online submission of metadata and results

Start a new study from scratch (most common option, especially for new users)

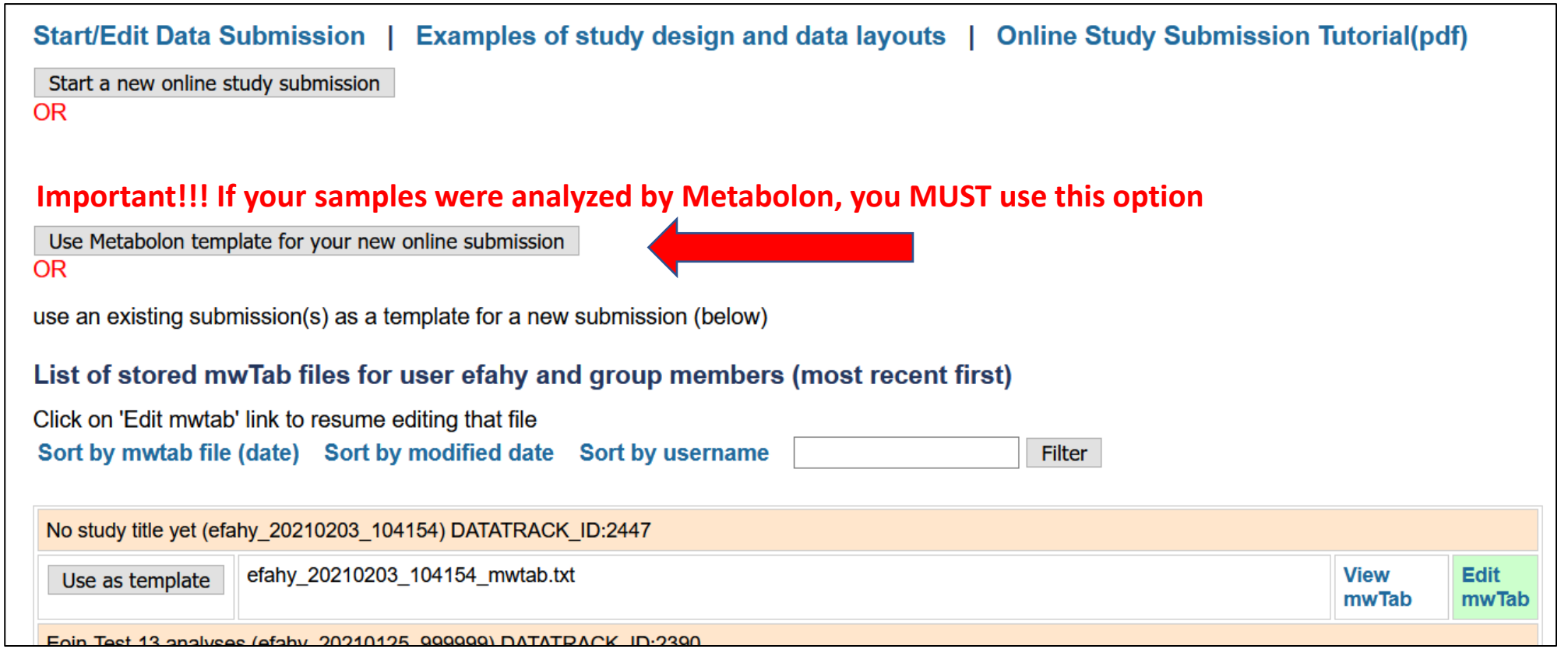
or

use the Metabolon template if the new submission is composed of Metabolon analyses

(If your samples were analyzed by Metabolon, you MUST use this option)

or

use an existing study as a template for a new submission



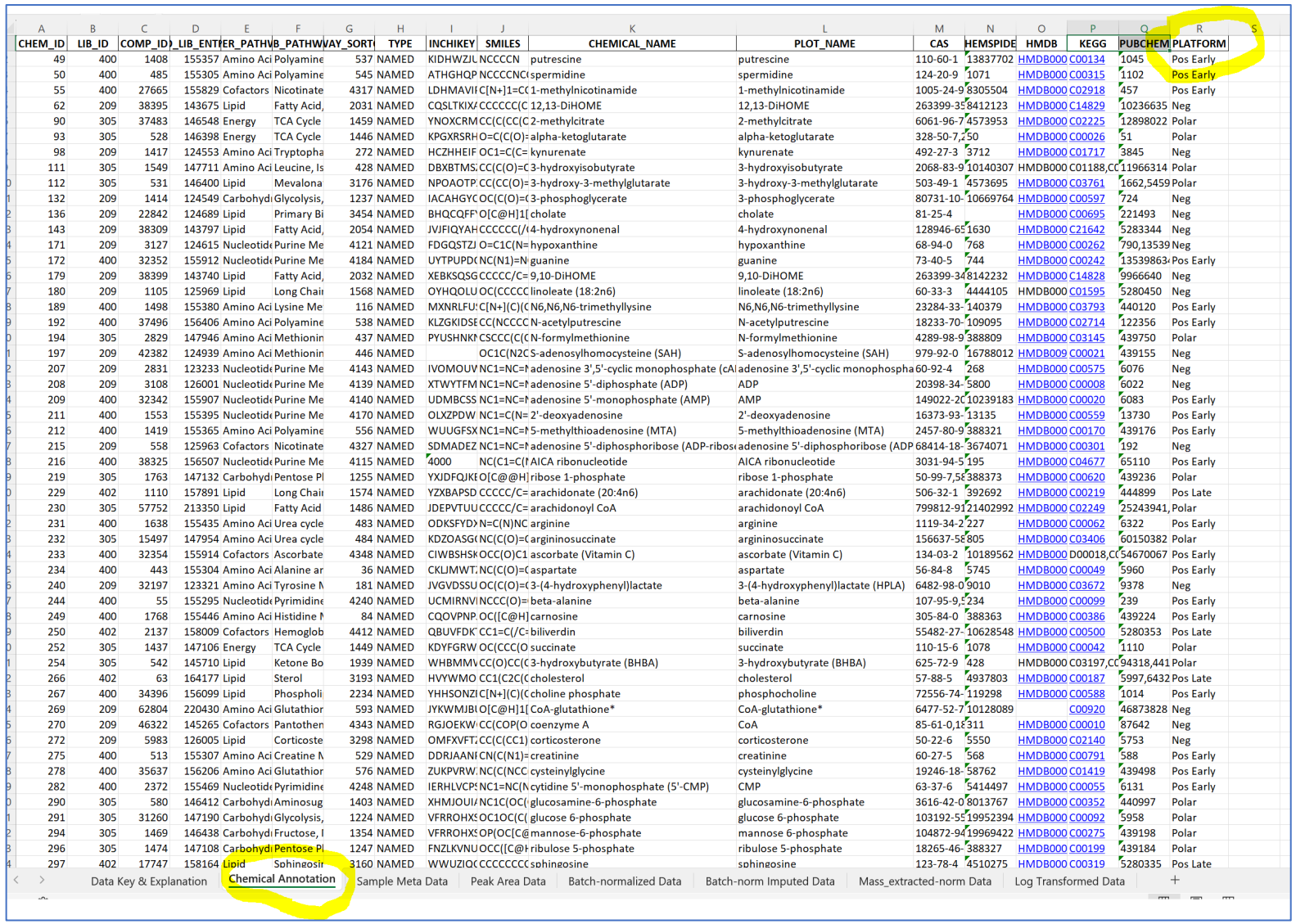
(b): Begin the online submission of metadata and results
Entering Metabolon data

The Metabolon template on the Metabolomics Workbench has 4 different combined LC/MS methods:
Low pH polar (LC/MS Pos early)
Low pH Lipophilic (LC/MS Pos late)
High pH (LC/MS Neg)
HILIC (LC/MS Polar Neg)
which correspond to 4 different sections (respectively) of the Metabolon results spreadsheet file:
Pos Early
Pos Late
Neg
Polar

Split your Metabolon results (1st column is metabolite names, subsequent columns are sample data) and metabolite metadata (1st column is metabolite names, subsequent columns are Pubchem id, KEGG, SMILES, etc) into these 4 sections based on the "PLATFORM" heading in the spreadsheet. Enter these data in the 4 "Data(Results)" sections of the submission form. Specify units of measurement for the data that you're providing (Unnormalized data, normalized-Imputed Data, log-transformed data, etc.)

PLATFORM in Metabolon results spreadsheet	Workbench template results section	LC/MS method	MS Polarity
Pos Early	1	Low pH polar (LC/MS Pos early)	POS
Pos Late	2	Low pH Lipophilic (LC/MS Pos late)	POS
Neg	3	High pH (LC/MS Neg)	NEG
Polar	4	HILIC (LC/MS Polar)	NEG

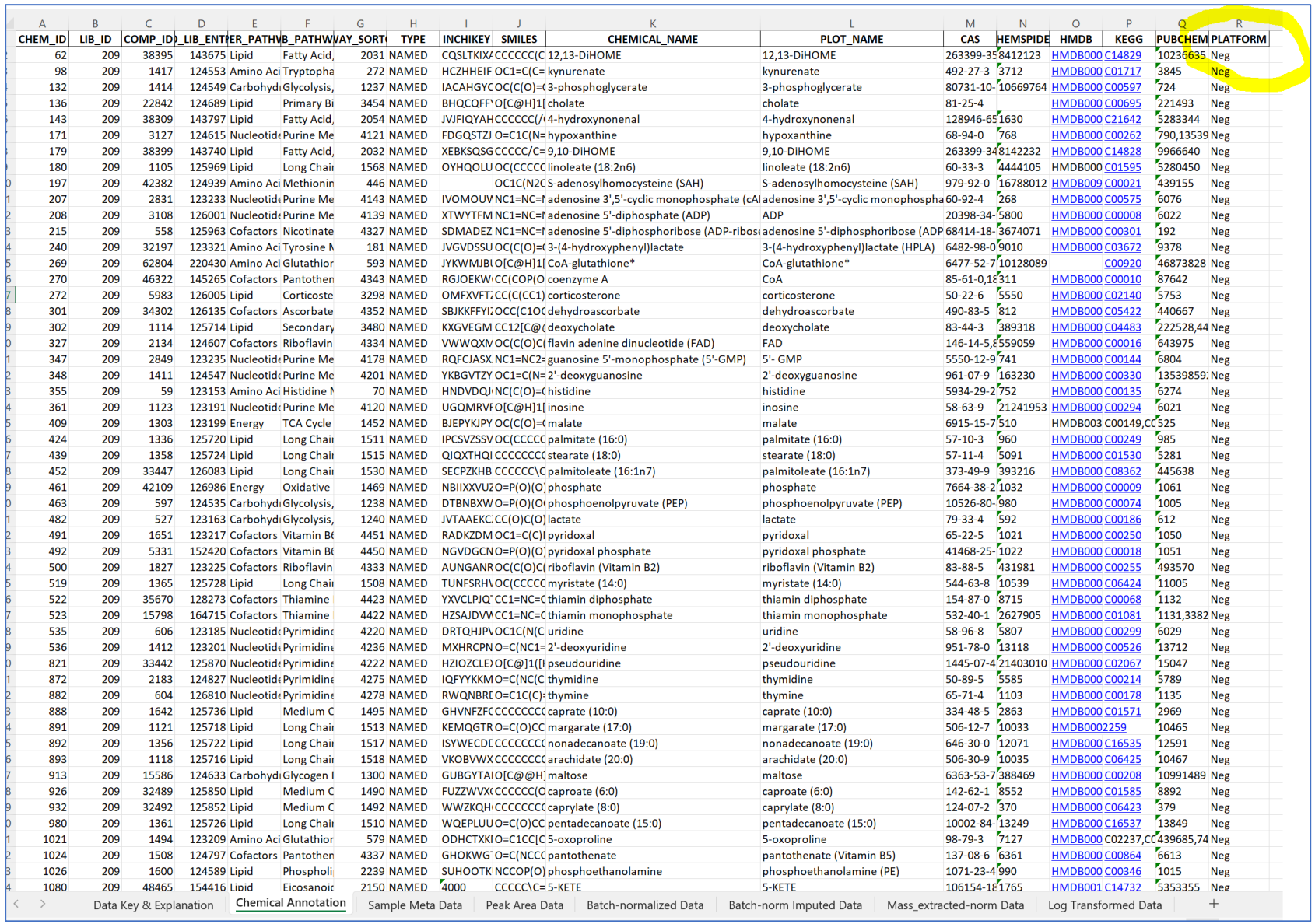
“Chemical annotation” tab in Metabolon results file



CHEM_ID	LIB_ID	COMP_ID	LIB_ENTR	ER_PATHW	B_PATHW	WAY_SORT	TYPE	INCHIKEY	SMILES	CHEMICAL_NAME	PLOT_NAME	CAS	HEMSPIDE	HMDB	KEGG	PUBCHEM	PLATFORM
49	400	1408	155357	Amino Aci	Polyamine	537	NAMED	KIDHWZJL	NCCCCN	putrescine	putrescine	110-60-1	13837702	HMDB000	C00134	1045	Pos Early
50	400	485	155305	Amino Aci	Polyamine	545	NAMED	ATHGHQP	NCCCCNC(	spermidine	spermidine	124-20-9	1071	HMDB000	C00315	1102	Pos Early
55	400	27665	155829	Cofactors	Nicotinate	4317	NAMED	LDHMAVIF	C[N+]1=CC	1-methylnicotinamide	1-methylnicotinamide	1005-24-9	8305504	HMDB000	C02918	457	Pos Early
62	209	38395	143675	Lipid	Fatty Acid,	2031	NAMED	CQSLTKIX/	CCCCCC(C	12,13-DiHOME	12,13-DiHOME	263399-35	8412123	HMDB000	C14829	10236635	Neg
90	305	37483	146548	Energy	TCA Cycle	1459	NAMED	YNOXCRM	CC(C(C(C	2-methylcitrate	2-methylcitrate	6061-96-7	4573953	HMDB000	C02225	12898022	Polar
93	305	528	146398	Energy	TCA Cycle	1446	NAMED	KPGXRSRH	O=C(C(O)=	alpha-ketoglutarate	alpha-ketoglutarate	328-50-7,2	50	HMDB000	C00026	51	Polar
98	209	1417	124553	Amino Aci	Tryptopha	272	NAMED	HCZHHEIF	OC1=C(C=	kynurenate	kynurenate	492-27-3	3712	HMDB000	C01717	3845	Neg
111	305	1549	147711	Amino Aci	Leucine, Is	428	NAMED	DBXBTMS	CC(C(O)=C	3-hydroxyisobutyrate	3-hydroxyisobutyrate	2068-83-9	10140307	HMDB000	C01188,CC	11966314	Polar
112	305	531	146400	Lipid	Mevalona	3176	NAMED	NPOAOTP	CC(CC(O)=	3-hydroxy-3-methylglutarate	3-hydroxy-3-methylglutarate	503-49-1	4573695	HMDB000	C03761	1662,5459	Polar
132	209	1414	124549	Carbohydi	Glycolysis,	1237	NAMED	IACAHGYC	OC(C(O)=C	3-phosphoglycerate	3-phosphoglycerate	80731-10-	10669764	HMDB000	C00597	724	Neg
136	209	22842	124689	Lipid	Primary Bi	3454	NAMED	BHQCQFF	O[C@H]1[	cholate	cholate	81-25-4		HMDB000	C00695	221493	Neg
143	209	38309	143797	Lipid	Fatty Acid,	2054	NAMED	JVJFIQYAH	CCCCCC(/(	4-hydroxynonenal	4-hydroxynonenal	128946-65	1630	HMDB000	C21642	5283344	Neg
171	209	3127	124615	Nucleotide	Purine Me	4121	NAMED	FDGQSTZJ	O=C1C(N=	hypoxanthine	hypoxanthine	68-94-0	768	HMDB000	C00262	790,13539	Neg
172	400	32352	155912	Nucleotide	Purine Me	4184	NAMED	UYTPUPD(	NC(N1)=N	guanine	guanine	73-40-5	744	HMDB000	C00242	13539863	Pos Early
179	209	38399	143740	Lipid	Fatty Acid,	2032	NAMED	XEBKSQSG	CCCCC/C=	9,10-DiHOME	9,10-DiHOME	263399-34	8142232	HMDB000	C14828	9966640	Neg
180	209	1105	125969	Lipid	Long Chair	1568	NAMED	OYHQOLU	OC(CCCC(	linoleate (18:2n6)	linoleate (18:2n6)	60-33-3	4444105	HMDB000	C01595	5280450	Neg
189	400	1498	155380	Amino Aci	Lysine Me	116	NAMED	MXNRLFU	C[N+](C)(C	N6,N6,N6-trimethyllysine	N6,N6,N6-trimethyllysine	23284-33-	140379	HMDB000	C03793	440120	Pos Early
192	400	37496	156406	Amino Aci	Polyamine	538	NAMED	KLZGKIDSE	CC(NCCCC	N-acetylputrescine	N-acetylputrescine	18233-70-	109095	HMDB000	C02714	122356	Pos Early
194	305	2829	147946	Amino Aci	Methionin	437	NAMED	PYUSHNK	CSCCC(C(C	N-formylmethionine	N-formylmethionine	4289-98-9	388809	HMDB000	C03145	439750	Polar
197	209	42382	124939	Amino Aci	Methionin	446	NAMED		OC1C(N2C	S-adenosylhomocysteine (SAH)	S-adenosylhomocysteine (SAH)	979-92-0	16788012	HMDB000	C00021	439155	Neg
207	209	2831	123233	Nucleotide	Purine Me	4143	NAMED	IVOMOUV	NC1=NC=N	adenosine 3',5'-cyclic monophosphate (cA	adenosine 3',5'-cyclic monophospha	60-92-4	268	HMDB000	C00575	6076	Neg
208	209	3108	126001	Nucleotide	Purine Me	4139	NAMED	XTWYTFM	NC1=NC=N	adenosine 5'-diphosphate (ADP)	ADP	20398-34-	5800	HMDB000	C00008	6022	Neg
209	400	32342	155907	Nucleotide	Purine Me	4140	NAMED	UDMBCSS	NC1=NC=N	adenosine 5'-monophosphate (AMP)	AMP	149022-20	10239183	HMDB000	C00020	6083	Pos Early
211	400	1553	155395	Nucleotide	Purine Me	4170	NAMED	OLXZPDW	NC1=C(N=	2'-deoxyadenosine	2'-deoxyadenosine	16373-93-	13135	HMDB000	C00559	13730	Pos Early
212	400	1419	155365	Amino Aci	Polyamine	556	NAMED	WUUGFSX	NC1=NC=N	5-methylthioadenosine (MTA)	5-methylthioadenosine (MTA)	2457-80-9	388321	HMDB000	C00170	439176	Pos Early
215	209	558	125963	Cofactors	Nicotinate	4327	NAMED	SDMADEZ	NC1=NC=N	adenosine 5'-diphosphoribose (ADP-ribos	adenosine 5'-diphosphoribose (ADP	68414-18-	3674071	HMDB000	C00301	192	Neg
216	400	38325	156507	Nucleotide	Purine Me	4115	NAMED	4000	NC(C1=C(N	AICA ribonucleotide	AICA ribonucleotide	3031-94-5	195	HMDB000	C04677	65110	Pos Early
219	305	1763	147132	Carbohydi	Pentose Pl	1255	NAMED	YXJDFQJKE	O[C@@H]	ribose 1-phosphate	ribose 1-phosphate	50-99-7,5	388373	HMDB000	C00620	439236	Polar
229	402	1110	157891	Lipid	Long Chair	1574	NAMED	YZXBAPSD	CCCCC/C=	arachidonate (20:4n6)	arachidonate (20:4n6)	506-32-1	392692	HMDB000	C00219	444899	Pos Late
230	305	57752	213350	Lipid	Fatty Acid	1486	NAMED	JDEPVTUU	CCCCC/C=	arachidonoyl CoA	arachidonoyl CoA	799812-91	21402992	HMDB000	C02249	25243941,	Polar
231	400	1638	155435	Amino Aci	Urea cycle	483	NAMED	ODKSFYDX	N=C(N)NC	arginine	arginine	1119-34-2	227	HMDB000	C00062	6322	Pos Early
232	305	15497	147954	Amino Aci	Urea cycle	484	NAMED	KDZOASG(	NC(C(O)=C	argininosuccinate	argininosuccinate	156637-58	805	HMDB000	C03406	60150382	Polar
233	400	32354	155914	Cofactors	Ascorbate	4348	NAMED	CIWBSHSK	OCC(O)C1	ascorbate (Vitamin C)	ascorbate (Vitamin C)	134-03-2	10189562	HMDB000	D00018,CC	54670067	Pos Early
234	400	443	155304	Amino Aci	Alanine ar	36	NAMED	CKLJMWT	NC(C(O)=C	aspartate	aspartate	56-84-8	5745	HMDB000	C00049	5960	Pos Early
240	209	32197	123321	Amino Aci	Tyrosine M	181	NAMED	JVGVDSSU	OC(C(O)=C	3-(4-hydroxyphenyl)lactate (HPLA)	3-(4-hydroxyphenyl)lactate (HPLA)	6482-98-0	9010	HMDB000	C03672	9378	Neg
244	400	55	155295	Nucleotide	Pyrimidine	4240	NAMED	UCMIRNVI	NCCC(O)=	beta-alanine	beta-alanine	107-95-9,5	234	HMDB000	C00099	239	Pos Early
249	400	1768	155446	Amino Aci	Histidine M	84	NAMED	CQOVPNP	OC([C@H]	carnosine	carnosine	305-84-0	388363	HMDB000	C00386	439224	Pos Early
250	402	2137	158009	Cofactors	Hemoglob	4412	NAMED	QBUVFDK	CC1=C(/C=	biliverdin	biliverdin	55482-27-	10628548	HMDB000	C00500	5280353	Pos Late
252	305	1437	147106	Energy	TCA Cycle	1449	NAMED	KDYFGRW	OC(CCC(O	succinate	succinate	110-15-6	1078	HMDB000	C00042	1110	Polar
254	305	542	145710	Lipid	Ketone Bo	1939	NAMED	WHBMMV	CC(O)CC(=	3-hydroxybutyrate (BHBA)	3-hydroxybutyrate (BHBA)	625-72-9	428	HMDB000	C03197,CC	94318,441	Polar
266	402	63	164177	Lipid	Sterol	3193	NAMED	HVYWMO	CC1(C2C(C	cholesterol	cholesterol	57-88-5	4937803	HMDB000	C00187	5997,6432	Pos Late
267	400	34396	156099	Lipid	Phospholi	2234	NAMED	YHHSONZI	C[N+](C)(C	choline phosphate	phosphocholine	72556-74-	119298	HMDB000	C00588	1014	Pos Early
269	209	62804	220430	Amino Aci	Glutathior	593	NAMED	JYKWMJBI	O[C@H]1[	CoA-glutathione*	CoA-glutathione*	6477-52-7	10128089		C00920	46873828	Neg
270	209	46322	145265	Cofactors	Pantothen	4343	NAMED	RGJOEKW	CC(COP(O	coenzyme A	CoA	85-61-0,16	311	HMDB000	C00010	87642	Neg
272	209	5983	126005	Lipid	Corticoste	3298	NAMED	OMFXVFT	CC(C(CC1)	corticosterone	corticosterone	50-22-6	5550	HMDB000	C02140	5753	Neg
275	400	513	155307	Amino Aci	Creatine M	529	NAMED	DDRJAANI	CN(C(N1)=	creatinine	creatinine	60-27-5	568	HMDB000	C00791	588	Pos Early
278	400	35637	156206	Amino Aci	Glutathior	576	NAMED	ZUKPVRW	NC(C(NCC	cysteinylglycine	cysteinylglycine	19246-18-	58762	HMDB000	C01419	439498	Pos Early
282	400	2372	155469	Nucleotide	Pyrimidine	4248	NAMED	IERHLVCP	NC1=NC(N	cytidine 5'-monophosphate (5'-CMP)	CMP	63-37-6	5414497	HMDB000	C00055	6131	Pos Early
290	305	580	146412	Carbohydi	Aminosug	1403	NAMED	XHMJOUI	NC1C(OC((	glucosamine-6-phosphate	glucosamine-6-phosphate	3616-42-0	8013767	HMDB000	C00352	440997	Polar
291	305	31260	147190	Carbohydi	Glycolysis,	1224	NAMED	VFRROHX	OC1OC(C(	glucose 6-phosphate	glucose 6-phosphate	103192-55	19952394	HMDB000	C00092	5958	Polar
294	305	1469	146438	Carbohydi	Fructose, I	1354	NAMED	VFRROHX	OP(OC[C@	mannose 6-phosphate	mannose 6-phosphate	104872-94	19969422	HMDB000	C00275	439198	Polar
296	305	1474	147108	Carbohydi	Pentose Pl	1247	NAMED	FNZLKVNU	OCC([C@H	ribulose 5-phosphate	ribulose 5-phosphate	18265-46-	388327	HMDB000	C00199	439184	Polar
297	402	17747	158164	Lipid	Sphingosir	3160	NAMED	WWUZIQ(	CCCCCCCC	sphingosine	sphingosine	123-78-4	4510275	HMDB000	C00319	5280335	Pos Late

Data Key & Explanation | Chemical Annotation | Sample Meta Data | Peak Area Data | Batch-normalized Data | Batch-norm Imputed Data | Mass_extracted-norm Data | Log Transformed Data

“Chemical annotation” tab in Metabolon results file:
Sort on “Platform” column to get 4 datasets (Pos Early, Pos Late, Neg and Polar)



CHEM_ID	LIB_ID	COMP_ID	_LIB_ENTR	ER_PATHW	B_PATHW	VAY_SORT	TYPE	INCHIKEY	SMILES	CHEMICAL_NAME	PLOT_NAME	CAS	HEMSPIDE	HMDB	KEGG	PUBCHEM	PLATFORM
62	209	38395	143675	Lipid	Fatty Acid,	2031	NAMED	CQSLTKIX/	CCCCCC(C	12,13-DiHOME	12,13-DiHOME	263399-35	8412123	HMDB000	C14829	10236635	Neg
98	209	1417	124553	Amino Aci	Tryptopha	272	NAMED	HCZHHEIF	OC1=C(C=	kynurenate	kynurenate	492-27-3	3712	HMDB000	C01717	3845	Neg
132	209	1414	124549	Carbohydı	Glycolysis,	1237	NAMED	IACAHGYC	OC(C(O)=	3-phosphoglycerate	3-phosphoglycerate	80731-10-	10669764	HMDB000	C00597	724	Neg
136	209	22842	124689	Lipid	Primary Bi	3454	NAMED	BHQCQFF	O[C@H]1[	cholate	cholate	81-25-4		HMDB000	C00695	221493	Neg
143	209	38309	143797	Lipid	Fatty Acid,	2054	NAMED	JVJFIQYAH	CCCCCC(/(	4-hydroxynonenal	4-hydroxynonenal	128946-65	1630	HMDB000	C21642	5283344	Neg
171	209	3127	124615	Nucleotide	Purine Me	4121	NAMED	FDGQSTZJ	O=C1C(N=	hypoxanthine	hypoxanthine	68-94-0	768	HMDB000	C00262	790,13539	Neg
179	209	38399	143740	Lipid	Fatty Acid,	2032	NAMED	XEBKSQSG	CCCCC/C=	9,10-DiHOME	9,10-DiHOME	263399-34	8142232	HMDB000	C14828	9966640	Neg
180	209	1105	125969	Lipid	Long Chair	1568	NAMED	OYHQOLU	OC(CCCC	linoleate (18:2n6)	linoleate (18:2n6)	60-33-3	4444105	HMDB000	C01595	5280450	Neg
197	209	42382	124939	Amino Aci	Methionin	446	NAMED		OC1C(N2C	S-adenosylhomocysteine (SAH)	S-adenosylhomocysteine (SAH)	979-92-0	16788012	HMDB009	C00021	439155	Neg
207	209	2831	123233	Nucleotide	Purine Me	4143	NAMED	IVOMOUV	NC1=NC=N	adenosine 3',5'-cyclic monophosphate (cA	adenosine 3',5'-cyclic monophospha	60-92-4	268	HMDB000	C00575	6076	Neg
208	209	3108	126001	Nucleotide	Purine Me	4139	NAMED	XTWYTFM	NC1=NC=N	adenosine 5'-diphosphate (ADP)	ADP	20398-34-	5800	HMDB000	C00008	6022	Neg
215	209	558	125963	Cofactors	Nicotinate	4327	NAMED	SDMADEZ	NC1=NC=N	adenosine 5'-diphosphoribose (ADP-ribos	adenosine 5'-diphosphoribose (ADP	68414-18-	3674071	HMDB000	C00301	192	Neg
240	209	32197	123321	Amino Aci	Tyrosine M	181	NAMED	JVGVDSSU	OC(C(O)=(	3-(4-hydroxyphenyl)lactate	3-(4-hydroxyphenyl)lactate (HPLA)	6482-98-0	9010	HMDB000	C03672	9378	Neg
269	209	62804	220430	Amino Aci	Glutathior	593	NAMED	JYKWMJBI	O[C@H]1[	CoA-glutathione*	CoA-glutathione*	6477-52-7	10128089		C00920	46873828	Neg
270	209	46322	145265	Cofactors	Pantothen	4343	NAMED	RGJOEKW	CC(COP(O	coenzyme A	CoA	85-61-0,18	311	HMDB000	C00010	87642	Neg
272	209	5983	126005	Lipid	Corticoste	3298	NAMED	OMFXVFT/	CC(C(CC1)	corticosterone	corticosterone	50-22-6	5550	HMDB000	C02140	5753	Neg
301	209	34302	126135	Cofactors	Ascorbate	4352	NAMED	SBJKKFFYI	OCC(C1OC	dehydroascorbate	dehydroascorbate	490-83-5	812	HMDB000	C05422	440667	Neg
302	209	1114	125714	Lipid	Secondary	3480	NAMED	KXGVEGM	CC12[C@(	deoxycholate	deoxycholate	83-44-3	389318	HMDB000	C04483	222528,44	Neg
327	209	2134	124607	Cofactors	Riboflavin	4334	NAMED	VWWQXM	OC(C(O)C(	flavin adenine dinucleotide (FAD)	FAD	146-14-5,8	559059	HMDB000	C00016	643975	Neg
347	209	2849	123235	Nucleotide	Purine Me	4178	NAMED	RQFCJASX	NC1=NC2=	guanosine 5'-monophosphate (5'-GMP)	5'- GMP	5550-12-9	741	HMDB000	C00144	6804	Neg
348	209	1411	124547	Nucleotide	Purine Me	4201	NAMED	YKBGVTZY	OC1=C(N=	2'-deoxyguanosine	2'-deoxyguanosine	961-07-9	163230	HMDB000	C00330	13539859	Neg
355	209	59	123153	Amino Aci	Histidine M	70	NAMED	HNDVDQJ	NC(C(O)=C	histidine	histidine	5934-29-2	752	HMDB000	C00135	6274	Neg
361	209	1123	123191	Nucleotide	Purine Me	4120	NAMED	UGQMRVF	O[C@H]1[	inosine	inosine	58-63-9	21241953	HMDB000	C00294	6021	Neg
409	209	1303	123199	Energy	TCA Cycle	1452	NAMED	BJEPYKJPY	OC(C(O)=(	malate	malate	6915-15-7	510	HMDB003	C00149,CC	525	Neg
424	209	1336	125720	Lipid	Long Chair	1511	NAMED	IPCSVZSSV	OC(CCCC	palmitate (16:0)	palmitate (16:0)	57-10-3	960	HMDB000	C00249	985	Neg
439	209	1358	125724	Lipid	Long Chair	1515	NAMED	QIQXTHQI	CCCCCCCC	stearate (18:0)	stearate (18:0)	57-11-4	5091	HMDB000	C01530	5281	Neg
452	209	33447	126083	Lipid	Long Chair	1530	NAMED	SECPZKHB	CCCCCC\C	palmitoleate (16:1n7)	palmitoleate (16:1n7)	373-49-9	393216	HMDB000	C08362	445638	Neg
461	209	42109	126986	Energy	Oxidative	1469	NAMED	NBIIXXVU	O=P(O)(O)	phosphate	phosphate	7664-38-2	1032	HMDB000	C00009	1061	Neg
463	209	597	124535	Carbohydı	Glycolysis,	1238	NAMED	DTBNBXW	O=P(O)(O(	phosphoenolpyruvate (PEP)	phosphoenolpyruvate (PEP)	10526-80-	980	HMDB000	C00074	1005	Neg
482	209	527	123163	Carbohydı	Glycolysis,	1240	NAMED	JVTAAEKC	CC(O)C(O)	lactate	lactate	79-33-4	592	HMDB000	C00186	612	Neg
491	209	1651	123217	Cofactors	Vitamin B(	4451	NAMED	RADKZDM	OC1=C(C)I	pyridoxal	pyridoxal	65-22-5	1021	HMDB000	C00250	1050	Neg
492	209	5331	152420	Cofactors	Vitamin B(	4450	NAMED	NGVDGCN	O=P(O)(O)	pyridoxal phosphate	pyridoxal phosphate	41468-25-	1022	HMDB000	C00018	1051	Neg
500	209	1827	123225	Cofactors	Riboflavin	4333	NAMED	AUNGANR	OC(C(O)C(	riboflavin (Vitamin B2)	riboflavin (Vitamin B2)	83-88-5	431981	HMDB000	C00255	493570	Neg
519	209	1365	125728	Lipid	Long Chair	1508	NAMED	TUNFSRH\	OC(CCCC	myristate (14:0)	myristate (14:0)	544-63-8	10539	HMDB000	C06424	11005	Neg
522	209	35670	128273	Cofactors	Thiamine	4423	NAMED	YXVCLPJQ	CC1=NC=C	thiamin diphosphate	thiamin diphosphate	154-87-0	8715	HMDB000	C00068	1132	Neg
523	209	15798	164715	Cofactors	Thiamine	4422	NAMED	HZSAJDVV	CC1=NC=C	thiamin monophosphate	thiamin monophosphate	532-40-1	2627905	HMDB000	C01081	1131,3382	Neg
535	209	606	123185	Nucleotide	Pyrimidine	4220	NAMED	DRTQHJP\	OC1C(N(C	uridine	uridine	58-96-8	5807	HMDB000	C00299	6029	Neg
536	209	1412	123201	Nucleotide	Pyrimidine	4236	NAMED	MXHRCPN	O=C(NC1=	2'-deoxyuridine	2'-deoxyuridine	951-78-0	13118	HMDB000	C00526	13712	Neg
821	209	33442	125870	Nucleotide	Pyrimidine	4222	NAMED	HZIOZCLE	O[C@]1([I	pseudouridine	pseudouridine	1445-07-4	21403010	HMDB000	C02067	15047	Neg
872	209	2183	124827	Nucleotide	Pyrimidine	4275	NAMED	IQFYYKKM	O=C(NC(C	thymidine	thymidine	50-89-5	5585	HMDB000	C00214	5789	Neg
882	209	604	126810	Nucleotide	Pyrimidine	4278	NAMED	RWQNBR	O=C1C(C)=	thymine	thymine	65-71-4	1103	HMDB000	C00178	1135	Neg
888	209	1642	125736	Lipid	Medium C	1495	NAMED	GHVNFZFC	CCCCCCCC	caprate (10:0)	caprate (10:0)	334-48-5	2863	HMDB000	C01571	2969	Neg
891	209	1121	125718	Lipid	Long Chair	1513	NAMED	KEMQGTR	O=C(O)CC	margarate (17:0)	margarate (17:0)	506-12-7	10033	HMDB0002259		10465	Neg
892	209	1356	125722	Lipid	Long Chair	1517	NAMED	ISYWECDI	CCCCCCCC	nonadecanoate (19:0)	nonadecanoate (19:0)	646-30-0	12071	HMDB000	C16535	12591	Neg
893	209	1118	125716	Lipid	Long Chair	1518	NAMED	VKOBVWX	CCCCCCCC	arachidate (20:0)	arachidate (20:0)	506-30-9	10035	HMDB000	C06425	10467	Neg
913	209	15586	124633	Carbohydı	Glycogen I	1300	NAMED	GUBGYTA	O[C@@H]	maltose	maltose	6363-53-7	388469	HMDB000	C00208	10991489	Neg
926	209	32489	125850	Lipid	Medium C	1490	NAMED	FUZZWVX	CCCCCC(O	caproate (6:0)	caproate (6:0)	142-62-1	8552	HMDB000	C01585	8892	Neg
932	209	32492	125852	Lipid	Medium C	1492	NAMED	WWZKQH	CCCCCCCC	caprylate (8:0)	caprylate (8:0)	124-07-2	370	HMDB000	C06423	379	Neg
980	209	1361	125726	Lipid	Long Chair	1510	NAMED	WQEPLUU	O=C(O)CC	pentadecanoate (15:0)	pentadecanoate (15:0)	10002-84-	13249	HMDB000	C16537	13849	Neg
1021	209	1494	123209	Amino Aci	Glutathior	579	NAMED	ODHCTXKI	O=C1CC[C	5-oxoproline	5-oxoproline	98-79-3	7127	HMDB000	C02237,CC	439685,74	Neg
1024	209	1508	124797	Cofactors	Pantothen	4337	NAMED	GHOKWG	O=C(NCCC	pantothenate	pantothenate (Vitamin B5)	137-08-6	6361	HMDB000	C00864	6613	Neg
1026	209	1600	124589	Lipid	Phospholi	2239	NAMED	SUHOOTK	NCCOP(O)	phosphoethanolamine	phosphoethanolamine (PE)	1071-23-4	990	HMDB000	C00346	1015	Neg
1080	209	48465	154416	Lipid	Eicosanoic	2150	NAMED	4000	CCCCC\C=	5-KETE	5-KETE	106154-18	1765	HMDB001	C14732	5353355	Neg

Data Key & Explanation | Chemical Annotation | Sample Meta Data | Peak Area Data | Batch-normalized Data | Batch-norm Imputed Data | Mass_extracted-norm Data | Log Transformed Data

“Peak area Data” tab in Metabolon results file

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	PARENT_SAMPLE_NAME	49	50	55	62	90	93	98	111	112	132	136	143	171	172	179	180	189	192	194	197
2	WASH-02116	452223	3895163	579521	468682	2970954	3749072			1863447	16833276	1038381	5527007	46310586	340131	392831	9.1E+09	19713662		911546	29923
3	WASH-02117	506717	4583423	828044	161483	3110717	3884827	75602	219800	2378842	17661327	286758	4265011	36109629	259006	224002	1.13E+10	26925663	54917	1259469	35259
4	WASH-02118	605861	6158099	610499	537652	3573398	6397640	78402		2106469	10742633	247487	4459762	42153612	294639	647369	1.28E+10	21871686	41862	1059919	25411
5	WASH-02119	441751	4153682	363872	318184	4430110	3640053	68765	109383	1908509	7755479	1898216	518338	38699707	202536	208805	6.61E+09	21386361	36088	1055856	31804
6	WASH-02120	805913	6989570	1282324	531691	4083535	5727567	68644	187985	2423502	16239975	468449	1680034	39559541	268711	582967	6.52E+09	23271494	56199	1208513	28027
7	WASH-02121	594692	6790709	1086786	126191	1568864	2662570	50185	127327	2016517	26838468	654614	6867986	40404808	293227	280209	1.12E+10	23661314	46941	1070039	25194
8	WASH-02122	1319533	10746472	1387408	117547	3035188	4686280	52258	133036	2175406	11988649	516443	5480533	37203751	324460	183632	9.15E+09	24150688	51185	1235271	16603
9	WASH-02123	832389	5788404	1615321	84901	2941955	3631780	85685		2163237	12449156	283164	9421384	46654715	302389		1.22E+10	27086612	68635	1245291	26775
10	WASH-02125	929364	7668152	1418806	250094	2509682	3774100	72811	254419	2210292	13282071	1184432	1403858	39859283	312510	248208	5.09E+09	24331196	66361	1328296	22646
11	WASH-02126	281687	2638282	531414	278891	1450477	5561934		212428	1061857	6827723	140095	1256697	38294424	243503	209622	9.82E+09	13786631	26364	704702	19960
12	WASH-02127	347989	2962047	776812	230655	2937948	6191605	41842	201933	1334843	6287164	593986	464709	41737056	255850	217231	2.63E+09	18826021	37906	914876	25983
13	WASH-02128	322323	2502108	541188		781021	3148661			1139584	8984219	163264	1449207	32051659	224466	104617	7.42E+09	11604740	19991	598135	20390
14	WASH-02129	322225	3387646	1029117	141466	4079801	7050846	26471		1579708	9515811	11880905	2280852	47597637	188203	101673	1.01E+10	15902259	33533	880489	32054
15	WASH-02130	541158	4761027	1032922	374300	4432035	7120633	81898	424133	2732850	5830215	293444	2252090	43984500	274982	246771	1.03E+10	20401007	55095	1165911	29760
16	WASH-02131	1351471	11226342	2557445	138535	3960003	2600718	76429	373898	2429806	10186090	357261	2270758	43668981	300358	178907	6.74E+09	21104936	83497	1223775	20455
17	WASH-02132	633176	4962499	1048678	238471	2513251	4068241		286872	1678963	7408478	149143	1299512	36857444	267244		9.87E+09	21054475	40134	1201646	18946
18	WASH-02133	476658	3239360	977307	118147	946545	2797872	76823	297922	1362085	7770003	97722	3639983	28679425	276517	129554	4.83E+09	9853218	37413	726802	13078
19	WASH-02134	1333529	12280021	1734416	226921	4299507	5015963	104724	430355	2781239	13707284	295223	4742948	40390420	293952	200701	6.81E+09	19733833	72700	1342306	14123
20	WASH-02135	1012028	5694174	1812076	133784	2500685	3773585	80607	297467	1780622	5530944	206118	1839597	47164794	330849		8.48E+09	18965672	64138	1246164	20254
21	WASH-02136	478579	9184206	1055198		5015913	6041946	90058	404987	2203541	9612669	565271	624946	40213318	244919		2.93E+09	20398081	43604	1299973	22050
22	WASH-02137	767842	7094598	1495681	267037	3291609	4501810	116855	403515	2282611	8698422	1684768	2918166	52139203	271598	158700	8.49E+09	21673162	51912	1299340	28650
23	WASH-02138	360871	6576576	985798	226303	113736	1180590	72911	232240	870818	2054978		345235	42207487	298546	339363	4.47E+09	3209201	49824	466205	12301
24	WASH-02139	286139	4562681	833049	280938	1652145	2503899	68502	518281	1013587	3028341		2125700	65404478	392940	448285	8.99E+09	9156338		938358	16613
25	WASH-02140	537298	8014111	1070191	368687	944889	1602599	52360	363098	1405278	2964360	122178	1066450	74314550	223748	425993	1.43E+10	8010512		823900	25417
26	WASH-02141	380950	4036562	1097747	291444	726152	1806675	73149	350249	1135204	3366571	123030	2767905	75358930	394703	258210	6.47E+09	6521075	21745		20677
27	WASH-02142	531362	4969552	1074331	197660	2754975	2620883	147219	779053	1698283	2470274	37690	1396714	95477943	558123	263579	9.41E+09	6724135	119504	1420421	22947
28	WASH-02143	350808	4267671	1010103	162104	1522391	2366760	32446	521508	991234	2439319		2570266	63411455	478931	309859	4.7E+09	8094222	36037	1061621	20748
29	WASH-02144	508999	5128872	1035422	640576	2581054	3249721	38858	344780	1100873	4220228	107887	1647480	80594236	313681	492380	1.56E+10	12845859		953729	29913
30	WASH-02145	594570	7311398	1114854	242101	1053573	2560641	97967	390064	4791523	11201316	47333	2580081	72326128	230203	202057	8.75E+09	14186025	27221	1133087	24593
31	WASH-02146	534526	5542335	1327826	119966	1612459	3330442	90879	456035	2292206	17647299		381029	70877806	224707	180199	9.62E+09	17446537	22125	1303324	25706
32	WASH-02147	473407	5294052	928595	147430	1489568	1884485	108889	599693	1127689	4211967	33224	1427310	82158155	495653	293791	8E+09	8368288	81018	870504	16124
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Data Key & Explanation | Chemical Annotation | Sample Meta Data | **Peak Area Data** | Batch-normalized Data | Batch-norm Imputed Data | Mass_extracted-norm Data | Log Transformed Data

“Peak area Data” needs to be transposed into a new tab (Transposed peak area data) and chem_id needs to be mapped to chemical name and Platform (from Chemical annotation tab)

CHEM_ID	CHEMICAL_NAME	PLATFORM		PLATFORM	CHEMICAL_NAME	PARENT_SAMPLE_NAME	WASH-02116	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WAS
62	12,13-DiHOME	Neg		Pos Early	putrescine	49	452223	506717	605861	441751	805913	594692	1319533	832389	929364	281687	347989	32
98	kynurenate	Neg		Pos Early	spermidine	50	3895163	4583423	6158099	4153682	6989570	6790709	10746472	5788404	7668152	2638282	2962047	250
132	3-phosphoglycerate	Neg		Pos Early	1-methylnicotinamide	55	579521	828044	610499	363872	1282324	1086786	1387408	1615321	1418806	531414	776812	54
136	cholate	Neg		Neg	12,13-DiHOME	62	468682	161483	537652	318184	531691	126191	117547	84901	250094	278891	230655	
143	4-hydroxynonenal	Neg		Polar	2-methylcitrate	90	2970954	3110717	3573398	4430110	4083535	1568864	3035188	2941955	2509682	1450477	2937948	78
171	hypoxanthine	Neg		Polar	alpha-ketoglutarate	93	3749072	3884827	6397640	3640053	5727567	2662570	4686280	3631780	3774100	5561934	6191605	314
179	9,10-DiHOME	Neg		Neg	kynurenate	98		75602	78402	68765	68644	50185	52258	85685	72811		41842	
180	linoleate (18:2n6)	Neg		Polar	3-hydroxyisobutyrate	111		219800		109383	187985	127327	133036		254419	212428	201933	
197	S-adenosylhomocysteine (SAH)	Neg		Polar	3-hydroxy-3-methylglut	112	1863447	2378842	2106469	1908509	2423502	2016517	2175406	2163237	2210292	1061857	1334843	113
207	adenosine 3',5'-cyclic monophosphate (cAMP)	Neg		Neg	3-phosphoglycerate	132	16833276	17661327	10742633	7755479	16239975	26838468	11988649	12449156	13282071	6827723	6287164	898
208	adenosine 5'-diphosphate (ADP)	Neg		Neg	cholate	136	1038381	286758	247487	1898216	468449	654614	516443	283164	1184432	140095	593986	16
215	adenosine 5'-diphosphoribose (ADP-ribose)	Neg		Neg	4-hydroxynonenal	143	5527007	4265011	4									
240	3-(4-hydroxyphenyl)lactate	Neg		Neg	hypoxanthine	171	46310586	36109629	42									
269	CoA-glutathione*	Neg		Pos Early	guanine	172	340131	259006										
270	coenzyme A	Neg		Neg	9,10-DiHOME	179	392831	224002										
272	corticosterone	Neg		Neg	linoleate (18:2n6)	180	9098076797	1.13E+10	1.									
301	dehydroascorbate	Neg		Pos Early	N6,N6,N6-trimethyllysir	189	19713662	26925663	21									
302	deoxycholate	Neg		Pos Early	N-acetylputrescine	192		54917										
327	flavin adenine dinucleotide (FAD)	Neg		Polar	N-formylmethionine	194	911546	1259469	1									
347	guanosine 5'-monophosphate (5'-GMP)	Neg		Neg	S-adenosylhomocystein	197	2992368	3525992	2									
348	2'-deoxyguanosine	Neg		Neg	adenosine 3',5'-cyclic m	207	420775	349546										
355	histidine	Neg		Neg	adenosine 5'-diphospha	208	17829829	19567207	19									
361	inosine	Neg		Pos Early	adenosine 5'-monopho	209	187872060	2.14E+08	2.									
409	malate	Neg		Pos Early	2'-deoxyadenosine	211	111429	119838										
424	palmitate (16:0)	Neg		Pos Early	5-methylthioadenosine	212	7230096	7490975	8									
439	stearate (18:0)	Neg		Neg	adenosine 5'-diphospho	215	5065001	5037979	8									
452	palmitoleate (16:1n7)	Neg		Pos Early	AICA ribonucleotide	216	65272	135229										
461	phosphate	Neg		Polar	ribose 1-phosphate	219	10035389	9081342	9									
463	phosphoenolpyruvate (PEP)	Neg		Pos Late	arachidonate (20:4n6)	229	946354	1322323	1									
482	lactate	Neg		Polar	arachidonoyl CoA	230	85290	81362										
491	pyridoxal	Neg		Pos Early	arginine	231	380650966	3.39E+08	3.									
492	pyridoxal phosphate	Neg		Polar	argininosuccinate	232	116510	127865										
500	riboflavin (Vitamin B2)	Neg		Pos Early	ascorbate (Vitamin C)	233	9907570	7928587	12									
519	myristate (14:0)	Neg		Pos Early	aspartate	234	352308882	5.21E+08	1.									
522	thiamin diphosphate	Neg		Neg	3-(4-hydroxyphenyl)lac	240	3192734	7253383	2									
523	thiamin monophosphate	Neg		Pos Early	beta-alanine	244	15556985	19434152	17300907	18599856	19894174	19443945	20062589	18117737	20276420	16475044	16727922	1453
535	uridine	Neg		Pos Early	carnosine	249	33880836	29607345	41380611	33054394	19667518	22549756	13300957	20282700	12400255	25782149	35001395	2144
536	2'-deoxyuridine	Neg		Pos Late	biliverdin	250	787256	931612	683782	876356	837303	782139	908806	751253	866764	618602	760121	48
821	pseudouridine	Neg		Polar	succinate	252	58324082	70123806	57228034	1.07E+08	47986814	60446788	79385158	65366972	62440908	44023117	65429215	3756
872	thymidine	Neg		Polar	3-hydroxybutyrate (BH	254	309817	227750	456673	220267	565219	261654	356287	250251	435055	1003685	951145	39
882	thymine	Neg		Pos Late	cholesterol	266	76831562	87118536	81402571	94741746	88796872	79139455	83496013	85110691	97077000	71130571	95826566	7359
888	caprate (10:0)	Neg		Pos Early	choline phosphate	267	133091811	1.07E+08	1.3E+08	1.32E+08	1.12E+08	96203030	1.3E+08	1.21E+08	1.27E+08	96371978	87655097	8166
891	margarate (17:0)	Neg		Neg	CoA-glutathione*	269	10177646	7299369	6994737	7620778	5361912	8924962	6956630	7482218	6810473	5251092	6810397	671
892	nonadecanoate (19:0)	Neg		Neg	coenzyme A	270	1089193	1006735	2265115	1164649	1383771	1647865	1147963	509139	1174901	927291	1568802	91
893	arachidate (20:0)	Neg		Neg	corticosterone	272	835316	568112	477274	518920	311460	606640	189446	690947	859007	246732	478892	38
913	maltose	Neg		Pos Early	creatinine	275	96237943	97823434	96696778	94271117	1.09E+08	1.08E+08	99343577	99584383	1.06E+08	78186706	92285583	6759
926	caproate (6:0)	Neg		Pos Early	cysteinylglycine	278	435015	409416	784755	481686	517466	432128	366438	438528	348707	178786	247395	18
932	caprylate (8:0)	Neg		Pos Early	cytidine 5'-monophosp	282	4067428	4679323	4769664	4749556	4512069	5873288	5883627	5088953	4743794	2478710	3143149	290
980	pentadecanoate (15:0)	Neg		Polar	glucosamine-6-phospha	290	1733002	2978093	5492398	2277192	6205981	4772909	4116051	3642374	2869232	657988	1268148	86
1021	5-oxoproline	Neg		Polar	glucose 6-phosphate	291	30225858	48045592	89557228	38148918	1.07E+08	80756267	76235759	64835766	45152902	12743833	28640559	1731
1024	pantothenate	Neg		Polar	mannose-6-phosphate	294	7243320	11066607	17831970	7885813	21542288	15279792	16250870	13768936	10273703	3523006	6603523	420
1026	phosphoethanolamine	Neg		Polar	ribulose 5-phosphate	296	19971	46207.8	99468.9	90402	224009.3	61758	153091	128851	10043.2	88010	182462.3	2
1080	5-KETE	Neg		Pos Late	sphingosine	297	7873434	9085811	9469731	10409694	9023074	8701405	10483862	9992608	11380069	6290479	7589568	710

Data Key & Explanation | Chemical Annotation | Sample Meta Data | Peak Area Data | Transposed Peak area data | Batch-normalized Data | Batch-norm Imputed Data | Mass_extracted-norm Data | Log Transformed Data

Ready | Accessibility: Investigate

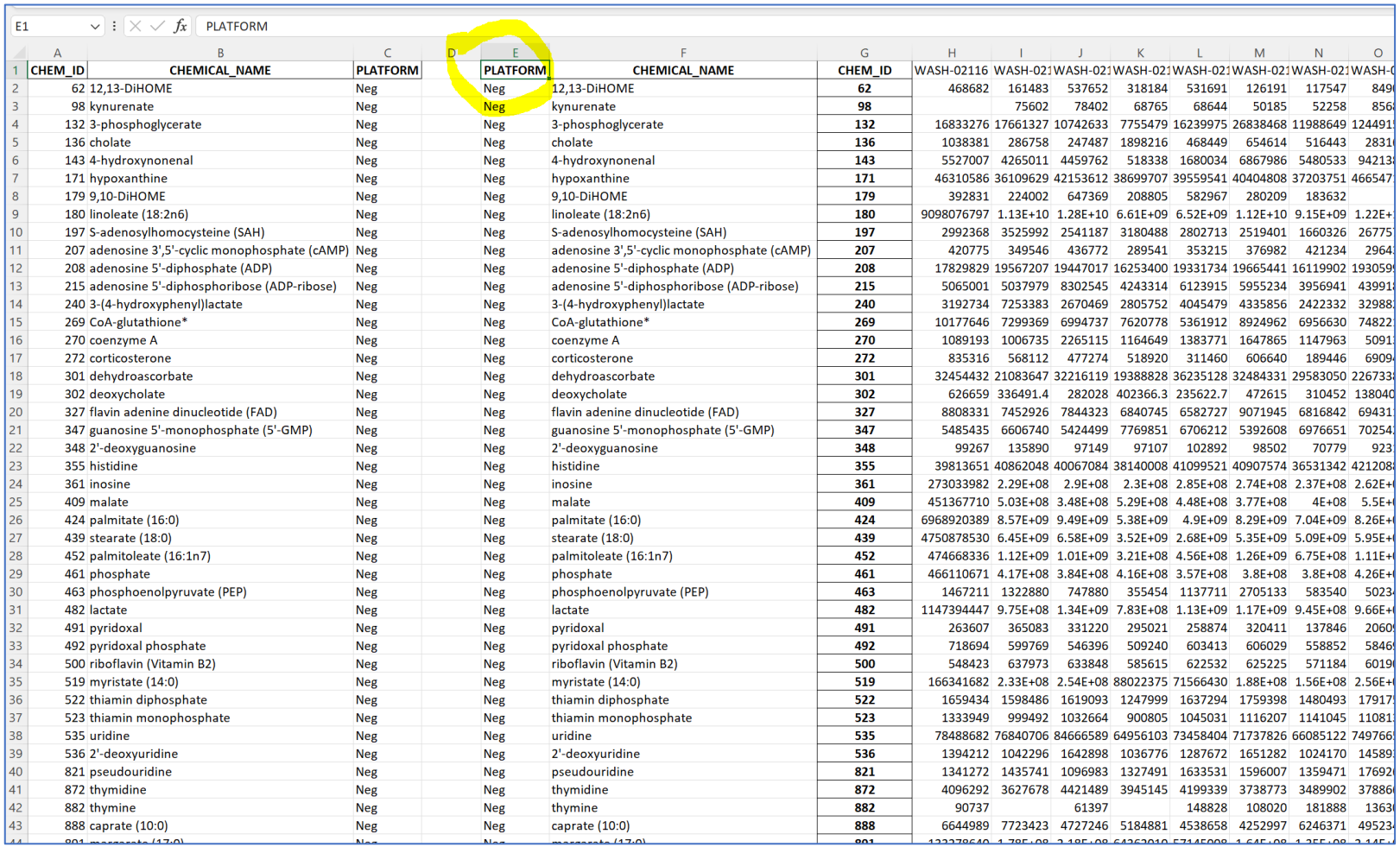
F2 =VLOOKUP(G2,A:B,2,FALSE)

CHEM_ID	CHEMICAL_NAME	PLATFORM		PLATFORM	CHEMICAL_NAME	CHEM_ID	WASH-02116	WASH-021	WASH-
62	12,13-DiHOME	Neg		Pos Early	putrescine	49	452223	506717	6058
98	kynurenate	Neg		Pos Early	spermidine	50	3895163	4583423	61580
132	3-phosphoglycerate	Neg		Pos Early	1-methylnicotinamide	55	579521	828044	6104
136	cholate	Neg		Neg	12,13-DiHOME	62	468682	161483	5376
143	4-hydroxynonenal	Neg		Polar	2-methylcitrate	90	2970954	3110717	35733
171	hypoxanthine	Neg		Polar	alpha-ketoglutarate	93	3749072	3884827	63976
179	9,10-DiHOME	Neg		Neg	kynurenate	98		75602	784
180	linoleate (18:2n6)	Neg		Polar	3-hydroxyisobutyrate	111		219800	
197	S-adenosylhomocysteine (SAH)	Neg		Polar	3-hydroxy-3-methylglut	112	1863447	2378842	21064
207	adenosine 3',5'-cyclic monophosphate (cAMP)	Neg		Neg	3-phosphoglycerate	132	16833276	17661327	107426
208	adenosine 5'-diphosphate (ADP)	Neg		Neg	cholate	136	1038381	286758	2474
215	adenosine 5'-diphosphoribose (ADP-ribose)	Neg		Neg	4-hydroxynonenal	143	5527007	4265011	44597
240	3-(4-hydroxyphenyl)lactate	Neg		Neg	hypoxanthine	171	46310586	36109629	421536
269	CoA-glutathione*	Neg		Pos Early	guanine	172	340131	259006	2946
270	coenzyme A	Neg		Neg	9,10-DiHOME	179	392831	224002	6473
272	corticosterone	Neg		Neg	linoleate (18:2n6)	180	9098076797	1.13E+10	1.28E+
301	dehydroascorbate	Neg		Pos Early	N6,N6,N6-trimethyllysir	189	19713662	26925663	218716

Use “vlookup” function to map chem_id to metabolite name and platform

Sort the results table on the “Platform “ column

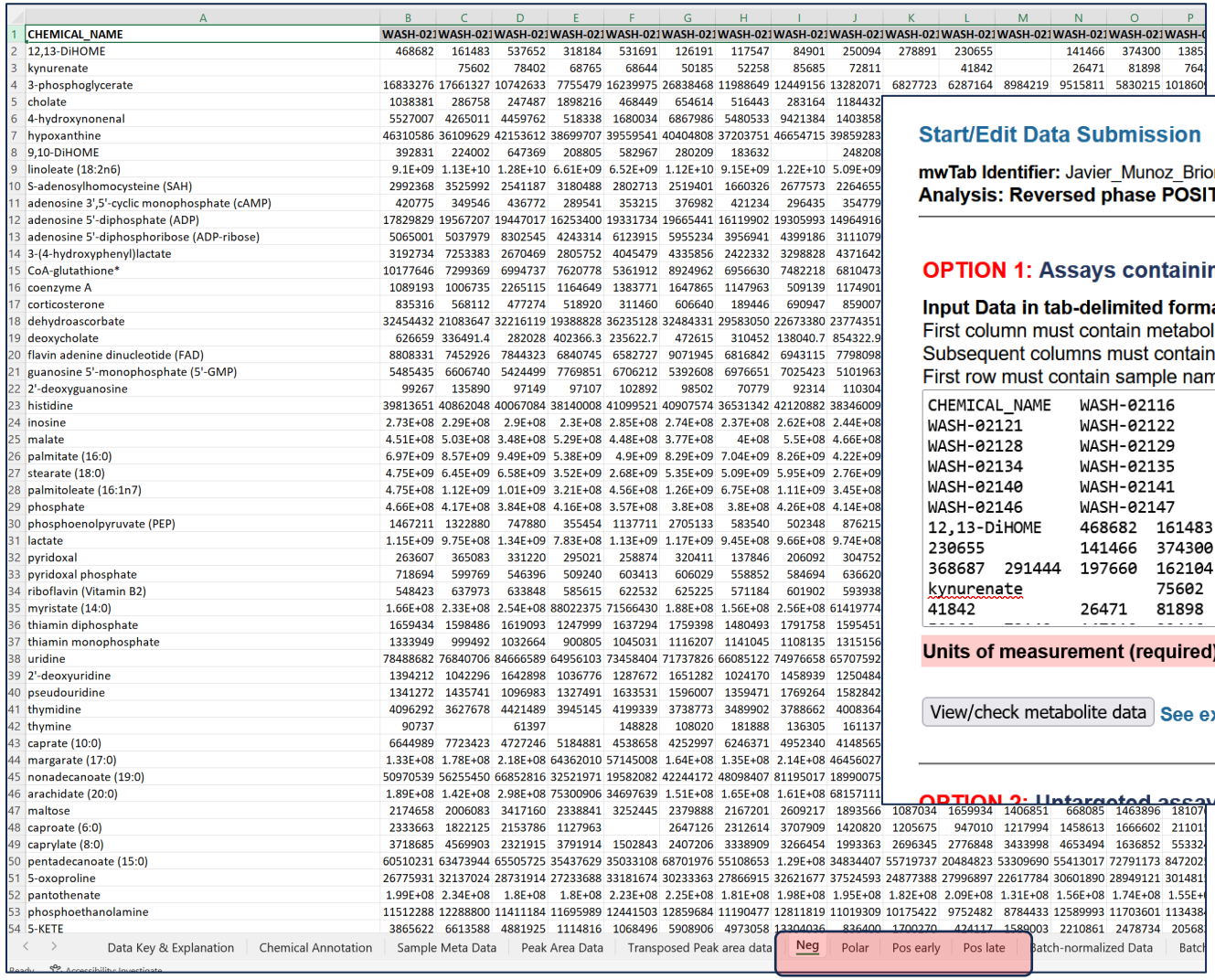
Now you’ve got all 4 results datasets separated in the “Transposed peak area data” tab and 4 metabolite metadata sets separated in the “Chemical Annotation” tab



E1 | PLATFORM

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	CHEM_ID	CHEMICAL_NAME	PLATFORM		PLATFORM	CHEMICAL_NAME	CHEM_ID	WASH-02116	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-021	WASH-(
2	62	12,13-DiHOME	Neg		Neg	12,13-DiHOME	62	468682	161483	537652	318184	531691	126191	117547	849
3	98	kynurenate	Neg		Neg	kynurenate	98		75602	78402	68765	68644	50185	52258	856
4	132	3-phosphoglycerate	Neg		Neg	3-phosphoglycerate	132	16833276	17661327	10742633	7755479	16239975	26838468	11988649	124491
5	136	cholate	Neg		Neg	cholate	136	1038381	286758	247487	1898216	468449	654614	516443	2831
6	143	4-hydroxynonenal	Neg		Neg	4-hydroxynonenal	143	5527007	4265011	4459762	518338	1680034	6867986	5480533	94213
7	171	hypoxanthine	Neg		Neg	hypoxanthine	171	46310586	36109629	42153612	38699707	39559541	40404808	37203751	466547
8	179	9,10-DiHOME	Neg		Neg	9,10-DiHOME	179	392831	224002	647369	208805	582967	280209	183632	
9	180	linoleate (18:2n6)	Neg		Neg	linoleate (18:2n6)	180	9098076797	1.13E+10	1.28E+10	6.61E+09	6.52E+09	1.12E+10	9.15E+09	1.22E+
10	197	S-adenosylhomocysteine (SAH)	Neg		Neg	S-adenosylhomocysteine (SAH)	197	2992368	3525992	2541187	3180488	2802713	2519401	1660326	26775
11	207	adenosine 3',5'-cyclic monophosphate (cAMP)	Neg		Neg	adenosine 3',5'-cyclic monophosphate (cAMP)	207	420775	349546	436772	289541	353215	376982	421234	2964
12	208	adenosine 5'-diphosphate (ADP)	Neg		Neg	adenosine 5'-diphosphate (ADP)	208	17829829	19567207	19447017	16253400	19331734	19665441	16119902	193059
13	215	adenosine 5'-diphosphoribose (ADP-ribose)	Neg		Neg	adenosine 5'-diphosphoribose (ADP-ribose)	215	5065001	5037979	8302545	4243314	6123915	5955234	3956941	43991
14	240	3-(4-hydroxyphenyl)lactate	Neg		Neg	3-(4-hydroxyphenyl)lactate	240	3192734	7253383	2670469	2805752	4045479	4335856	2422332	32988
15	269	CoA-glutathione*	Neg		Neg	CoA-glutathione*	269	10177646	7299369	6994737	7620778	5361912	8924962	6956630	74822
16	270	coenzyme A	Neg		Neg	coenzyme A	270	1089193	1006735	2265115	1164649	1383771	1647865	1147963	5091
17	272	corticosterone	Neg		Neg	corticosterone	272	835316	568112	477274	518920	311460	606640	189446	6909
18	301	dehydroascorbate	Neg		Neg	dehydroascorbate	301	32454432	21083647	32216119	19388828	36235128	32484331	29583050	226733
19	302	deoxycholate	Neg		Neg	deoxycholate	302	626659	336491.4	282028	402366.3	235622.7	472615	310452	138040
20	327	flavin adenine dinucleotide (FAD)	Neg		Neg	flavin adenine dinucleotide (FAD)	327	8808331	7452926	7844323	6840745	6582727	9071945	6816842	69431
21	347	guanosine 5'-monophosphate (5'-GMP)	Neg		Neg	guanosine 5'-monophosphate (5'-GMP)	347	5485435	6606740	5424499	7769851	6706212	5392608	6976651	70254
22	348	2'-deoxyguanosine	Neg		Neg	2'-deoxyguanosine	348	99267	135890	97149	97107	102892	98502	70779	923
23	355	histidine	Neg		Neg	histidine	355	39813651	40862048	40067084	38140008	41099521	40907574	36531342	421208
24	361	inosine	Neg		Neg	inosine	361	273033982	2.29E+08	2.9E+08	2.3E+08	2.85E+08	2.74E+08	2.37E+08	2.62E+
25	409	malate	Neg		Neg	malate	409	451367710	5.03E+08	3.48E+08	5.29E+08	4.48E+08	3.77E+08	4E+08	5.5E+
26	424	palmitate (16:0)	Neg		Neg	palmitate (16:0)	424	6968920389	8.57E+09	9.49E+09	5.38E+09	4.9E+09	8.29E+09	7.04E+09	8.26E+
27	439	stearate (18:0)	Neg		Neg	stearate (18:0)	439	4750878530	6.45E+09	6.58E+09	3.52E+09	2.68E+09	5.35E+09	5.09E+09	5.95E+
28	452	palmitoleate (16:1n7)	Neg		Neg	palmitoleate (16:1n7)	452	474668336	1.12E+09	1.01E+09	3.21E+08	4.56E+08	1.26E+09	6.75E+08	1.11E+
29	461	phosphate	Neg		Neg	phosphate	461	466110671	4.17E+08	3.84E+08	4.16E+08	3.57E+08	3.8E+08	3.8E+08	4.26E+
30	463	phosphoenolpyruvate (PEP)	Neg		Neg	phosphoenolpyruvate (PEP)	463	1467211	1322880	747880	355454	1137711	2705133	583540	5023
31	482	lactate	Neg		Neg	lactate	482	1147394447	9.75E+08	1.34E+09	7.83E+08	1.13E+09	1.17E+09	9.45E+08	9.66E+
32	491	pyridoxal	Neg		Neg	pyridoxal	491	263607	365083	331220	295021	258874	320411	137846	2060
33	492	pyridoxal phosphate	Neg		Neg	pyridoxal phosphate	492	718694	599769	546396	509240	603413	606029	558852	5846
34	500	riboflavin (Vitamin B2)	Neg		Neg	riboflavin (Vitamin B2)	500	548423	637973	633848	585615	622532	625225	571184	6019
35	519	myristate (14:0)	Neg		Neg	myristate (14:0)	519	166341682	2.33E+08	2.54E+08	88022375	71566430	1.88E+08	1.56E+08	2.56E+
36	522	thiamin diphosphate	Neg		Neg	thiamin diphosphate	522	1659434	1598486	1619093	1247999	1637294	1759398	1480493	17917
37	523	thiamin monophosphate	Neg		Neg	thiamin monophosphate	523	1333949	999492	1032664	900805	1045031	1116207	1141045	11081
38	535	uridine	Neg		Neg	uridine	535	78488682	76840706	84666589	64956103	73458404	71737826	66085122	749766
39	536	2'-deoxyuridine	Neg		Neg	2'-deoxyuridine	536	1394212	1042296	1642898	1036776	1287672	1651282	1024170	14589
40	821	pseudouridine	Neg		Neg	pseudouridine	821	1341272	1435741	1096983	1327491	1633531	1596007	1359471	17692
41	872	thymidine	Neg		Neg	thymidine	872	4096292	3627678	4421489	3945145	4199339	3738773	3489902	37886
42	882	thymine	Neg		Neg	thymine	882	90737		61397		148828	108020	181888	1363
43	888	caprate (10:0)	Neg		Neg	caprate (10:0)	888	6644989	7723423	4727246	5184881	4538658	4252997	6246371	49523

Create separate tabs for Pos Early, Pos Late, Neg and Polar datasets
Delete the chem_id and platform columns
These datasets are then ready to be copied/pasted into the results sections of the online submission form
Order of analyses: 1:Pos Early, 2:Pos Late, 3:Neg 4:Polar



CHEMICAL_NAME	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02	WASH-02
12,13-DiHOME	468682	161483	537652	318184	531691	126191	117547	84901	250094	278891	230655		141466	374300	1385
kynurenate		75602	78402	68765	68644	50185	52258	85685	72811		41842		26471	81898	764
3-phosphoglycerate	16833276	17661327	10742633	7755479	16239975	26838468	11988649	12449156	13282071	6827723	6287164	8984219	9515811	5830215	101860
cholate	1038381	286758	247487	1898216	468449	654614	516443	283164	1184432						
4-hydroxynonenal	5527007	4265011	4459762	518338	1680034	6867986	5480533	9421384	1403858						
hypoxanthine	46310586	36109629	42153612	38699707	39559541	40404808	37203751	46654715	39859283						
9,10-DiHOME	392831	224002	647369	208805	582967	280209	183632		248208						
linoleate (18:2n6)	9.1E+09	1.13E+10	1.28E+10	6.61E+09	6.52E+09	1.12E+10	9.15E+09	1.22E+10	5.09E+09						
S-adenosylhomocysteine (SAH)	2992368	3525992	2541187	3180488	2802713	2519401	1660326	2677573	2264655						
adenosine 3',5'-cyclic monophosphate (cAMP)	420775	349546	436772	289541	353215	376982	421234	296435	354779						
adenosine 5'-diphosphate (ADP)	17829829	19567207	19447017	16253400	19331734	19665441	16119902	19305993	14964916						
adenosine 5'-diphosphoribose (ADP-ribose)	5065001	5037979	8302545	4243314	6123915	5955234	3956941	4399186	3111079						
3-(4-hydroxyphenyl)lactate	3192734	7253383	2670469	2805752	4045479	4335856	2422332	3298828	4371642						
CoA-glutathione*	10177646	7299369	6994737	7620778	5361912	8924962	6956630	7482218	6810473						
coenzyme A	1089193	1006735	2265115	1164649	1383771	1647865	1147963	509139	1174901						
corticosterone	835316	568112	477274	518920	311460	606640	189446	690947	859007						
dehydroascorbate	32454432	21083647	32216119	19388828	36235128	32484331	29583050	22673380	23774351						
deoxycholate	626659	336491.4	282028	402366.3	235622.7	472615	310452	138040.7	854322.9						
flavin adenine dinucleotide (FAD)	8808331	7452926	7844323	6840745	6582727	9071945	6816842	6943115	7798098						
guanosine 5'-monophosphate (5'-GMP)	5485435	6606740	5424499	7769851	6706212	5392608	6976651	7025423	5101963						
2'-deoxyguanosine	99267	135890	97149	97107	102892	98502	70779	92314	110304						
histidine	39813651	40862048	40067084	38140008	41099521	40907574	36531342	42120882	38346009						
inosine	2.73E+08	2.29E+08	2.9E+08	2.3E+08	2.85E+08	2.74E+08	2.37E+08	2.62E+08	2.44E+08						
malate	4.51E+08	5.03E+08	3.48E+08	5.29E+08	4.48E+08	3.77E+08	4E+08	5.5E+08	4.66E+08						
palmitate (16:0)	6.97E+09	8.57E+09	9.49E+09	5.38E+09	4.9E+09	8.29E+09	7.04E+09	8.26E+09	4.22E+09						
stearate (18:0)	4.75E+09	6.45E+09	6.58E+09	3.52E+09	2.68E+09	5.35E+09	5.09E+09	5.95E+09	2.76E+09						
palmitoleate (16:1n7)	4.75E+08	1.12E+09	1.01E+09	3.21E+08	4.56E+08	1.26E+09	6.75E+08	1.11E+09	3.45E+08						
phosphate	4.66E+08	4.17E+08	3.84E+08	4.16E+08	3.57E+08	3.8E+08	3.8E+08	4.26E+08	4.14E+08						
phosphoenolpyruvate (PEP)	1467211	1322880	747880	355454	1137711	2705133	583540	502348	876215						
lactate	1.15E+09	9.75E+08	1.34E+09	7.83E+08	1.13E+09	1.17E+09	9.45E+08	9.66E+08	9.74E+08						
pyridoxal	263607	365083	331220	295021	258874	320411	137846	206092	304752						
pyridoxal phosphate	718694	599769	546396	509240	603413	606029	558852	584694	636620						
riboflavin (Vitamin B2)	548423	637973	633848	585615	622532	625225	571184	601902	593938						
myristate (14:0)	1.66E+08	2.33E+08	2.54E+08	88022375	71566430	1.88E+08	1.56E+08	2.56E+08	61419774						
thiamin diphosphate	1659434	1598486	1619093	1247999	1637294	1759398	1480493	1791758	1595451						
thiamin monophosphate	1333949	999492	1032664	900805	1045031	1116207	1141045	1108135	1315156						
uridine	78488682	76840706	84666589	64956103	73458404	71737826	66085122	74976658	65707592						
2'-deoxyuridine	1394212	1042296	1642898	1036776	1287672	1651282	1024170	1458939	1250484						
pseudouridine	1341272	1435741	1096983	1327491	1633531	1596007	1359471	1769264	1582842						
thymidine	4096292	3627678	4421489	3945145	4199339	3738773	3489902	3788662	4008364						
thymine	90737		61397		148828	108020	181888	136305	161137						
caprate (10:0)	6644989	7723423	4727246	5184881	4538658	4252997	6246371	4952340	4148565						
margarate (17:0)	1.33E+08	1.78E+08	2.18E+08	64362010	57145008	1.64E+08	1.35E+08	2.14E+08	46456027						
nonadecanoate (19:0)	50970539	56255450	66852816	32521971	19582082	42244172	48098407	81195017	18990075						
arachidate (20:0)	1.89E+08	1.42E+08	2.98E+08	75300906	34697639	1.51E+08	1.65E+08	1.61E+08	68157111						
maltose	2174658	2006083	3417160	2338841	3252445	2379888	2167201	2609217	1893566	1087034	1659934	1406851	668085	1463896	18107
caproate (6:0)	2333663	1822125	2153786	1127963		2647126	2312614	3707909	1420820	1205675	947010	1217994	1458613	1666602	21101
caprylate (8:0)	3718685	4569903	2321915	3791914	1502843	2407206	3338909	3266454	1993363	2696345	2776848	3433998	4653494	1636852	55332
pentadecanoate (15:0)	60510231	63473944	65505725	35437629	35033108	68701976	55108653	1.29E+08	34834407	55719737	20484823	53309690	55413017	72791173	847202
5-oxoproline	26775931	32137024	28731914	27233688	33181674	30233363	27866915	32621677	37524593	24877388	27996897	22617784	30601890	28949121	301481
pantothenate	1.99E+08	2.34E+08	1.8E+08	1.8E+08	2.23E+08	2.25E+08	1.81E+08	1.98E+08	1.95E+08	1.82E+08	2.09E+08	1.31E+08	1.56E+08	1.74E+08	1.55E+
phosphoethanolamine	11512288	12288800	11411184	11695989	12441503	12859684	11190477	12811819	11019309	10175422	9752482	8784433	12589993	11703601	113438
5-KETE	3865622	6613588	4881925	1114816	1068496	5908906	4973058	13304036	836400	1700270	424117	1589003	2210861	2478734	20568

Data Key & Explanation | Chemical Annotation | Sample Meta Data | Peak Area Data | Transposed Peak area data | Neg | Polar | Pos early | Pos late | Batch-normalized Data | Batch

Start/Edit Data Submission | Examples of study design and data layouts | Online Study Submission Tutorial(pdf)

mwTab Identifier: Javier_Munoz_Briones_24_20230930_161810 Return to start
Analysis: Reversed phase POSITIVE (1)

OPTION 1: Assays containing identified (named) metabolite species

Input Data in tab-delimited format in the text area below.
First column must contain metabolite names.
Subsequent columns must contain sample data with identical sample names as in Study Design submission.
First row must contain sample names.

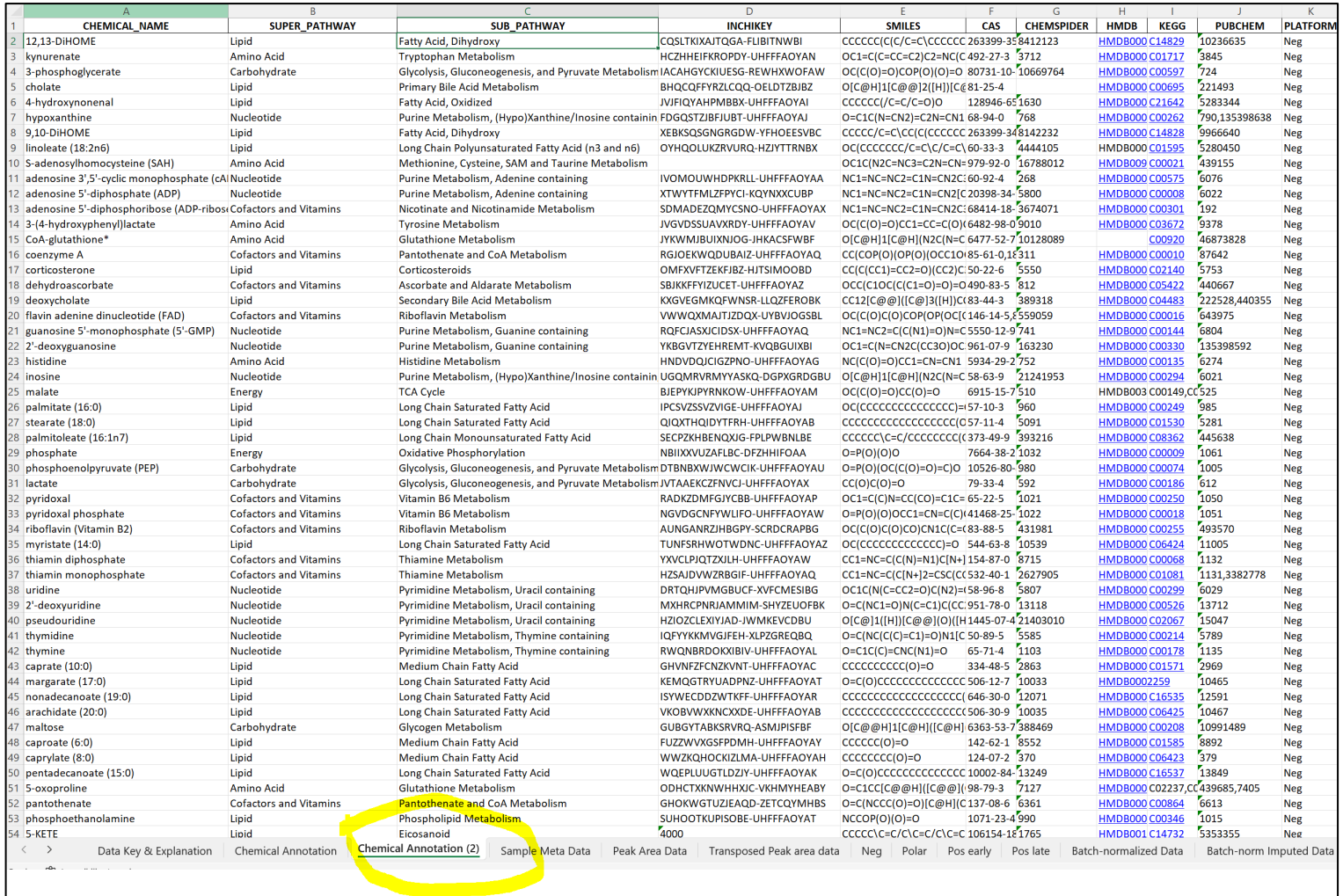
```
CHEMICAL_NAME   WASH-02116   WASH-02117   WASH-02118   WASH-02119   WASH-02120
WASH-02121      WASH-02122   WASH-02123   WASH-02125   WASH-02126   WASH-02127
WASH-02128      WASH-02129   WASH-02130   WASH-02131   WASH-02132   WASH-02133
WASH-02134      WASH-02135   WASH-02136   WASH-02137   WASH-02138   WASH-02139
WASH-02140      WASH-02141   WASH-02142   WASH-02143   WASH-02144   WASH-02145
WASH-02146      WASH-02147
12,13-DiHOME    468682  161483  537652  318184  531691  126191  117547  84901  250094  278891
230655          141466  374300  138535  238471  118147  226921  133784         267037  226303  280938
368687  291444  197660  162104  640576  242101  119966  147430
kynurenate              75602   78402   68765   68644   50185   52258   85685  72811
41842           26471   81898   76429           76823   104724  80607   90058  116855  72911   68502
```

Units of measurement (required): Peak area

View/check metabolite data | See examples of metabolite data layout | Delete existing metabolite data (this analysis only)

OPTION 2: Untargeted assays not containing identified (named) metabolite species

Make a copy of the “Chemical annotation” tab and put “Chemical name” on the left
This column must EXACTLY match that of results datasets with regard to metabolite names
Note that several columns may be deleted for the purpose of submission upload (Metabolon identifiers, etc)
Split this table into 4 sub-tables corresponding to Pos Early, Pos Late, Neg and Polar metadata



	A	B	C	D	E	F	G	H	I	J	K
1	CHEMICAL_NAME	SUPER_PATHWAY	SUB_PATHWAY	INCHIKEY	SMILES	CAS	CHEMSPIDER	HMDB	KEGG	PUBCHEM	PLATFORM
2	12,13-DiHOME	Lipid	Fatty Acid, Dihydroxy	CQSLTKIXAJTQGA-FLIBITNWBI	CCCCCC(C(C/C=C\CCCCCC	263399-35	8412123	HMDB000	C14829	10236635	Neg
3	kynurenate	Amino Acid	Tryptophan Metabolism	HCZHHEIFKROPDY-UHFFFAOYAN	OC1=C(C=CC=C2)C2=NC(C	492-27-3	3712	HMDB000	C01717	3845	Neg
4	3-phosphoglycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	IACAHGYCKIUESG-REWHXWOFAW	OC(C(O)=O)COP(O)(O)=O	80731-10	10669764	HMDB000	C00597	724	Neg
5	cholate	Lipid	Primary Bile Acid Metabolism	BHQCQFFYRZLCQQ-OELDTZBJBZ	O[C@H]1[C@@]2([H])[C(	81-25-4		HMDB000	C00695	221493	Neg
6	4-hydroxynonenal	Lipid	Fatty Acid, Oxidized	JVJFIQYAHPMBBX-UHFFFAOYAI	CCCCCC(/C=C/C=O)O	128946-65	1630	HMDB000	C21642	5283344	Neg
7	hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containin	FDGQSTZJBFJUBT-UHFFFAOYAJ	O=C1C(N=CN2)=C2N=CN1	68-94-0	768	HMDB000	C00262	790,135398638	Neg
8	9,10-DiHOME	Lipid	Fatty Acid, Dihydroxy	XEBKSQSGNGRGDW-YFHOEESVBC	CCCCC/C=C\CC(C(CCCCCC	263399-34	8142232	HMDB000	C14828	9966640	Neg
9	linoleate (18:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	OYHQOLUKZRVURQ-HZJYTTRNBX	OC(CCCCCCC/C=C\C/C=C\	60-33-3	4444105	HMDB000	C01595	5280450	Neg
10	S-adenosylhomocysteine (SAH)	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism		OC1C(N2C=NC3=C2N=CN=	979-92-0	16788012	HMDB009	C00021	439155	Neg
11	adenosine 3',5'-cyclic monophosphate (cAI	Nucleotide	Purine Metabolism, Adenine containing	IVOMOUWHDPKRLL-UHFFFAOYAA	NC1=NC=NC2=C1N=CN2C	60-92-4	268	HMDB000	C00575	6076	Neg
12	adenosine 5'-diphosphate (ADP)	Nucleotide	Purine Metabolism, Adenine containing	XTWYTFMLZFPYCI-KQYNXXCUBP	NC1=NC=NC2=C1N=CN2[C	20398-34	5800	HMDB000	C00008	6022	Neg
13	adenosine 5'-diphosphoribose (ADP-ribos	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	SDMADEZQMYCSNO-UHFFFAOYAX	NC1=NC=NC2=C1N=CN2C	68414-18	3674071	HMDB000	C00301	192	Neg
14	3-(4-hydroxyphenyl)lactate	Amino Acid	Tyrosine Metabolism	JVGVDSSUAVXRDY-UHFFFAOYAV	OC(C(O)=O)CC1=CC=C(O)(	6482-98-0	9010	HMDB000	C03672	9378	Neg
15	CoA-glutathione*	Amino Acid	Glutathione Metabolism	JYKWMJBUIXNJOG-JHKACSFWBF	O[C@H]1[C@H](N2C(N=C	6477-52-7	10128089		C00920	46873828	Neg
16	coenzyme A	Cofactors and Vitamins	Pantothenate and CoA Metabolism	RGJOEKWQDUBAIZ-UHFFFAOYAQ	CC(COP(O)(OP(O)(OCC1O	85-61-0,1	311	HMDB000	C00010	87642	Neg
17	corticosterone	Lipid	Corticosteroids	OMFXVFTZEKFJBZ-HJTSIMOOBD	CC(C(CC1)=CC2=O)(CC2)C	50-22-6	5550	HMDB000	C02140	5753	Neg
18	dehydroascorbate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	SBJKKFFYIZUCET-UHFFFAOYAZ	OCC(C1OC(C(C1=O)=O)=O	490-83-5	812	HMDB000	C05422	440667	Neg
19	deoxycholate	Lipid	Secondary Bile Acid Metabolism	KXGVEGMKQFWNSR-LLQZFEROBK	CC12[C@@]([C@]3([H])C(	83-44-3	389318	HMDB000	C04483	222528,440355	Neg
20	flavin adenine dinucleotide (FAD)	Cofactors and Vitamins	Riboflavin Metabolism	VWWQXMAJTJZDQX-UYBVJOGSBL	OC(C(O)C(O)COP(OP(OC[	146-14-5,5	559059	HMDB000	C00016	643975	Neg
21	guanosine 5'-monophosphate (5'-GMP)	Nucleotide	Purine Metabolism, Guanine containing	RQFCJASXJCIDSX-UHFFFAOYAQ	NC1=NC2=C(C(N1)=O)N=C	5550-12-9	741	HMDB000	C00144	6804	Neg
22	2'-deoxyguanosine	Nucleotide	Purine Metabolism, Guanine containing	YKBGVTZYEHREMT-KVQBGUIXBI	OC1=C(N=CN2C(CC3O)OC	961-07-9	163230	HMDB000	C00330	135398592	Neg
23	histidine	Amino Acid	Histidine Metabolism	HNDVDQJCIGZPNO-UHFFFAOYAG	NC(C(O)=O)CC1=CN=CN1	5934-29-2	752	HMDB000	C00135	6274	Neg
24	inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containin	UGQMRVRMYYASKQ-DGPXGRDGBU	O[C@H]1[C@H](N2C(N=C	58-63-9	21241953	HMDB000	C00294	6021	Neg
25	malate	Energy	TCA Cycle	BJEPYKJPYRNKOW-UHFFFAOYAM	OC(C(O)=O)CC(O)=O	6915-15-7	510	HMDB003	C00149,CC	525	Neg
26	palmitate (16:0)	Lipid	Long Chain Saturated Fatty Acid	IPCSVZSSVZVIGE-UHFFFAOYAJ	OC(CCCCCCCCCCCCCCC)=(	57-10-3	960	HMDB000	C00249	985	Neg
27	stearate (18:0)	Lipid	Long Chain Saturated Fatty Acid	QIQXTHQIDYTFRH-UHFFFAOYAB	CCCCCCCCCCCCCCCCCC(O	57-11-4	5091	HMDB000	C01530	5281	Neg
28	palmitoleate (16:1n7)	Lipid	Long Chain Monounsaturated Fatty Acid	SECPZKHBENQXJG-FPLPWBNLBE	CCCCCC\C=C/CCCCCCCC(	373-49-9	393216	HMDB000	C08362	445638	Neg
29	phosphate	Energy	Oxidative Phosphorylation	NBIIXXVUZAFLBC-DFZHHIFOAA	O=P(O)(O)O	7664-38-2	1032	HMDB000	C00009	1061	Neg
30	phosphoenolpyruvate (PEP)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	DTBNBXWJWCWCIK-UHFFFAOYAU	O=P(O)(OC(C(O)=O)=C)O	10526-80-	980	HMDB000	C00074	1005	Neg
31	lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	JVTAAEKCZFNVCJ-UHFFFAOYAX	CC(O)C(O)=O	79-33-4	592	HMDB000	C00186	612	Neg
32	pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	RADKZDMFGJYCBB-UHFFFAOYAP	OC1=C(C)N=CC(CO)=C1C=	65-22-5	1021	HMDB000	C00250	1050	Neg
33	pyridoxal phosphate	Cofactors and Vitamins	Vitamin B6 Metabolism	NGVDGCNFYWLIFO-UHFFFAOYAW	O=P(O)(O)OCC1=CN=C(C)(	41468-25	1022	HMDB000	C00018	1051	Neg
34	riboflavin (Vitamin B2)	Cofactors and Vitamins	Riboflavin Metabolism	AUNGANRZJHBGPY-SCRDCRAPBG	OC(C(O)C(O)CO)CN1C(C=(	83-88-5	431981	HMDB000	C00255	493570	Neg
35	myristate (14:0)	Lipid	Long Chain Saturated Fatty Acid	TUNFSRHWOTWDNC-UHFFFAOYAZ	OC(CCCCCCCCCCCCC)=O	544-63-8	10539	HMDB000	C06424	11005	Neg
36	thiamin diphosphate	Cofactors and Vitamins	Thiamine Metabolism	YXVCLPJQTZXJLH-UHFFFAOYAW	CC1=NC=C(C(N)=N1)C[N+]	154-87-0	8715	HMDB000	C00068	1132	Neg
37	thiamin monophosphate	Cofactors and Vitamins	Thiamine Metabolism	HZSAJDVWZRBGIF-UHFFFAOYAQ	CC1=NC=C(C[N+]2=CSC(CC	532-40-1	2627905	HMDB000	C01081	1131,3382778	Neg
38	uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	DRTQHJPVMGBUCF-XVFCMESIBG	OC1C(N(C=CC2=O)C(N2)=(	58-96-8	5807	HMDB000	C00299	6029	Neg
39	2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	MXHRCPNRJAMMIM-SHYZEUOFBK	O=C(NC1=O)N(C=C1)C(CC	951-78-0	13118	HMDB000	C00526	13712	Neg
40	pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	HZIOZCLEXIYJAD-JWMKEVCDBU	O[C@]1([H])[C@@](O)([H	1445-07-4	21403010	HMDB000	C02067	15047	Neg
41	thymidine	Nucleotide	Pyrimidine Metabolism, Thymine containing	IQFYYKKMVGJFEH-XLPZGREQBQ	O=C(NC(C(C)=C1)=O)N1[C	50-89-5	5585	HMDB000	C00214	5789	Neg
42	thymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	RWQNBRDOKXIBIV-UHFFFAOYAL	O=C1C(C)=CNC(N1)=O	65-71-4	1103	HMDB000	C00178	1135	Neg
43	caprate (10:0)	Lipid	Medium Chain Fatty Acid	GHVNFZFCNZKVNT-UHFFFAOYAC	CCCCCCCCCC(O)=O	334-48-5	2863	HMDB000	C01571	2969	Neg
44	margarate (17:0)	Lipid	Long Chain Saturated Fatty Acid	KEMQGTRYUADPNZ-UHFFFAOYAT	O=C(O)CCCCCCCCCCCCCCC	506-12-7	10033	HMDB0002259		10465	Neg
45	nonadecanoate (19:0)	Lipid	Long Chain Saturated Fatty Acid	ISYWECDDZWTKFF-UHFFFAOYAR	CCCCCCCCCCCCCCCCCCC(	646-30-0	12071	HMDB000	C16535	12591	Neg
46	arachidate (20:0)	Lipid	Long Chain Saturated Fatty Acid	VKOBVWXKNCXXDE-UHFFFAOYAB	CCCCCCCCCCCCCCCCCCCC	506-30-9	10035	HMDB000	C06425	10467	Neg
47	maltose	Carbohydrate	Glycogen Metabolism	GUBGYTABKSRVRQ-ASMJPISFBF	O[C@@H]1[C@H]([C@H]	6363-53-7	388469	HMDB000	C00208	10991489	Neg
48	caproate (6:0)	Lipid	Medium Chain Fatty Acid	FUZZWVXGSFPDMH-UHFFFAOYAY	CCCCCC(O)=O	142-62-1	8552	HMDB000	C01585	8892	Neg
49	caprylate (8:0)	Lipid	Medium Chain Fatty Acid	WWZKQHOCKIZLMA-UHFFFAOYAH	CCCCCCCC(O)=O	124-07-2	370	HMDB000	C06423	379	Neg
50	pentadecanoate (15:0)	Lipid	Long Chain Saturated Fatty Acid	WQEPLUUGTLDZJY-UHFFFAOYAK	O=C(O)CCCCCCCCCCCCCC	10002-84-	13249	HMDB000	C16537	13849	Neg
51	5-oxoproline	Amino Acid	Glutathione Metabolism	ODHCTXKNWHHXJC-VKHMYHEABY	O=C1CC[C@@H]([C@@](	98-79-3	7127	HMDB000	C02237,CC	439685,7405	Neg
52	pantothenate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	GHOKWGTUZJEAQD-ZETCQYMHBS	O=C(NCCC(O)=O)[C@H](C	137-08-6	6361	HMDB000	C00864	6613	Neg
53	phosphoethanolamine	Lipid	Phospholipid Metabolism	SUHOOTKUPISOBE-UHFFFAOYAT	NCCOP(O)(O)=O	1071-23-4	990	HMDB000	C00346	1015	Neg
54	5-KETE	Lipid	Eicosanoid	4000	CCCCC\C=C/C\C=C/C\C=C	106154-16	1765	HMDB001	C14732	5353355	Neg

Data Key & Explanation | Chemical Annotation | Chemical Annotation (2) | Sample Meta Data | Peak Area Data | Transposed Peak area data | Neg | Polar | Pos early | Pos late | Batch-normalized Data | Batch-norm Imputed Data

These sub-tables are then ready to be copied/pasted into the online submission form at the "metabolite metadata" steps
Order of analyses: 1:Pos Early, 2:Pos Late, 3:Neg 4:Polar

Start/Edit Data Submission | Examples of study design and data layouts | Online Study Submission Tutorial(pdf)

mwTab Identifier: Javier_Munoz_Briones_24_20230930_161810 Return to start

Analysis: Reversed phase POSITIVE(1)

Metabolite metadata in tab-delimited format. First column must contain metabolite names.
Subsequent columns should contain KEGG,PubChem identifiers, retention index,quantitated m/z, etc.
First row must contain headings.

```
metabolite_name SUPER_PATHWAY   SUB_PATHWAY     TYPE    INCHIKEY        SMILES  CAS     CHEMSPIDER
HMDB    KEGG    PUBCHEM
S-1-pyrroline-5-carboxylate     Amino Acid      Glutamate Metabolism    NAMED   DWAKNKKXGALPNW-
UHFFFAOYSA-N    OC(C1CCC=N1)=O  2906-39-0       10140206        HMDB0001301     C04322  11966181
1,3-diaminopropane      Amino Acid      Polyamine Metabolism    NAMED   XFNJVJPLKCPIBV-UHFFFAOYSA-N
NCCCN   109-76-2        415     HMDB0000002     C00986  428
putrescine      Amino Acid      Polyamine Metabolism    NAMED   KIDHWZJUCRJVML-UHFFFAOYSA-N     NCCCCN
110-60-1        13837702        HMDB0001414     C00134  1045
spermidine      Amino Acid      Polyamine Metabolism    NAMED   ATHGHQPFGPMSJY-UHFFFAOYSA-N
NCCCCNCCCN      124-20-9        1071    HMDB0001257     C00315  1102
1-methyladenine Nucleotide      Purine Metabolism, Adenine containing   NAMED   SATCOUWSAZBIJO-
```

View/check metabolite metadata See examples of metabolite metadata layout

Data upload is complete when you have copied/pasted results and metadata tables for each of the 4 Metabolon analyses
Order of analyses: 1:Pos Early, 2:Pos Late, 3:Neg 4:Polar

Click the “Finalize” button in the form when complete