

# PEC1

```
# Definir las URLs de descarga de los archivos desde GitHub
metadatosURL <- "https://raw.githubusercontent.com/nutrimetabolomics/metaboData/main/Datasets/2018-MetaboData"
datosURL <- "https://raw.githubusercontent.com/nutrimetabolomics/metaboData/main/Datasets/2018-Metabotype"
```

```
# Descargar los archivos y guardarlos localmente
download.file(metadatosURL, destfile = "metadatosPEC1.csv")
download.file(datosURL, destfile = "datosPEC1.csv")
```

```
# Leer los archivos CSV y asignar la primera columna como nombres de fila
metadatosPEC1 <- read.csv("./metadatosPEC1.csv", row.names = 1)
datosPEC1 <- read.csv("./datosPEC1.csv", row.names = 1)
```

```
# Exploración de los objetos
class(datosPEC1)
```

```
## [1] "data.frame"
```

```
class(metadatosPEC1)
```

```
## [1] "data.frame"
```

```
# Visualizar las primeras filas de cada objeto para comprobar su contenido
head(datosPEC1)
```

```
##   SUBJECTS SURGERY AGE GENDER Group MEDDM_TO MEDCOL_TO MEDINF_TO MEDHTA_TO
## 1         1 by pass  27      F      1         0         0         0         1
## 2         2 by pass  19      F      2         0         0         0         0
## 3         3 by pass  42      F      1         0         0         0         0
## 4         4 by pass  37      F      2         0         0         0         0
## 5         5 tubular  42      F      1         0         0         0         0
## 6         6 by pass  24      F      2         0         0         0         0
##   GLU_TO INS_TO HOMA_TO HBA1C_TO HBA1C.mmol.mol_TO PESO_TO bmi_TO CC_TO CINT_TO
## 1     85  11.40   2.40      NA              NA      151  62.9   0.7    116
## 2     78  12.10   2.32      NA              NA      139  47.0   NA     NA
## 3     75   8.41   1.56    5.4          35.51      84   29.8   0.7     90
## 4     71  12.80   2.25    5.1          32.23     136  53.1   1.0    157
## 5     82   6.01   1.22    5.6          37.69     121  46.6   0.9    123
## 6     71   9.88   1.73    5.1          32.23     148  48.8   0.7    110
##   CAD_TO TAD_TO TAS_TO TG_TO COL_TO LDL_TO HDL_TO VLDL_TO PCR_TO LEP_TO
## 1    167   125   174   147   256  167.0    60   29.4  10.20   155
## 2     NA    NA    NA   150   180   94.0    56   30.0   9.00    84
## 3    126    79   111    45   211  114.0    88    9.0   3.05    27
## 4    162    73   127   109   205  146.0    37   21.8   8.89    46
```

## 5	132	84	122	30	102	24.0	72	6.0	NA	NA	
## 6	148	74	131	61	121	60.8	48	12.2	1.60	38	
##	ADIPO_TO	GOT_TO	GPT_TO	GGT_TO	URICO_TO	CREAT_TO	UREA_TO	HIERRO_TO	TRANSF_TO		
## 1	8.15	21	33	22		5.7	0.8	33	77	NA	
## 2	7.94	16	40	25		NA	0.8	29	113	290	
## 3	16.70	24	39	20		2.7	0.8	28	142	251	
## 4	4.68	21	37	20		4.9	0.7	22	64	289	
## 5	NA	42	68	18		5.2	0.8	29	94	252	
## 6	11.80	11	26	12		3.7	0.7	14	102	200	
##	FERR_TO	Ile_TO	Leu_TO	Val_TO	Ala_TO	Pro_TO	Gly_TO	Ser_TO	Trp_TO	Phe_TO	Met_TO
## 1	53.0	53.9	105	192	498	160	270	161	52.4	62.1	19.7
## 2	25.0	95.7	188	317	558	249	288	174	72.0	98.3	36.6
## 3	15.0	57.8	119	183	194	153	252	143	42.6	50.8	23.3
## 4	18.0	84.5	180	296	439	216	298	144	74.4	94.8	28.3
## 5	39.4	72.0	140	247	267	156	348	184	68.6	75.4	36.8
## 6	25.0	109.0	205	376	654	498	586	310	123.0	121.0	53.0
##	Orn_TO	Arg_TO	His_TO	Asn_TO	Asp_TO	Glu_TO	Gln_TO	Cit_TO	Tyr_TO	Thr_TO	Lys_TO
## 1	89.2	110	81.6	40.8	21.00	38.7	631	30.3	68.9	150	296
## 2	104.0	166	106.0	50.4	21.30	66.9	845	37.9	114.0	203	434
## 3	90.4	101	73.5	36.7	7.54	16.9	625	22.9	50.1	107	271
## 4	104.0	142	95.2	46.1	17.90	44.6	750	35.0	92.8	107	378
## 5	139.0	133	108.0	58.7	15.60	54.1	900	45.8	108.0	144	350
## 6	152.0	204	167.0	82.1	28.30	60.8	1320	54.3	140.0	280	549
##	Creatinine_TO	Kynurenine_TO	Putrescine_TO	Sarcosine_TO	Serotonin_TO						
## 1		66.9		2.55		0.100		7.70		0.650	
## 2		75.3		3.30		0.290		11.70		0.640	
## 3		39.1		1.77		0.000		2.05		0.400	
## 4		79.3		3.16		-99.000		8.11		0.345	
## 5		66.4		3.57		0.279		3.77		0.441	
## 6		113.0		6.51		0.209		12.20		0.894	
##	Taurine_TO	SDMA_TO	CO_TO	C2_TO	C3.OH_TO	C6..C4.1.DC.._TO	C5.DC..C6.OH.._TO				
## 1	107.0	0.88	34.1	5.25	0.26		0.000			0.050	
## 2	90.9	1.64	45.2	8.51	0.27		0.150			0.070	
## 3	64.3	0.93	23.9	6.00	0.24		0.000			0.000	
## 4	125.0	1.36	48.6	8.94	0.23		-9.000			0.044	
## 5	97.1	1.08	51.2	5.18	0.28		0.179			0.076	
## 6	181.0	1.85	79.3	9.89	0.37		0.086			-9.000	
##	C7.DC_TO	C8_TO	C10_TO	C10.1_TO	C10.2_TO	C14.1_TO	C14.2_TO	C16.1_TO	C16.2_TO		
## 1	0.040	0.500	0.52	0.18	0.18	0.17	0.12	0.10	0.03		
## 2	0.060	0.600	0.70	0.35	0.21	0.28	0.21	0.18	0.06		
## 3	0.040	0.440	0.35	0.20	0.12	0.09	0.07	0.07	0.03		
## 4	-9.000	0.429	0.39	0.17	0.13	0.18	0.09	0.09	0.03		
## 5	0.071	0.807	0.33	0.16	0.14	0.12	0.10	0.08	0.04		
## 6	-9.000	0.402	0.83	0.42	0.25	0.30	0.19	0.17	0.06		
##	C16.2.OH_TO	C18.1_TO	C18.1.OH_TO	C18.2_TO	lysoPC.a.C16.0_TO	lysoPC.a.C16.1_TO					
## 1	0.04	0.18		0.05	0.07		167.0		6.14		
## 2	0.06	0.22		0.07	0.13		149.0		3.92		
## 3	0.04	0.10		0.04	0.06		82.2		2.15		
## 4	0.04	0.23		0.05	0.11		187.0		5.28		
## 5	0.04	0.12		0.05	0.09		86.1		2.48		
## 6	0.05	0.25		0.07	0.17		228.0		6.80		
##	lysoPC.a.C17.0_TO	lysoPC.a.C18.0_TO	lysoPC.a.C18.1_TO	lysoPC.a.C18.2_TO							
## 1		3.05		48.9			42.6		39.0		
## 2		1.69		45.6			28.4		46.0		

## 3	1.91	32.0	21.7	39.9	
## 4	3.26	71.8	50.8	47.7	
## 5	1.13	32.6	22.4	35.8	
## 6	3.58	88.5	58.2	109.0	
##	lysoPC.a.C20.3_T0	lysoPC.a.C20.4_T0	lysoPC.a.C24.0_T0	lysoPC.a.C26.0_T0	
## 1	4.84	16.00	0.47	0.49	
## 2	3.51	12.90	0.35	0.40	
## 3	2.54	7.23	0.41	0.40	
## 4	8.33	16.90	0.54	0.30	
## 5	1.57	4.50	0.46	0.40	
## 6	7.50	19.60	0.56	0.41	
##	lysoPC.a.C26.1_T0	lysoPC.a.C28.0_T0	lysoPC.a.C28.1_T0	PC.aa.C24.0_T0	
## 1	0.35	0.41	0.62	0.24	
## 2	0.46	0.35	0.58	0.21	
## 3	0.33	0.40	0.38	0.18	
## 4	0.19	0.30	0.52	0.14	
## 5	0.30	0.30	0.36	0.20	
## 6	0.50	0.44	0.56	0.27	
##	PC.aa.C28.1_T0	PC.aa.C30.0_T0	PC.aa.C32.0_T0	PC.aa.C32.1_T0	PC.aa.C32.3_T0
## 1	3.23	1.37	9.87	13.00	0.24
## 2	4.09	1.29	8.09	10.20	0.25
## 3	2.46	1.88	8.19	5.80	0.16
## 4	3.75	2.20	10.50	11.80	0.21
## 5	2.20	1.50	9.71	5.86	0.15
## 6	4.77	1.58	12.10	8.63	0.34
##	PC.aa.C34.1_T0	PC.aa.C34.2_T0	PC.aa.C34.3_T0	PC.aa.C34.4_T0	PC.aa.C36.0_T0
## 1	136.0	233	9.73	0.65	0.95
## 2	138.0	394	11.00	0.81	1.30
## 3	89.2	258	6.13	0.39	1.23
## 4	162.0	257	10.20	0.81	1.16
## 5	77.6	276	5.37	0.23	0.80
## 6	136.0	466	14.90	0.81	1.30
##	PC.aa.C36.1_T0	PC.aa.C36.2_T0	PC.aa.C36.3_T0	PC.aa.C36.4_T0	PC.aa.C36.5_T0
## 1	13.9	68.9	59.4	120.0	8.79
## 2	18.5	161.0	75.3	147.0	10.00
## 3	10.1	104.0	48.3	71.2	4.20
## 4	26.6	131.0	96.8	126.0	11.40
## 5	14.4	119.0	49.9	57.1	2.90
## 6	25.9	204.0	118.0	158.0	6.99
##	PC.aa.C38.0_T0	PC.aa.C38.1_T0	PC.aa.C38.3_T0	PC.aa.C38.4_T0	PC.aa.C38.5_T0
## 1	2.43	0.98	27.7	88.8	32.8
## 2	2.47	0.92	39.6	106.0	29.5
## 3	2.35	0.27	22.8	59.3	20.8
## 4	3.55	1.21	58.5	113.0	32.5
## 5	1.95	1.03	21.2	47.3	13.6
## 6	3.30	1.72	56.6	139.0	40.5
##	PC.aa.C38.6_T0	PC.aa.C40.1_T0	PC.aa.C40.2_T0	PC.aa.C40.3_T0	PC.aa.C40.4_T0
## 1	58.7	0.43	0.23	0.58	2.04
## 2	71.3	0.48	0.38	0.59	2.50
## 3	36.1	-9.00	0.19	0.51	1.89
## 4	66.1	0.58	0.42	0.81	2.74
## 5	13.9	0.37	0.36	0.54	1.65
## 6	50.8	0.55	0.53	0.77	3.99
##	PC.aa.C40.5_T0	PC.aa.C40.6_T0	PC.aa.C42.0_T0	PC.aa.C42.1_T0	PC.aa.C42.2_T0

## 1	4.60	18.80	0.73	0.36	0.27
## 2	5.49	20.70	0.71	0.37	0.28
## 3	3.53	12.30	0.56	0.31	0.22
## 4	5.61	25.30	0.66	0.32	0.31
## 5	2.88	5.39	0.64	0.27	0.29
## 6	6.80	15.70	0.83	0.38	0.33
##	PC.aa.C42.4_T0	PC.aa.C42.5_T0	PC.aa.C42.6_T0	PC.ae.C30.0_T0	PC.ae.C32.1_T0
## 1	0.22	0.26	0.32	0.41	1.93
## 2	0.17	0.27	0.28	0.31	2.25
## 3	0.20	0.26	0.34	0.36	2.60
## 4	0.24	0.35	0.42	0.41	2.28
## 5	0.22	0.25	0.31	0.30	2.37
## 6	0.37	0.40	0.39	0.35	3.37
##	PC.ae.C32.2_T0	PC.ae.C34.0_T0	PC.ae.C34.1_T0	PC.ae.C34.2_T0	PC.ae.C34.3_T0
## 1	0.63	0.42	5.63	5.20	2.35
## 2	0.72	0.35	5.07	6.77	5.05
## 3	0.81	0.54	4.71	7.64	4.81
## 4	0.75	0.71	6.71	8.40	4.92
## 5	0.80	0.44	4.87	7.78	4.75
## 6	1.07	0.60	6.68	13.40	8.56
##	PC.ae.C36.0_T0	PC.ae.C36.1_T0	PC.ae.C36.2_T0	PC.ae.C36.3_T0	PC.ae.C36.4_T0
## 1	0.96	3.12	5.19	2.31	6.79
## 2	0.67	3.31	6.15	3.11	8.50
## 3	0.75	2.60	6.43	3.12	6.57
## 4	1.15	4.22	6.11	4.76	9.33
## 5	0.86	1.91	4.53	3.98	9.26
## 6	1.03	3.61	7.90	7.81	16.10
##	PC.ae.C36.5_T0	PC.ae.C38.0_T0	PC.ae.C38.2_T0	PC.ae.C38.3_T0	PC.ae.C38.4_T0
## 1	5.42	1.69	1.61	1.55	5.71
## 2	6.30	1.84	2.00	1.43	6.60
## 3	5.34	1.03	1.68	1.15	4.98
## 4	6.41	1.77	2.02	2.42	6.88
## 5	4.84	0.57	1.99	0.83	4.00
## 6	10.10	1.38	2.21	2.20	11.10
##	PC.ae.C38.5_T0	PC.ae.C38.6_T0	PC.ae.C40.1_T0	PC.ae.C40.2_T0	PC.ae.C40.3_T0
## 1	7.61	3.27	1.39	1.40	0.76
## 2	8.67	3.67	1.19	1.15	0.97
## 3	7.19	2.69	0.88	0.90	0.75
## 4	11.80	4.63	1.09	1.72	1.13
## 5	8.06	2.46	0.68	0.62	0.84
## 6	18.10	5.61	1.17	1.32	1.27
##	PC.ae.C40.4_T0	PC.ae.C40.5_T0	PC.ae.C40.6_T0	PC.ae.C42.1_T0	PC.ae.C42.2_T0
## 1	1.98	1.71	2.39	0.45	0.44
## 2	2.16	1.79	2.37	0.39	0.52
## 3	1.74	1.49	2.03	0.45	0.35
## 4	2.42	2.39	2.63	0.42	0.70
## 5	1.94	1.35	1.34	0.33	0.35
## 6	3.44	3.31	3.03	0.56	0.75
##	PC.ae.C42.3_T0	PC.ae.C42.4_T0	PC.ae.C42.5_T0	PC.ae.C44.3_T0	PC.ae.C44.4_T0
## 1	0.76	0.86	2.34	0.14	0.56
## 2	0.91	1.34	2.37	0.17	0.49
## 3	0.60	0.79	1.95	0.15	0.43
## 4	0.88	0.93	2.43	0.15	0.48
## 5	0.83	0.99	2.14	0.28	0.51

## 6	0.94	1.67	3.01	0.24	0.56						
##	PC.ae.C44.5_T0	PC.ae.C44.6_T0	SM..OH..C14.1_T0	SM..OH..C16.1_T0							
## 1	2.56	1.59	4.09	1.69							
## 2	2.34	1.96	3.98	1.95							
## 3	1.96	1.70	3.73	1.33							
## 4	2.65	1.63	5.31	2.06							
## 5	2.28	2.29	2.10	0.82							
## 6	3.27	2.51	4.88	1.89							
##	SM..OH..C22.1_T0	SM..OH..C22.2_T0	SM..OH..C24.1_T0	SM.C16.0_T0	SM.C16.1_T0						
## 1	4.08	4.47	0.47	59.8	10.60						
## 2	8.01	7.05	0.74	82.8	16.10						
## 3	3.66	3.96	0.38	58.1	9.06						
## 4	8.50	8.00	0.82	87.5	15.30						
## 5	2.39	2.91	0.31	52.4	8.36						
## 6	6.32	6.03	0.80	105.0	19.50						
##	SM.C18.0_T0	SM.C18.1_T0	SM.C20.2_T0	SM.C24.0_T0	SM.C24.1_T0	MEDDM_T2					
## 1	9.03	6.17	0.26	4.60	22.2	0					
## 2	15.50	11.20	0.27	10.80	29.8	0					
## 3	6.46	4.14	0.21	5.35	17.5	0					
## 4	10.70	6.40	0.35	10.90	36.2	0					
## 5	4.13	3.30	0.14	3.63	13.3	0					
## 6	11.40	8.37	0.28	10.60	30.3	0					
##	MEDCOL_T2	MEDINF_T2	MEDHTA_T2	GLU_T2	INS_T2	HOMA_T2	HBA1C_T2				
## 1	0	0	1	97	16.90	4.05	NA				
## 2	0	0	0	74	9.99	1.83	5.0				
## 3	0	0	0	85	10.40	2.18	5.2				
## 4	0	0	0	66	4.52	0.74	4.7				
## 5	0	0	0	86	5.94	1.26	NA				
## 6	0	0	0	68	11.00	1.84	4.9				
##	HBA1C.mmol.mol_T2	PESO_T2	bmi_T2	CC_T2	CINT_T2	CAD_T2	TAD_T2	TAS_T2	TG_T2		
## 1	NA	117.0	48.7	0.7	115	156	NA	NA	163		
## 2	31.13	120.0	40.6	1.0	136	140	61	122	118		
## 3	33.32	75.7	26.8	0.7	78	105	67	111	63		
## 4	27.85	124.0	48.2	0.9	134	149	73	123	75		
## 5	NA	116.0	44.8	0.9	122	136	74	108	52		
## 6	30.04	127.0	41.9	0.7	106	144	71	136	80		
##	COL_T2	LDL_T2	HDL_T2	VLDL_T2	PCR_T2	LEP_T2	ADIPO_T2	GOT_T2	GPT_T2	GGT_T2	
## 1	158	78.4	47	32.6	9.42	130	13.20	25	27	14	
## 2	129	65.4	40	23.6	2.15	31	8.32	57	128	29	
## 3	178	94.4	71	12.6	1.79	16	14.70	28	31	34	
## 4	124	77.0	32	15.0	2.29	29	8.67	34	58	11	
## 5	105	59.0	44	NA	NA	NA	NA	74	104	19	
## 6	93	45.0	32	16.0	4.80	28	7.04	20	38	16	
##	URICO_T2	CREAT_T2	UREA_T2	HIERRO_T2	TRANSF_T2	FERR_T2	Ile_T2	Leu_T2	Val_T2		
## 1	10.4	1.2	27	49	221	151.0	61.4	115.0	162		
## 2	7.8	0.6	16	28	259	12.0	116.0	156.0	224		
## 3	2.5	0.6	25	40	254	13.0	63.4	120.0	194		
## 4	5.9	0.9	14	43	216	15.0	98.6	145.0	230		
## 5	4.5	0.7	17	119	207	58.5	59.5	99.9	152		
## 6	7.7	0.8	4	81	156	97.0	79.5	136.0	199		
##	Ala_T2	Pro_T2	Gly_T2	Ser_T2	Trp_T2	Phe_T2	Met_T2	Orn_T2	Arg_T2	His_T2	Asn_T2
## 1	451	186	459	183	15.4	56.1	20.4	46.7	97.7	73.5	34.8
## 2	352	282	465	210	45.4	68.7	29.4	71.2	101.0	75.9	47.1
## 3	324	219	378	233	44.7	63.3	28.2	120.0	128.0	87.6	43.8

## 4	409	223	473	199	41.8	58.3	26.3	99.0	106.0	79.5	38.4
## 5	369	141	453	225	45.8	53.5	26.0	95.1	137.0	75.0	49.4
## 6	379	258	402	179	29.4	61.5	26.5	46.2	82.8	70.7	35.7
##	Asp_T2	Glu_T2	Gln_T2	Cit_T2	Tyr_T2	Thr_T2	Lys_T2	Creatinine_T2	Kynurenine_T2		
## 1	12.30	27.0	774	21.0	41.6	61.5	249	99.5		1.09	
## 2	27.00	63.0	951	26.5	68.3	185.0	331	76.7		2.20	
## 3	19.50	30.8	723	29.7	55.0	150.0	331	56.4		1.94	
## 4	15.20	37.9	868	28.6	60.1	128.0	355	76.5		2.10	
## 5	8.96	35.8	1050	39.2	70.9	162.0	231	72.3		2.59	
## 6	17.40	58.6	579	17.7	46.9	177.0	270	82.6		1.73	
##	Putrescine_T2	Sarcosine_T2	Serotonin_T2	Taurine_T2	SDMA_T2	C0_T2	C2_T2				
## 1	0.134	6.55	0.818	106.0	1.90	33.4	22.10				
## 2	0.322	15.40	0.591	148.0	1.66	20.2	13.00				
## 3	-99.000	4.66	0.521	82.6	1.15	29.8	7.04				
## 4	0.256	9.76	0.397	176.0	1.54	32.3	24.60				
## 5	-99.000	2.75	0.522	50.7	1.44	36.0	9.30				
## 6	0.216	5.99	0.324	149.0	1.23	26.7	30.30				
##	C3.OH_T2	C6..C4.1.DC_T2	C5.DC..C6.OH_T2	C7.DC_T2	C8_T2	C10_T2	C10.1_T2				
## 1	0.23	-99.000	0.049	0.058	0.609	0.70	0.31				
## 2	0.15	0.089	0.040	-9.000	0.352	0.38	0.20				
## 3	0.28	-99.000	0.037	0.060	0.703	0.67	0.31				
## 4	0.19	0.085	0.038	0.047	0.393	0.44	0.22				
## 5	0.29	0.096	0.050	0.039	0.543	0.58	0.33				
## 6	0.17	0.240	0.038	0.048	0.703	1.15	0.48				
##	C10.2_T2	C14.1_T2	C14.2_T2	C16.1_T2	C16.2_T2	C16.2.OH_T2	C18.1_T2	C18.1.OH_T2			
## 1	0.17	0.26	0.18	0.15	0.04	0.04	0.29	0.04			
## 2	0.13	0.14	0.07	0.08	0.03	0.03	0.30	0.03			
## 3	0.22	0.16	0.16	0.10	0.04	0.06	0.16	0.06			
## 4	0.13	0.22	0.11	0.09	0.04	0.04	0.31	0.03			
## 5	0.13	0.20	0.13	0.09	0.04	0.04	0.15	0.04			
## 6	0.12	0.38	0.19	0.12	0.05	0.04	0.29	0.06			
##	C18.2_T2	X lysoPC.a.C14.0_T2	lysoPC.a.C16.0_T2	lysoPC.a.C16.1_T2							
## 1	0.10	NA	-9	107	3.31						
## 2	0.12	NA	-9	167	2.81						
## 3	0.10	NA	-9	110	2.49						
## 4	0.09	NA	-9	143	2.20						
## 5	0.08	NA	-9	104	2.50						
## 6	0.15	NA	-9	153	3.02						
##	lysoPC.a.C17.0_T2	lysoPC.a.C18.0_T2	lysoPC.a.C18.1_T2	lysoPC.a.C18.2_T2							
## 1	1.71	22.9	33.1	25.9							
## 2	1.53	39.9	29.1	31.8							
## 3	2.16	36.0	32.6	50.3							
## 4	1.55	25.5	27.6	25.3							
## 5	1.25	31.9	23.2	33.9							
## 6	1.31	27.4	32.8	36.2							
##	lysoPC.a.C20.3_T2	lysoPC.a.C20.4_T2	lysoPC.a.C24.0_T2	lysoPC.a.C26.0_T2							
## 1	2.05	16.70	0.27	-9.000							
## 2	1.59	17.40	0.37	0.301							
## 3	2.69	9.94	0.45	0.230							
## 4	1.30	11.80	0.33	0.219							
## 5	1.36	7.07	0.36	0.308							
## 6	1.37	15.70	0.29	0.193							
##	lysoPC.a.C26.1_T2	lysoPC.a.C28.0_T2	lysoPC.a.C28.1_T2	PC.aa.C24.0_T2							
## 1	0.220	0.225	0.299	0.170							

## 2	0.474	0.248	0.401	0.219	
## 3	0.182	0.234	0.327	0.173	
## 4	0.344	0.255	0.394	-9.000	
## 5	0.251	0.252	0.349	0.158	
## 6	0.119	-9.000	0.226	-9.000	
##	PC.aa.C28.1_T2	PC.aa.C30.0_T2	PC.aa.C32.0_T2	PC.aa.C32.1_T2	PC.aa.C32.3_T2
## 1	2.07	1.10	11.50	7.62	0.25
## 2	1.73	1.41	11.40	6.35	0.28
## 3	3.06	1.88	10.20	6.26	0.23
## 4	2.17	1.26	12.50	4.72	0.25
## 5	1.68	1.05	9.67	7.35	0.14
## 6	1.75	1.67	10.20	4.91	0.21
##	PC.aa.C34.1_T2	PC.aa.C34.2_T2	PC.aa.C34.3_T2	PC.aa.C34.4_T2	PC.aa.C36.0_T2
## 1	131	181	3.22	0.26	0.80
## 2	116	258	3.65	0.28	0.96
## 3	111	285	6.46	0.39	1.17
## 4	135	218	2.70	0.18	0.87
## 5	107	261	5.13	0.18	0.58
## 6	102	219	2.76	0.14	0.50
##	PC.aa.C36.1_T2	PC.aa.C36.2_T2	PC.aa.C36.3_T2	PC.aa.C36.4_T2	PC.aa.C36.5_T2
## 1	7.65	44.6	27.3	146.0	5.44
## 2	8.18	64.0	30.4	192.0	7.21
## 3	14.20	101.0	54.7	91.1	4.22
## 4	8.78	52.7	29.9	144.0	4.47
## 5	9.11	78.2	34.7	65.0	2.72
## 6	6.83	43.5	27.1	152.0	3.66
##	PC.aa.C38.0_T2	PC.aa.C38.1_T2	PC.aa.C38.3_T2	PC.aa.C38.4_T2	PC.aa.C38.5_T2
## 1	2.21	0.440	14.6	74.2	25.1
## 2	2.47	1.040	15.5	110.0	24.4
## 3	2.26	0.898	23.3	67.9	22.9
## 4	2.52	0.992	15.7	75.3	20.0
## 5	1.87	0.528	13.3	49.4	14.8
## 6	1.67	0.600	12.8	77.1	24.1
##	PC.aa.C38.6_T2	PC.aa.C40.1_T2	PC.aa.C40.2_T2	PC.aa.C40.3_T2	PC.aa.C40.4_T2
## 1	68.1	-9.000	0.18	0.42	1.35
## 2	84.3	0.440	0.32	0.49	1.50
## 3	44.1	0.352	0.20	0.46	2.27
## 4	68.1	-9.000	0.25	0.48	1.23
## 5	35.7	0.389	0.18	0.34	1.47
## 6	55.9	-9.000	0.21	0.48	1.58
##	PC.aa.C40.5_T2	PC.aa.C40.6_T2	PC.aa.C42.0_T2	PC.aa.C42.1_T2	PC.aa.C42.2_T2
## 1	3.41	18.40	0.54	0.26	0.15
## 2	3.18	24.20	0.77	0.36	0.21
## 3	3.87	13.60	0.58	0.34	0.22
## 4	2.60	17.00	0.64	0.27	0.22
## 5	2.88	9.63	0.59	0.30	0.19
## 6	3.11	12.30	0.70	0.32	0.15
##	PC.aa.C42.4_T2	PC.aa.C42.5_T2	PC.aa.C42.6_T2	PC.aa.C30.0_T2	PC.aa.C32.1_T2
## 1	0.16	0.28	0.222	0.253	2.11
## 2	0.17	0.31	0.316	0.201	2.22
## 3	0.16	0.32	0.308	0.398	2.65
## 4	0.15	0.29	0.278	0.199	2.03
## 5	0.12	0.26	0.197	0.217	2.13
## 6	0.13	0.25	0.246	0.160	1.45

##	PC.ae.C32.2_T2	PC.ae.C34.0_T2	PC.ae.C34.1_T2	PC.ae.C34.2_T2	PC.ae.C34.3_T2	
## 1	0.64	0.53	5.38	3.85	2.04	
## 2	0.69	0.28	4.09	3.86	3.66	
## 3	0.74	0.67	5.54	6.83	5.62	
## 4	0.67	0.32	4.81	4.34	4.13	
## 5	0.59	0.38	4.24	4.43	3.64	
## 6	0.51	0.23	3.63	3.50	2.78	
##	PC.ae.C36.0_T2	PC.ae.C36.1_T2	PC.ae.C36.2_T2	PC.ae.C36.3_T2	PC.ae.C36.4_T2	
## 1	0.75	2.42	3.29	1.55	5.55	
## 2	0.64	1.63	3.16	1.95	5.85	
## 3	0.96	2.65	6.70	3.04	7.14	
## 4	0.91	2.10	3.25	2.09	5.60	
## 5	0.75	1.57	3.30	2.21	5.83	
## 6	0.64	1.40	2.57	1.88	5.26	
##	PC.ae.C36.5_T2	PC.ae.C38.0_T2	PC.ae.C38.2_T2	PC.ae.C38.3_T2	PC.ae.C38.4_T2	
## 1	5.00	0.98	0.60	0.90	5.65	
## 2	6.05	0.92	0.65	0.77	5.40	
## 3	5.95	1.06	1.52	1.27	5.65	
## 4	5.42	0.72	0.79	0.93	4.28	
## 5	4.74	0.69	0.85	0.52	3.33	
## 6	3.84	0.73	0.62	0.72	4.57	
##	PC.ae.C38.5_T2	PC.ae.C38.6_T2	PC.ae.C40.1_T2	PC.ae.C40.2_T2	PC.ae.C40.3_T2	
## 1	8.44	2.47	0.84	1.32	0.61	
## 2	9.60	3.05	0.90	1.02	0.76	
## 3	9.21	2.79	0.97	1.16	0.78	
## 4	9.75	2.82	0.76	1.20	0.67	
## 5	6.82	2.14	0.68	0.76	0.55	
## 6	8.44	2.18	0.57	0.81	0.59	
##	PC.ae.C40.4_T2	PC.ae.C40.5_T2	PC.ae.C40.6_T2	PC.ae.C42.1_T2	PC.ae.C42.2_T2	
## 1	1.61	1.93	2.31	0.28	0.32	
## 2	1.64	2.36	2.35	0.35	0.36	
## 3	1.75	1.72	2.25	0.36	0.40	
## 4	1.43	2.14	2.01	0.36	0.34	
## 5	1.43	1.38	1.40	0.26	0.32	
## 6	1.59	2.00	1.77	0.32	0.28	
##	PC.ae.C42.3_T2	PC.ae.C42.4_T2	PC.ae.C42.5_T2	PC.ae.C44.3_T2	PC.ae.C44.4_T2	
## 1	0.48	0.72	2.38	0.10	0.37	
## 2	0.57	0.59	3.11	0.14	0.32	
## 3	0.61	0.90	2.12	0.09	0.41	
## 4	0.50	0.54	2.38	0.11	0.33	
## 5	0.51	0.61	2.16	0.13	0.38	
## 6	0.54	0.75	2.89	0.12	0.28	
##	PC.ae.C44.5_T2	PC.ae.C44.6_T2	SM..OH..C14.1_T2	SM..OH..C16.1_T2		
## 1	2.23	1.11	4.10	2.06		
## 2	2.71	2.06	3.05	1.69		
## 3	2.12	1.54	4.75	2.01		
## 4	2.57	1.40	4.43	1.88		
## 5	1.93	1.49	2.24	1.09		
## 6	2.81	2.06	3.18	1.32		
##	SM..OH..C22.1_T2	SM..OH..C22.2_T2	SM..OH..C24.1_T2	SM.C16.0_T2	SM.C16.1_T2	
## 1	2.52	4.19	0.30	68.3	12.20	
## 2	2.82	4.09	0.37	69.9	15.80	
## 3	3.74	4.74	0.40	84.6	13.50	
## 4	2.54	4.61	0.32	84.6	16.00	



## 5	2.14		2.57		0.15	53.0	9.98				
## 6	1.86		3.25		0.32	71.2	16.00				
##	SM.C18.0_T2	SM.C18.1_T2	SM.C20.2_T2	SM.C24.0_T2	SM.C24.1_T2	MEDDM_T4					
## 1	15.80	10.00	0.22	3.73	28.6	1					
## 2	18.00	12.80	0.36	4.03	29.6	0					
## 3	12.70	7.80	0.28	5.29	25.3	0					
## 4	16.00	11.10	0.30	4.50	33.7	0					
## 5	8.03	5.48	0.14	2.56	13.3	0					
## 6	13.20	8.82	0.30	4.66	29.1	0					
##	MEDCOL_T4	MEDINF_T4	MEDHTA_T4	GLU_T4	INS_T4	HOMA_T4	HBA1C_T4				
## 1	0	0	0	82	10.80	2.18	NA				
## 2	0	0	0	85	NA	NA	NA				
## 3	0	0	0	72	8.99	1.60	5.2				
## 4	0	0	0	73	8.55	1.54	4.9				
## 5	0	0	0	83	11.30	2.32	NA				
## 6	0	0	0	66	4.36	0.71	4.7				
##	HBA1C.mmol.mol_T4	PESO_T4	bmi_T4	CC_T4	CINT_T4	CAD_T4	TAD_T4	TAS_T4	TG_T4		
## 1	NA	106.0	44.1	0.7	105	154	NA	NA	136		
## 2	NA	106.0	35.8	NA	121	132	62	128	115		
## 3	33.32	74.5	26.4	0.8	81	105	62	97	39		
## 4	30.04	110.0	43.0	0.9	123	140	77	124	80		
## 5	NA	104.0	40.0	0.9	111	128	88	115	49		
## 6	27.85	113.0	37.2	0.8	100	128	65	115	54		
##	COL_T4	LDL_T4	HDL_T4	VLDL_T4	PCR_T4	LEP_T4	ADIPO_T4	GOT_T4	GPT_T4	GGT_T4	
## 1	185	112.0	46	27.2	7.07	48.2	19.60	32	32	12	
## 2	142	69.0	50	23.0	NA	NA	NA	50	55	20	
## 3	186	101.0	77	7.8	2.91	15.0	14.60	23	24	18	
## 4	164	104.0	44	16.0	1.51	21.0	13.00	41	65	11	
## 5	107	51.0	49	NA	NA	NA	NA	117	147	28	
## 6	110	57.2	42	10.8	0.38	11.0	2.92	30	24	7	
##	URICO_T4	CREAT_T4	UREA_T4	HIERRO_T4	TRANSF_T4	FERR_T4	Ile_T4	Leu_T4	Val_T4		
## 1	6.8	0.9	17	482	227	70.0	51.9	96.3	166		
## 2	5.6	0.7	17	32	NA	NA	NA	NA	NA		
## 3	2.5	0.5	35	33	256	5.0	71.7	130.0	230		
## 4	4.3	0.6	19	53	247	10.0	68.2	124.0	200		
## 5	5.4	0.8	23	43	290	19.5	107.0	163.0	269		
## 6	4.1	0.6	19	114	172	42.0	86.7	222.0	301		
##	Ala_T4	Pro_T4	Gly_T4	Ser_T4	Trp_T4	Phe_T4	Met_T4	Orn_T4	Arg_T4	His_T4	Asn_T4
## 1	396	216	385	212	22.4	50.2	16.1	57.6	106	81.1	35.8
## 2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
## 3	358	276	366	217	60.2	73.0	37.0	116.0	138	93.6	51.9
## 4	389	267	506	230	54.4	62.3	27.6	127.0	137	93.3	48.9
## 5	408	212	439	229	65.2	82.9	38.4	148.0	115	94.0	59.0
## 6	412	265	414	247	69.8	98.0	29.2	84.5	128	142.0	51.3
##	Asp_T4	Glu_T4	Gln_T4	Cit_T4	Tyr_T4	Thr_T4	Lys_T4	Creatinine_T4	Kynurenine_T4		
## 1	12.5	28.2	876	27.2	45.8	100	252	82.6	2.20		
## 2	NA	NA	NA	NA	NA	NA	NA	NA	NA		
## 3	16.9	31.0	683	35.6	79.6	174	412	57.8	2.14		
## 4	24.0	53.5	987	42.9	75.1	127	320	75.8	2.35		
## 5	12.8	39.6	1070	41.4	102.0	163	294	80.1	2.19		
## 6	33.7	76.5	823	27.1	65.1	127	350	99.6	3.56		
##	Putrescine_T4	Sarcosine_T4	Serotonin_T4	Taurine_T4	SDMA_T4	C0_T4	C2_T4				
## 1	-99.000	3.58	0.708	61.7	1.76	31.1	17.40				
## 2	NA	NA	NA	NA	NA	NA	NA				

## 3	0.103	4.76	0.572	57.8	0.98	36.3	4.01	
## 4	0.201	11.70	0.364	165.0	1.69	39.4	12.90	
## 5	-99.000	8.03	0.495	115.0	1.23	46.3	11.50	
## 6	-9.000	9.47	0.462	-99.0	1.96	41.7	23.90	
##	C3.OH_T4	C6..C4.1.DC._T4	C5.DC..C6.OH._T4	C7.DC_T4	C8_T4	C10_T4	C10.1_T4	
## 1	0.19	-99.000	0.038	0.044	0.499	0.72	0.29	
## 2	NA	NA	NA	NA	NA	NA	NA	
## 3	0.23	-9.000	0.047	0.044	0.481	0.38	0.17	
## 4	0.26	0.088	0.053	0.057	0.474	0.44	0.20	
## 5	0.26	-99.000	0.051	0.047	0.589	0.78	0.40	
## 6	0.38	0.166	0.068	0.089	0.958	1.17	0.41	
##	C10.2_T4	C14.1_T4	C14.2_T4	C16.1_T4	C16.2_T4	C16.2.OH_T4	C18.1_T4	C18.1.OH_T4
## 1	0.10	0.29	0.12	0.12	0.04	0.04	0.27	0.03
## 2	NA	NA	NA	NA	NA	NA	NA	NA
## 3	0.20	0.16	0.13	0.12	0.03	0.04	0.10	0.04
## 4	0.16	0.20	0.08	0.10	0.04	0.05	0.22	0.04
## 5	0.18	0.24	0.15	0.09	0.04	0.03	0.24	0.05
## 6	0.24	0.43	0.23	0.20	0.08	0.08	0.26	0.06
##	C18.2_T4	lysoPC.a.C16.0_T4	lysoPC.a.C16.1_T4	lysoPC.a.C17.0_T4				
## 1	0.10	152	3.98	2.52				
## 2	NA	NA	NA	NA				
## 3	0.07	108	2.96	2.43				
## 4	0.09	141	3.28	1.84				
## 5	0.14	117	2.95	1.54				
## 6	0.17	222	4.22	2.13				
##	lysoPC.a.C18.0_T4	lysoPC.a.C18.1_T4	lysoPC.a.C18.2_T4	lysoPC.a.C20.3_T4				
## 1	39.7	45.2	35.0	2.66				
## 2	NA	NA	NA	NA				
## 3	36.1	34.1	48.9	2.66				
## 4	36.9	35.9	36.5	2.29				
## 5	31.7	35.8	59.2	1.85				
## 6	59.0	43.2	49.5	2.21				
##	lysoPC.a.C20.4_T4	lysoPC.a.C24.0_T4	lysoPC.a.C26.0_T4	lysoPC.a.C26.1_T4				
## 1	19.00	0.25	0.19	0.12				
## 2	NA	NA	NA	NA				
## 3	9.35	0.50	0.38	0.26				
## 4	12.50	0.37	0.35	0.43				
## 5	9.71	0.41	0.20	0.29				
## 6	15.60	0.52	0.38	0.54				
##	lysoPC.a.C28.0_T4	lysoPC.a.C28.1_T4	PC.aa.C24.0_T4	PC.aa.C28.1_T4				
## 1	-9.00	0.31	-9.00	2.20				
## 2	NA	NA	NA	NA				
## 3	0.30	0.56	0.23	3.69				
## 4	-9.00	0.47	0.14	2.74				
## 5	0.32	0.28	0.16	2.06				
## 6	0.30	0.49	0.23	2.86				
##	PC.aa.C30.0_T4	PC.aa.C32.0_T4	PC.aa.C32.1_T4	PC.aa.C32.3_T4	PC.aa.C34.1_T4			
## 1	1.00	11.8	7.75	0.26	145.0			
## 2	NA	NA	NA	NA	NA			
## 3	2.03	10.7	6.90	0.19	120.0			
## 4	1.66	12.0	6.53	0.29	145.0			
## 5	1.87	11.3	6.76	0.20	91.6			
## 6	1.27	12.9	6.01	0.27	133.0			
##	PC.aa.C34.2_T4	PC.aa.C34.3_T4	PC.aa.C34.4_T4	PC.aa.C36.0_T4	PC.aa.C36.1_T4			

## 1	207	3.70	0.20	0.98	9.54
## 2	NA	NA	NA	NA	NA
## 3	256	7.01	0.36	1.24	15.30
## 4	302	6.45	0.34	1.10	13.90
## 5	299	6.09	0.30	1.05	10.40
## 6	324	4.68	0.24	1.02	14.90
##	PC.aa.C36.2_T4	PC.aa.C36.3_T4	PC.aa.C36.4_T4	PC.aa.C36.5_T4	PC.aa.C38.0_T4
## 1	53.6	28.8	132.0	5.82	2.44
## 2	NA	NA	NA	NA	NA
## 3	102.0	54.5	83.4	4.65	2.94
## 4	104.0	50.9	131.0	5.04	2.60
## 5	92.5	40.5	77.7	4.64	2.43
## 6	102.0	59.3	151.0	3.80	3.20
##	PC.aa.C38.1_T4	PC.aa.C38.3_T4	PC.aa.C38.4_T4	PC.aa.C38.5_T4	PC.aa.C38.6_T4
## 1	0.60	16.3	73.4	27.1	66.0
## 2	NA	NA	NA	NA	NA
## 3	0.66	26.3	66.8	24.3	45.6
## 4	0.94	22.4	86.4	24.7	57.7
## 5	0.73	12.9	53.0	15.5	33.2
## 6	0.79	25.7	97.7	30.6	52.7
##	PC.aa.C40.1_T4	PC.aa.C40.2_T4	PC.aa.C40.3_T4	PC.aa.C40.4_T4	PC.aa.C40.5_T4
## 1	0.33	0.19	0.41	1.43	3.42
## 2	NA	NA	NA	NA	NA
## 3	0.44	0.28	0.58	2.25	3.94
## 4	-9.00	0.24	0.54	1.65	3.66
## 5	0.36	0.20	0.36	1.39	2.18
## 6	0.57	0.43	0.69	3.25	5.45
##	PC.aa.C40.6_T4	PC.aa.C42.0_T4	PC.aa.C42.1_T4	PC.aa.C42.2_T4	PC.aa.C42.4_T4
## 1	17.7	0.63	0.27	0.18	0.14
## 2	NA	NA	NA	NA	NA
## 3	15.4	0.81	0.38	0.26	0.19
## 4	17.6	0.59	0.26	0.19	0.16
## 5	10.5	0.74	0.32	0.20	0.17
## 6	15.0	0.79	0.43	0.17	0.30
##	PC.aa.C42.5_T4	PC.aa.C42.6_T4	PC.aa.C30.0_T4	PC.aa.C32.1_T4	PC.aa.C32.2_T4
## 1	0.27	0.18	0.23	2.70	0.79
## 2	NA	NA	NA	NA	NA
## 3	0.31	0.33	0.43	2.67	0.77
## 4	0.29	0.23	0.34	2.37	0.78
## 5	0.26	0.21	0.35	2.54	0.66
## 6	0.39	0.36	0.30	2.90	0.85
##	PC.aa.C34.0_T4	PC.aa.C34.1_T4	PC.aa.C34.2_T4	PC.aa.C34.3_T4	PC.aa.C36.0_T4
## 1	0.55	5.61	5.38	3.85	0.84
## 2	NA	NA	NA	NA	NA
## 3	0.64	5.74	9.33	6.46	1.09
## 4	0.53	5.97	6.94	5.69	0.91
## 5	0.44	5.00	6.01	3.95	0.85
## 6	0.38	5.73	7.86	6.71	0.96
##	PC.aa.C36.1_T4	PC.aa.C36.2_T4	PC.aa.C36.3_T4	PC.aa.C36.4_T4	PC.aa.C36.5_T4
## 1	2.52	4.25	1.91	7.01	6.58
## 2	NA	NA	NA	NA	NA
## 3	3.48	7.40	3.84	7.16	6.80
## 4	2.69	5.72	3.47	7.18	7.53
## 5	1.93	4.64	2.71	7.04	6.07

## 6	2.46	5.26	4.41	13.30	9.11			
##	PC.ae.C38.0_T4	PC.ae.C38.2_T4	PC.ae.C38.3_T4	PC.ae.C38.4_T4	PC.ae.C38.5_T4			
## 1	1.00	0.55	0.84	5.17	9.11			
## 2	NA	NA	NA	NA	NA			
## 3	1.15	1.57	1.15	5.71	9.43			
## 4	1.03	0.86	1.21	5.44	10.50			
## 5	0.75	1.50	0.72	4.39	9.08			
## 6	0.84	0.75	1.47	7.26	16.80			
##	PC.ae.C38.6_T4	PC.ae.C40.1_T4	PC.ae.C40.2_T4	PC.ae.C40.3_T4	PC.ae.C40.4_T4			
## 1	3.22	0.80	1.13	0.56	1.54			
## 2	NA	NA	NA	NA	NA			
## 3	3.70	1.04	1.21	0.84	2.11			
## 4	4.04	0.90	1.49	0.77	1.72			
## 5	2.88	0.90	0.86	0.78	2.11			
## 6	5.26	1.10	1.11	0.78	2.29			
##	PC.ae.C40.5_T4	PC.ae.C40.6_T4	PC.ae.C42.1_T4	PC.ae.C42.2_T4	PC.ae.C42.3_T4			
## 1	1.74	1.86	0.30	0.32	0.46			
## 2	NA	NA	NA	NA	NA			
## 3	1.72	2.35	0.35	0.54	0.64			
## 4	2.13	2.18	0.27	0.36	0.58			
## 5	1.94	1.71	0.26	0.43	0.78			
## 6	3.36	2.81	0.49	0.45	0.80			
##	PC.ae.C42.4_T4	PC.ae.C42.5_T4	PC.ae.C44.3_T4	PC.ae.C44.4_T4	PC.ae.C44.5_T4			
## 1	0.61	2.28	0.11	0.35	2.14			
## 2	NA	NA	NA	NA	NA			
## 3	1.23	2.32	0.19	0.45	2.48			
## 4	0.75	2.35	0.13	0.31	2.49			
## 5	1.16	2.99	0.11	0.45	2.98			
## 6	1.40	3.38	0.10	0.39	3.69			
##	PC.ae.C44.6_T4	SM..OH..C14.1_T4	SM..OH..C16.1_T4	SM..OH..C22.1_T4				
## 1	1.26	5.02	2.40	2.16				
## 2	NA	NA	NA	NA				
## 3	2.00	4.40	1.77	3.29				
## 4	1.36	4.99	2.13	4.21				
## 5	2.17	2.43	1.02	1.90				
## 6	2.40	4.29	1.48	4.30				
##	SM..OH..C22.2_T4	SM..OH..C24.1_T4	SM.C16.0_T4	SM.C16.1_T4	SM.C18.0_T4			
## 1	4.32	0.23	78.5	15.5	16.20			
## 2	NA	NA	NA	NA	NA			
## 3	4.58	0.37	69.5	10.6	10.20			
## 4	5.99	0.52	96.7	17.3	16.60			
## 5	2.79	0.32	62.3	11.7	8.48			
## 6	5.18	0.45	107.0	20.1	12.60			
##	SM.C18.1_T4	SM.C20.2_T4	SM.C24.0_T4	SM.C24.1_T4	MEDDM_T5	MEDCOL_T5	MEDINF_T5	
## 1	11.30	0.22	3.15	26.4	0	0	0	
## 2	NA	NA	NA	NA	0	0	0	
## 3	6.47	0.25	5.55	25.6	0	0	0	
## 4	10.50	0.41	6.12	39.2	0	0	0	
## 5	5.65	0.18	3.50	18.0	1	1	1	
## 6	10.00	0.25	8.63	38.6	0	0	0	
##	MEDHTA_T5	GLU_T5	INS_T5	HOMA_T5	HBA1C_T5	HBA1C.mmol.mol_T5	PESO_T5	bmi_T5
## 1	1	101	10.60	2.65	5.1	32.23	NA	NA
## 2	0	77	5.08	0.97	5.2	33.32	94.2	31.8
## 3	0	95	3.66	0.86	5.3	34.41	72.1	25.5

## 4	0	70	4.71	0.81	4.9		30.04	101.0	39.1		
## 5	1	85	10.80	2.28	NA		NA	90.0	34.7		
## 6	0	76	9.89	1.86	5.0		31.13	101.0	33.4		
##	CC_T5	CINT_T5	CAD_T5	TAD_T5	TAS_T5	TG_T5	COL_T5	LDL_T5	HDL_T5	VLDL_T5	PCR_T5
## 1	0.7	100.0	150	NA	NA	118	209	128.0	57	23.6	3.71
## 2	0.9	117.0	127	65	127	63	135	65.4	57	12.6	1.78
## 3	0.8	79.5	106	70	130	48	192	92.4	90	9.6	0.91
## 4	0.8	111.0	132	60	115	73	163	105.0	43	14.6	0.97
## 5	0.9	97.0	103	79	108	37	98	37.6	53	NA	NA
## 6	0.8	97.5	129	71	125	75	124	65.0	44	15.0	0.57
##	LEP_T5	ADIPO_T5	GOT_T5	GPT_T5	GGT_T5	URICO_T5	CREAT_T5	UREA_T5	HIERRO_T5		
## 1	37.7	20.90	37	33	18	5.7	1.0	11	59		
## 2	27.0	13.60	25	39	14	4.2	0.6	19	26		
## 3	10.0	23.40	22	33	19	2.3	0.6	30	35		
## 4	22.0	12.90	23	32	5	4.4	0.6	22	49		
## 5	NA	NA	55	74	20	4.9	0.7	20	118		
## 6	13.0	8.54	13	21	6	4.4	0.7	21	131		
##	TRANSF_T5	FERR_T5	Ile_T5	Leu_T5	Val_T5	Ala_T5	Pro_T5	Gly_T5	Ser_T5	Trp_T5	
## 1	250	69.0	33.6	72.2	112	368	127	353	200	23.4	
## 2	328	6.0	62.0	93.1	156	407	253	290	177	45.7	
## 3	268	4.0	48.8	95.3	145	272	165	293	159	40.2	
## 4	256	13.0	76.8	139.0	224	342	173	360	162	52.1	
## 5	237	18.3	72.3	133.0	202	364	192	367	216	68.7	
## 6	180	51.0	69.6	139.0	205	339	202	314	164	36.0	
##	Phe_T5	Met_T5	Orn_T5	Arg_T5	His_T5	Asn_T5	Asp_T5	Glu_T5	Gln_T5	Cit_T5	Tyr_T5
## 1	48.6	15.7	76.6	97.2	72.6	35.6	18.20	23.4	729	23.4	46.2
## 2	58.3	25.6	71.6	98.2	73.8	45.1	21.80	46.5	717	24.7	56.7
## 3	47.2	24.8	95.7	101.0	73.0	38.1	9.41	19.0	598	29.1	55.7
## 4	59.6	23.6	96.6	119.0	85.6	42.5	18.10	46.8	737	42.1	60.5
## 5	71.1	26.3	102.0	130.0	99.8	55.7	10.50	35.9	996	44.4	78.2
## 6	50.5	22.9	53.3	92.0	81.9	35.2	14.10	30.8	606	20.9	44.6
##	Thr_T5	Lys_T5	Creatinine_T5	Kynurenine_T5	Putrescine_T5	Sarcosine_T5					
## 1	64.6	200	64.9	1.39	0.189	8.27					
## 2	149.0	227	76.0	1.95	0.260	8.63					
## 3	114.0	263	47.3	1.45	-99.000	2.84					
## 4	140.0	329	64.0	2.23	0.196	7.57					
## 5	101.0	223	105.0	2.80	0.166	6.99					
## 6	98.3	274	63.6	2.00	NA	5.88					
##	Serotonin_T5	Taurine_T5	SDMA_T5	C0_T5	C2_T5	C3.OH_T5	C6..C4.1.DC_T5				
## 1	0.647	87.8	1.460	29.3	8.94	0.22	-99.000				
## 2	0.859	97.3	1.240	32.2	4.10	0.22	0.089				
## 3	0.562	61.3	0.789	25.8	4.52	0.27	-9.000				
## 4	0.421	132.0	1.430	37.6	9.22	0.18	-9.000				
## 5	0.930	72.0	1.520	45.0	13.00	0.16	0.097				
## 6	0.420	94.3	1.250	28.4	13.50	0.26	0.158				
##	C5.DC..C6.OH_T5	C7.DC_T5	C8_T5	C10_T5	C10.1_T5	C10.2_T5	C14.1_T5	C14.2_T5			
## 1	0.05	0.05	0.57	0.78	0.31	0.18	0.20	0.14			
## 2	0.05	0.00	0.46	0.48	0.20	0.14	0.13	0.08			
## 3	0.05	0.05	0.44	0.39	0.20	0.15	0.13	0.09			
## 4	0.04	0.04	0.38	0.36	0.14	0.15	0.16	0.10			
## 5	0.04	0.05	0.42	0.51	0.30	0.12	0.22	0.12			
## 6	0.06	0.06	0.59	0.65	0.29	0.17	0.24	0.16			
##	C16.1_T5	C16.2_T5	C16.2.OH_T5	C18.1_T5	C18.1.OH_T5	C18.2_T5	lysoPC.a.C16.0_T5				
## 1	0.11	0.05	0.05	0.21	0.05	0.08	120.0				

## 2	0.09	0.04	0.03	0.13	0.03	0.09	131.0
## 3	0.11	0.03	0.04	0.12	0.04	0.07	64.7
## 4	0.11	0.06	0.04	0.19	0.04	0.10	123.0
## 5	0.09	0.04	0.04	0.22	0.03	0.10	161.0
## 6	0.14	0.05	0.05	0.17	0.07	0.13	115.0
##	lysoPC.a.C16.1_T5	lysoPC.a.C17.0_T5	lysoPC.a.C18.0_T5	lysoPC.a.C18.1_T5			
## 1		3.45	2.20	36.2		34.6	
## 2		2.61	1.44	38.6		33.2	
## 3		1.78	1.37	21.7		21.1	
## 4		2.83	2.13	36.6		34.4	
## 5		3.82	2.11	47.5		55.1	
## 6		2.37	1.59	33.3		29.2	
##	lysoPC.a.C18.2_T5	lysoPC.a.C20.3_T5	lysoPC.a.C20.4_T5	lysoPC.a.C24.0_T5			
## 1		31.8	2.04	9.71		0.35	
## 2		42.7	1.93	11.70		0.46	
## 3		28.1	1.77	5.64		0.40	
## 4		27.8	2.12	11.70		0.43	
## 5		72.1	2.32	12.30		0.33	
## 6		33.1	1.68	10.00		0.24	
##	lysoPC.a.C26.0_T5	lysoPC.a.C26.1_T5	lysoPC.a.C28.0_T5	lysoPC.a.C28.1_T5			
## 1		0.17	0.22	-9.00		0.38	
## 2		0.19	0.19	0.26		0.31	
## 3		0.20	0.18	0.23		0.31	
## 4		0.28	0.43	0.26		0.47	
## 5		0.22	0.13	0.24		0.25	
## 6		0.18	0.35	-9.00		0.31	
##	PC.aa.C24.0_T5	PC.aa.C28.1_T5	PC.aa.C30.0_T5	PC.aa.C32.0_T5	PC.aa.C32.1_T5		
## 1		0.16	1.93	0.97	9.95	9.29	
## 2		0.14	1.53	0.76	8.81	4.61	
## 3		0.15	2.39	1.46	8.64	6.04	
## 4		0.19	2.54	0.78	9.32	4.54	
## 5		-9.00	2.23	1.87	14.00	7.67	
## 6		-9.00	1.88	0.98	7.85	3.42	
##	PC.aa.C32.3_T5	PC.aa.C34.1_T5	PC.aa.C34.2_T5	PC.aa.C34.3_T5	PC.aa.C34.4_T5		
## 1		0.21	170.0	258	6.51	0.27	
## 2		0.18	102.0	244	4.26	0.24	
## 3		0.19	102.0	242	6.70	0.44	
## 4		0.18	117.0	210	4.48	0.29	
## 5		0.13	142.0	307	4.75	0.21	
## 6		0.15	82.2	183	3.33	0.19	
##	PC.aa.C36.0_T5	PC.aa.C36.1_T5	PC.aa.C36.2_T5	PC.aa.C36.3_T5	PC.aa.C36.4_T5		
## 1		1.03	14.50	88.5	44.5	97.0	
## 2		1.17	12.80	95.3	38.6	114.0	
## 3		1.11	13.50	89.2	54.3	75.6	
## 4		0.90	12.80	78.9	42.4	120.0	
## 5		1.07	16.00	114.0	46.0	75.2	
## 6		0.69	9.17	61.5	32.0	85.5	
##	PC.aa.C36.5_T5	PC.aa.C38.0_T5	PC.aa.C38.1_T5	PC.aa.C38.3_T5	PC.aa.C38.4_T5		
## 1		4.86	2.28	0.58	18.2	66.2	
## 2		3.73	2.63	1.18	19.0	71.8	
## 3		4.14	2.39	1.44	20.9	58.8	
## 4		6.85	2.84	1.17	20.4	84.9	
## 5		3.25	2.91	1.27	17.3	51.0	
## 6		3.00	2.14	0.56	14.7	57.2	

##	PC.aa.C38.5_T5	PC.aa.C38.6_T5	PC.aa.C40.1_T5	PC.aa.C40.2_T5	PC.aa.C40.3_T5
## 1	22.4	47.1	-9.00	0.19	0.43
## 2	19.4	42.0	0.47	0.26	0.47
## 3	23.1	31.5	0.36	0.27	0.56
## 4	27.9	55.4	0.45	0.33	0.51
## 5	17.3	33.6	0.45	0.30	0.59
## 6	18.3	35.4	-9.00	0.19	0.39
##	PC.aa.C40.4_T5	PC.aa.C40.5_T5	PC.aa.C40.6_T5	PC.aa.C42.0_T5	PC.aa.C42.1_T5
## 1	1.43	3.46	13.80	0.55	0.30
## 2	1.70	3.09	15.20	0.78	0.35
## 3	1.79	3.75	9.24	0.65	0.31
## 4	1.58	3.79	16.70	0.61	0.36
## 5	1.75	3.49	10.60	0.78	0.37
## 6	1.77	3.33	10.40	0.57	0.27
##	PC.aa.C42.2_T5	PC.aa.C42.4_T5	PC.aa.C42.5_T5	PC.aa.C42.6_T5	PC.aa.C30.0_T5
## 1	0.19	0.12	0.29	0.20	0.21
## 2	0.20	0.19	0.29	0.23	0.17
## 3	0.21	0.19	0.33	0.32	0.35
## 4	0.28	0.19	0.34	0.36	0.25
## 5	0.21	0.20	0.30	0.27	0.33
## 6	0.14	0.15	0.22	0.25	0.20
##	PC.aa.C32.1_T5	PC.aa.C32.2_T5	PC.aa.C34.0_T5	PC.aa.C34.1_T5	PC.aa.C34.2_T5
## 1	2.28	0.70	0.47	5.98	5.59
## 2	1.98	0.64	0.24	3.84	5.08
## 3	2.41	0.73	0.62	5.02	7.91
## 4	1.95	0.68	0.34	4.95	5.69
## 5	3.53	0.85	0.54	5.56	8.75
## 6	1.51	0.46	0.23	4.03	4.46
##	PC.aa.C34.3_T5	PC.aa.C36.0_T5	PC.aa.C36.1_T5	PC.aa.C36.2_T5	PC.aa.C36.3_T5
## 1	4.34	0.75	3.15	5.73	2.45
## 2	5.41	0.67	1.82	3.66	2.86
## 3	6.45	0.82	2.65	5.24	3.63
## 4	4.12	0.86	2.45	4.67	2.61
## 5	6.47	1.39	2.58	5.04	3.88
## 6	4.03	0.56	1.66	3.16	2.74
##	PC.aa.C36.4_T5	PC.aa.C36.5_T5	PC.aa.C38.0_T5	PC.aa.C38.2_T5	PC.aa.C38.3_T5
## 1	6.48	6.95	1.05	1.05	1.03
## 2	7.28	7.59	0.76	0.93	0.95
## 3	6.55	6.67	0.97	1.28	1.29
## 4	7.26	6.36	1.23	1.17	1.27
## 5	10.40	7.92	0.80	1.26	1.09
## 6	7.24	5.84	0.53	0.68	0.82
##	PC.aa.C38.4_T5	PC.aa.C38.5_T5	PC.aa.C38.6_T5	PC.aa.C40.1_T5	PC.aa.C40.2_T5
## 1	4.65	7.82	3.02	0.91	1.17
## 2	4.64	11.00	3.72	1.05	0.70
## 3	4.42	7.42	2.92	0.78	0.97
## 4	5.05	10.30	3.68	1.08	1.27
## 5	4.34	11.90	3.70	0.82	0.95
## 6	4.38	9.89	2.81	0.61	0.89
##	PC.aa.C40.3_T5	PC.aa.C40.4_T5	PC.aa.C40.5_T5	PC.aa.C40.6_T5	PC.aa.C42.1_T5
## 1	0.60	1.45	1.61	1.87	0.29
## 2	0.64	1.62	2.47	2.00	0.35
## 3	0.69	1.90	1.66	1.78	0.30
## 4	0.84	1.90	2.26	2.47	0.45

```
## 5      0.85      2.34      2.42      2.15      0.32
## 6      0.50      1.50      2.09      2.05      0.29
## PC.ae.C42.2_T5 PC.ae.C42.3_T5 PC.ae.C42.4_T5 PC.ae.C42.5_T5 PC.ae.C44.3_T5
## 1      0.35      0.58      0.70      2.08      0.14
## 2      0.31      0.57      0.74      2.73      0.09
## 3      0.49      0.59      0.91      2.16      0.11
## 4      0.44      0.75      0.89      2.48      0.13
## 5      0.41      0.74      1.14      3.34      0.14
## 6      0.30      0.52      0.72      2.33      0.11
## PC.ae.C44.4_T5 PC.ae.C44.5_T5 PC.ae.C44.6_T5 SM..OH..C14.1_T5
## 1      0.34      2.10      1.26      4.33
## 2      0.33      2.63      1.93      2.38
## 3      0.57      2.12      1.72      3.61
## 4      0.33      2.69      1.78      3.69
## 5      0.53      2.79      2.19      2.92
## 6      0.36      2.20      1.39      3.17
## SM..OH..C16.1_T5 SM..OH..C22.1_T5 SM..OH..C22.2_T5 SM..OH..C24.1_T5
## 1      1.93      2.44      3.93      0.24
## 2      1.05      2.60      3.76      0.27
## 3      1.49      2.77      3.70      0.40
## 4      1.62      3.54      4.85      0.53
## 5      1.19      2.55      3.31      0.39
## 6      1.33      3.04      3.90      0.38
## SM.C16.0_T5 SM.C16.1_T5 SM.C18.0_T5 SM.C18.1_T5 SM.C20.2_T5 SM.C24.0_T5
## 1      67.3      11.50      12.30      8.17      0.19      4.44
## 2      62.2      11.60      9.90      7.34      0.18      4.75
## 3      62.8      8.85      6.64      4.33      0.17      4.01
## 4      76.6      12.60      9.51      6.52      0.25      5.90
## 5      74.0      12.60      8.97      6.62      0.16      4.14
## 6      67.0      11.80      9.82      6.89      0.21      5.62
## SM.C24.1_T5
## 1      26.6
## 2      24.7
## 3      19.8
## 4      32.1
## 5      23.9
## 6      28.6
```

```
head(metadatosPEC1)
```

```
##      VarName      varTpe Description
## SUBJECTS SUBJECTS   integer  dataDesc
## SURGERY   SURGERY   character dataDesc
## AGE       AGE       integer  dataDesc
## GENDER    GENDER    character dataDesc
## Group     Group     integer  dataDesc
## MEDDM_TO  MEDDM_TO  integer  dataDesc
```

```
# Carga de paquetes
library(dplyr)
```

```
##
## Adjuntando el paquete: 'dplyr'
```



```
## The following objects are masked from 'package:stats':  
##  
##   filter, lag
```

```
## The following objects are masked from 'package:base':  
##  
##   intersect, setdiff, setequal, union
```

```
library(tidyr)  
library(SummarizedExperiment)
```

```
## Cargando paquete requerido: MatrixGenerics
```

```
## Cargando paquete requerido: matrixStats
```

```
##  
## Adjuntando el paquete: 'matrixStats'
```

```
## The following object is masked from 'package:dplyr':  
##  
##   count
```

```
##  
## Adjuntando el paquete: 'MatrixGenerics'
```

```
## The following objects are masked from 'package:matrixStats':  
##  
##   colAlls, colAnyNAs, colAnys, colAveragesPerRowSet, colCollapse,  
##   colCounts, colCummaxs, colCummins, colCumprods, colCumsums,  
##   colDiffs, colIQRDiffs, colIQRs, colLogSumExps, colMadDiffs,  
##   colMads, colMaxs, colMeans2, colMedians, colMins, colOrderStats,  
##   colProds, colQuantiles, colRanges, colRanks, colSdDiffs, colSds,  
##   colSums2, colTabulates, colVarDiffs, colVars, colWeightedMads,  
##   colWeightedMeans, colWeightedMedians, colWeightedSds,  
##   colWeightedVars, rowAlls, rowAnyNAs, rowAnys, rowAveragesPerColSet,  
##   rowCollapse, rowCounts, rowCummaxs, rowCummins, rowCumprods,  
##   rowCumsums, rowDiffs, rowIQRDiffs, rowIQRs, rowLogSumExps,  
##   rowMadDiffs, rowMads, rowMaxs, rowMeans2, rowMedians, rowMins,  
##   rowOrderStats, rowProds, rowQuantiles, rowRanges, rowRanks,  
##   rowSdDiffs, rowSds, rowSums2, rowTabulates, rowVarDiffs, rowVars,  
##   rowWeightedMads, rowWeightedMeans, rowWeightedMedians,  
##   rowWeightedSds, rowWeightedVars
```

```
## Cargando paquete requerido: GenomicRanges
```

```
## Cargando paquete requerido: stats4
```

```
## Cargando paquete requerido: BiocGenerics
```

```
##  
## Adjuntando el paquete: 'BiocGenerics'
```

```

## The following objects are masked from 'package:dplyr':
##
##   combine, intersect, setdiff, union

## The following objects are masked from 'package:stats':
##
##   IQR, mad, sd, var, xtabs

## The following objects are masked from 'package:base':
##
##   anyDuplicated, aperm, append, as.data.frame, basename, cbind,
##   colnames, dirname, do.call, duplicated, eval, evalq, Filter, Find,
##   get, grep, grepl, intersect, is.unsorted, lapply, Map, mapply,
##   match, mget, order, paste, pmax, pmax.int, pmin, pmin.int,
##   Position, rank, rbind, Reduce, rownames, sapply, saveRDS, setdiff,
##   table, tapply, union, unique, unsplit, which.max, which.min

## Cargando paquete requerido: S4Vectors

##
## Adjuntando el paquete: 'S4Vectors'

## The following object is masked from 'package:tidyr':
##
##   expand

## The following objects are masked from 'package:dplyr':
##
##   first, rename

## The following object is masked from 'package:utils':
##
##   findMatches

## The following objects are masked from 'package:base':
##
##   expand.grid, I, unname

## Cargando paquete requerido: IRanges

##
## Adjuntando el paquete: 'IRanges'

## The following objects are masked from 'package:dplyr':
##
##   collapse, desc, slice

## The following object is masked from 'package:grDevices':
##
##   windows

```

```
## Cargando paquete requerido: GenomeInfoDb

## Cargando paquete requerido: Biobase

## Welcome to Bioconductor
##
##     Vignettes contain introductory material; view with
##     'browseVignettes()'. To cite Bioconductor, see
##     'citation("Biobase")', and for packages 'citation("pkgname)".

##
## Adjuntando el paquete: 'Biobase'
```

```
## The following object is masked from 'package:MatrixGenerics':
##
##     rowMedians

## The following objects are masked from 'package:matrixStats':
##
##     anyMissing, rowMedians
```

```
library(naniar)
library(ggplot2)
library(pheatmap)
library(PCAtools)
```

```
## Cargando paquete requerido: ggrepel

##
## Adjuntando el paquete: 'PCAtools'
```

```
## The following objects are masked from 'package:stats':
##
##     biplot, screeplot
```

```
library(dendextend)
```

```
##
## -----
## Welcome to dendextend version 1.19.0
## Type citation('dendextend') for how to cite the package.
##
## Type browseVignettes(package = 'dendextend') for the package vignette.
## The github page is: https://github.com/talgalili/dendextend/
##
## Suggestions and bug-reports can be submitted at: https://github.com/talgalili/dendextend/issues
## You may ask questions at stackoverflow, use the r and dendextend tags:
##     https://stackoverflow.com/questions/tagged/dendextend
##
## To suppress this message use: suppressPackageStartupMessages(library(dendextend))
## -----
```

```
##
## Adjuntando el paquete: 'dendextend'

## The following object is masked from 'package:stats':
##
##      cutree

# Preparar los datos:
# Separamos la información de las muestras (primeras 5 columnas) de los datos metabolómicos (restantes
infoSamples <- datosPEC1[, 1:5]          # Información sobre individuos
datosPEC1 <- datosPEC1[, -c(1:5)]       # Datos metabolómicos puros (690 columnas)
metadatosPEC1 <- metadatosPEC1[-c(1:5), ] # Metadatos correspondientes (690 filas)

# Convertir las variables de información de muestras a factores y crear nombres de fila informativos

# Convertir a factor las columnas SURGERY, GENDER y Group
infoSamples <- infoSamples %>%
  mutate(SURGERY = as.factor(SURGERY), GENDER = as.factor(GENDER), Group = as.factor(Group))

# Crear un identificador único para cada muestra usando SUBJECTS, Group y la primera letra de SURGERY e
infoSamples <- infoSamples %>%
  mutate(RowName = paste0(SUBJECTS, "_", Group, "_", toupper(substr(SURGERY, 1, 1))))

# Asignar los nombres de fila generados a infoSamples y usarlos para las filas de datosPEC1
rownames(infoSamples) <- infoSamples$RowName
rownames(datosPEC1) <- rownames(infoSamples)
# Eliminar la columna auxiliar RowName para mantener el data frame limpio
infoSamples <- infoSamples %>% select(-RowName)

# Visualizar las primeras filas del data frame infoSamples modificado
head(infoSamples)

##      SUBJECTS SURGERY AGE GENDER Group
## 1_1_B        1 by pass  27      F      1
## 2_2_B        2 by pass  19      F      2
## 3_1_B        3 by pass  42      F      1
## 4_2_B        4 by pass  37      F      2
## 5_1_T        5 tubular  42      F      1
## 6_2_B        6 by pass  24      F      2

# Validar que los nombres de fila de infoSamples y datosPEC1 coinciden
stopifnot(all(rownames(infoSamples) == rownames(datosPEC1)))

# Crear el objeto SummarizedExperiment usando los datos y metadatos preparados
sePEC1 <- SummarizedExperiment(
  assays = list(valores = as.matrix(datosPEC1)),
  rowData = infoSamples,
  colData = metadatosPEC1,
  metadata = list(descripcion = "Dataset metabolómico 2018-MetabotypingPaper")
)
# Guardar el objeto SummarizedExperiment para uso posterior
save(sePEC1, file = "sePEC1.Rda")
```

```
# Mostrar las dimensiones del objeto SummarizedExperiment
dim(sePEC1)
```

```
## [1] 39 690
```

```
# Exploración inicial de los datos:
# Convertir el rowData a data.frame para explorar y seleccionar las variables de interés
datosDF <- data.frame(rowData(sePEC1)[, c("SURGERY", "AGE", "GENDER", "Group")]) %>%
  mutate(across(c("SURGERY", "GENDER", "Group"), as.factor))

# Mostrar las primeras filas del data frame de metadatos
datosDF %>%
  head() %>%
  print()
```

```
##      SURGERY AGE GENDER Group
## 1_1_B by pass 27      F     1
## 2_2_B by pass 19      F     2
## 3_1_B by pass 42      F     1
## 4_2_B by pass 37      F     2
## 5_1_T tubular 42      F     1
## 6_2_B by pass 24      F     2
```

```
# Mostrar un resumen estadístico de las variables
summary(datosDF)
```

```
##      SURGERY      AGE      GENDER Group
## by pass:26  Min.   :19.00  F:27   1:24
## tubular:13  1st Qu.:35.00  M:12   2:15
##              Median :41.00
##              Mean    :40.79
##              3rd Qu.:46.00
##              Max.    :59.00
```

```
# Explorar la distribución de las variables categóricas y numéricas
(freq_surgery <- table(datosDF$SURGERY)) # Frecuencia de cada valor en SURGERY
```

```
##
## by pass tubular
##      26      13
```

```
(freq_gender <- table(datosDF$GENDER)) # Frecuencia de cada valor en GENDER
```

```
##
## F M
## 27 12
```

```
(freq_group <- table(datosDF$Group)) # Frecuencia de cada valor en Group
```

```
##
## 1 2
## 24 15
```

```
# Frecuencia conjunta de SURGERY y Group
(freq_surgery_Group <- table(datosDF$SURGERY, datosDF$Group))
```

```
##
##          1  2
## by pass 13 13
## tubular 11  2
```

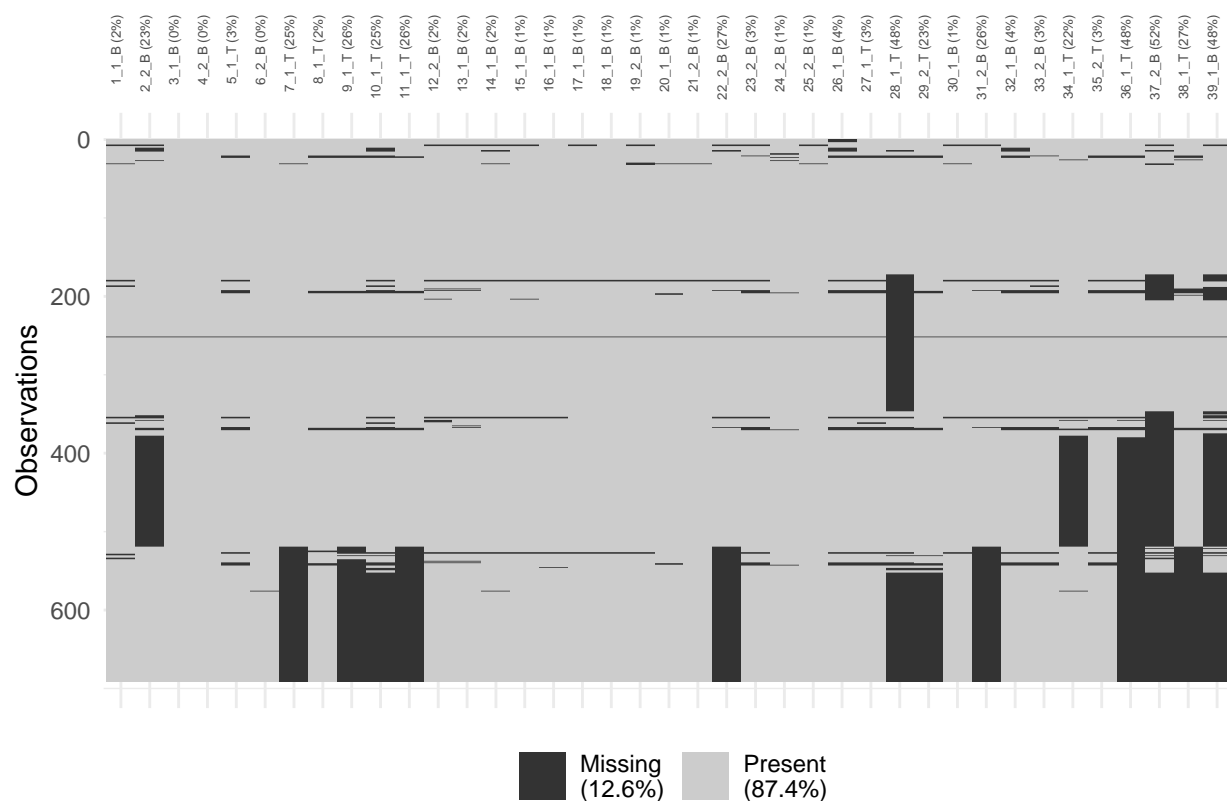
```
# Frecuencia conjunta de SURGERY, Group y GENDER
(freq_surgery_Group_Gender <- table(datosDF$SURGERY, datosDF$Group, datosDF$GENDER))
```

```
## , , = F
##
##
##          1  2
## by pass 10 10
## tubular  6  1
##
## , , = M
##
##
##          1  2
## by pass  3  3
## tubular  5  1
```

```
# Resumen estadístico de la variable numérica AGE
(summary(datosDF$AGE))
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
## 19.00  35.00  41.00  40.79  46.00  59.00
```

```
# Exploración visual de los valores faltantes en la matriz transpuesta del ensayo "valores"
traspuesta <- (as.data.frame(t(assay(sePEC1)), warn_large_data = FALSE))
# Visualizar la matriz de valores faltantes con vis_miss y ajustar las etiquetas del eje X
vis_miss(traspuesta) + theme(axis.text.x = element_text(size = 5, angle = 90, hjust = 1))
```



*# Calcular y mostrar el número y proporción de valores faltantes y completos*

```
n_miss(traspuesta)
```

```
## [1] 3390
```

```
n_complete(traspuesta)
```

```
## [1] 23520
```

```
prop_miss(traspuesta)
```

```
## [1] 0.1259755
```

```
prop_complete(traspuesta)
```

```
## [1] 0.8740245
```

```
pct_miss(traspuesta)
```

```
## [1] 12.59755
```

```
pct_complete(traspuesta)
```

```
## [1] 87.40245
```

```
# Manejo de valores faltantes en el ensayo "valores":  
# Extraer la matriz de datos  
valores <- assay(sePEC1)  
# Copiar la matriz para crear una versión donde se arreglen los valores faltantes  
valores_na_fix <- valores  
  
# Reemplazar -9 y -99 por NA  
valores_na_fix[valores_na_fix == -9] <- NA  
valores_na_fix[valores_na_fix == -99] <- NA  
  
# Imputar los NA con 1  
valores_na_fix[is.na(valores_na_fix)] <- 1  
  
# Comprobar que ya no queden NA en la matriz  
sum(is.na(valores_na_fix))
```

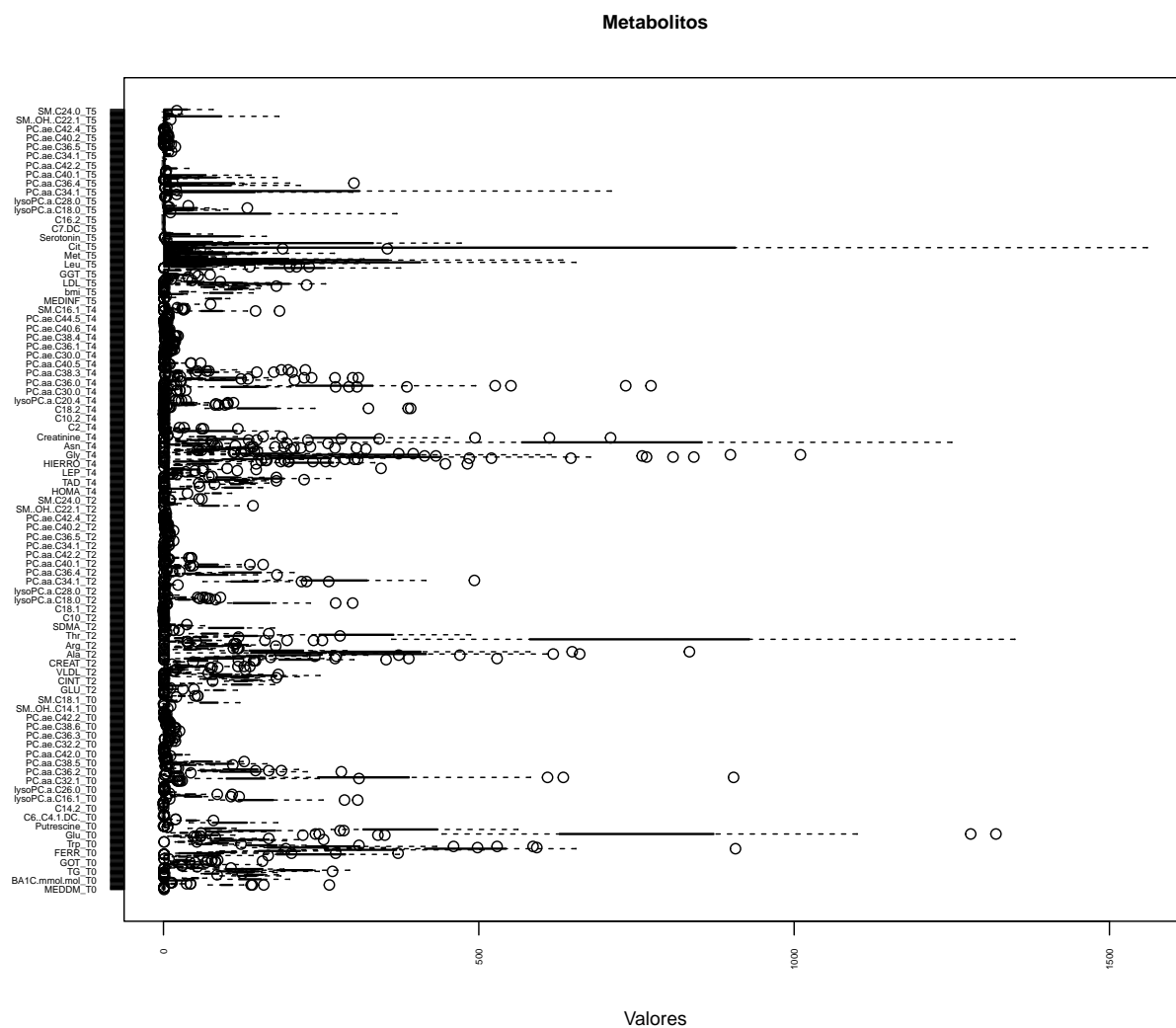
```
## [1] 0
```

```
# Agregar la matriz arreglada (valores_na_fix) como un nuevo ensayo en sePEC1  
assays(sePEC1)$valores_na_fix <- valores_na_fix  
# Mostrar la estructura actualizada del objeto SummarizedExperiment  
show(sePEC1)
```

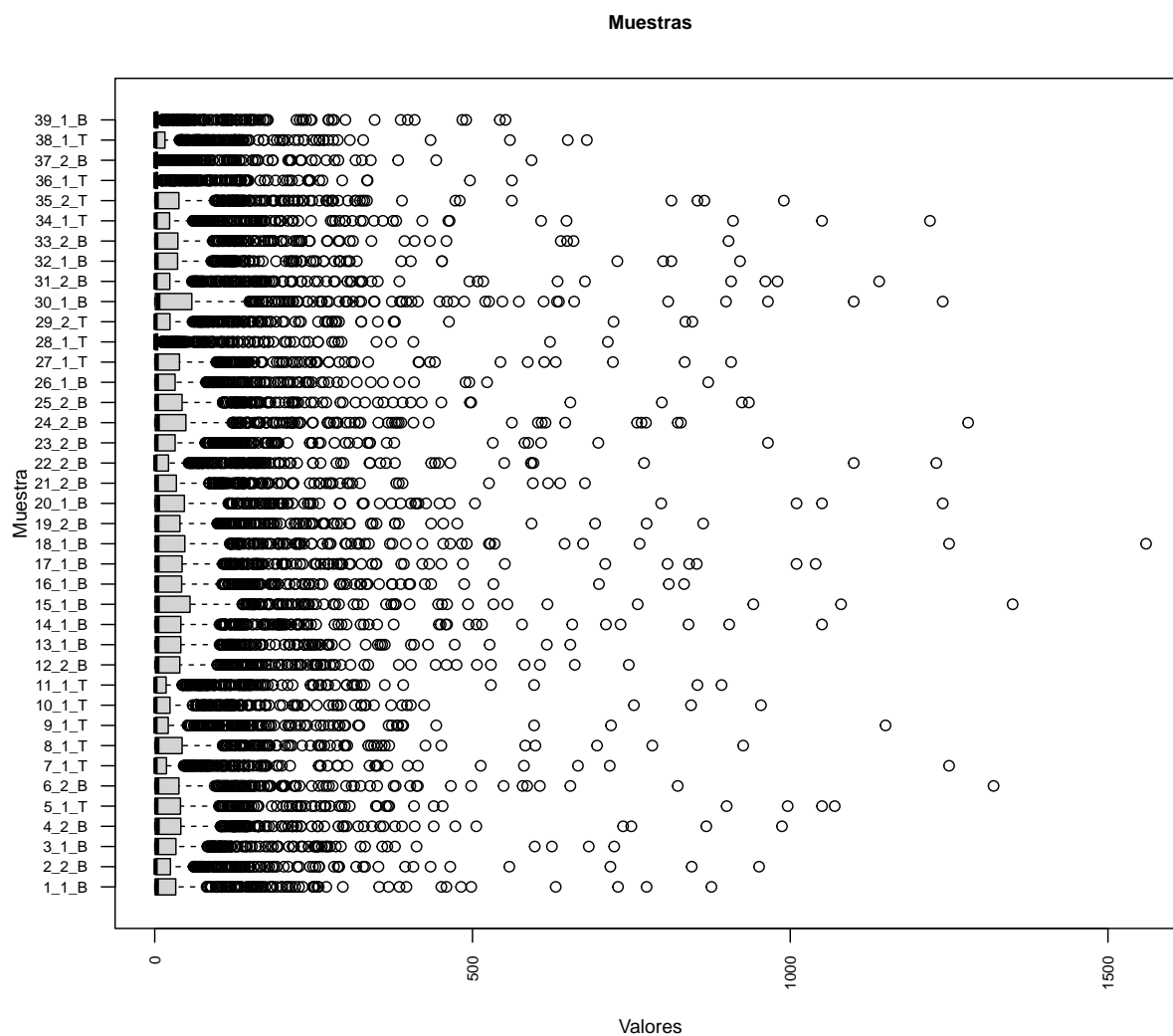
```
## class: SummarizedExperiment  
## dim: 39 690  
## metadata(1): descripcion  
## assays(2): valores valores_na_fix  
## rownames(39): 1_1_B 2_2_B ... 38_1_T 39_1_B  
## rowData names(5): SUBJECTS SURGERY AGE GENDER Group  
## colnames(690): MEDDM_TO MEDCOL_TO ... SM.C24.0_T5 SM.C24.1_T5  
## colData names(3): VarName varTpe Description
```

```
# Boxplot de los metabolitos (cada caja representa un metabolito)  
boxplot(assay(sePEC1, "valores_na_fix"),  
        xlab = "Valores",  
        cex.lab = 0.8,  
        horizontal = TRUE,  
        cex.axis = 0.4,  
        las = 2,  
        main = "Metabolitos",  
        cex.main = 0.8)
```





```
# Boxplot de las muestras (trasponer para que cada caja represente una muestra)
boxplot(t(assay(sePEC1, "valores_na_fix")),
  ylab = "Muestra",
  xlab = "Valores",
  cex.lab = 0.8,
  horizontal = TRUE,
  cex.axis = 0.7,
  las = 2,
  main = "Muestras",
  cex.main = 0.8)
```



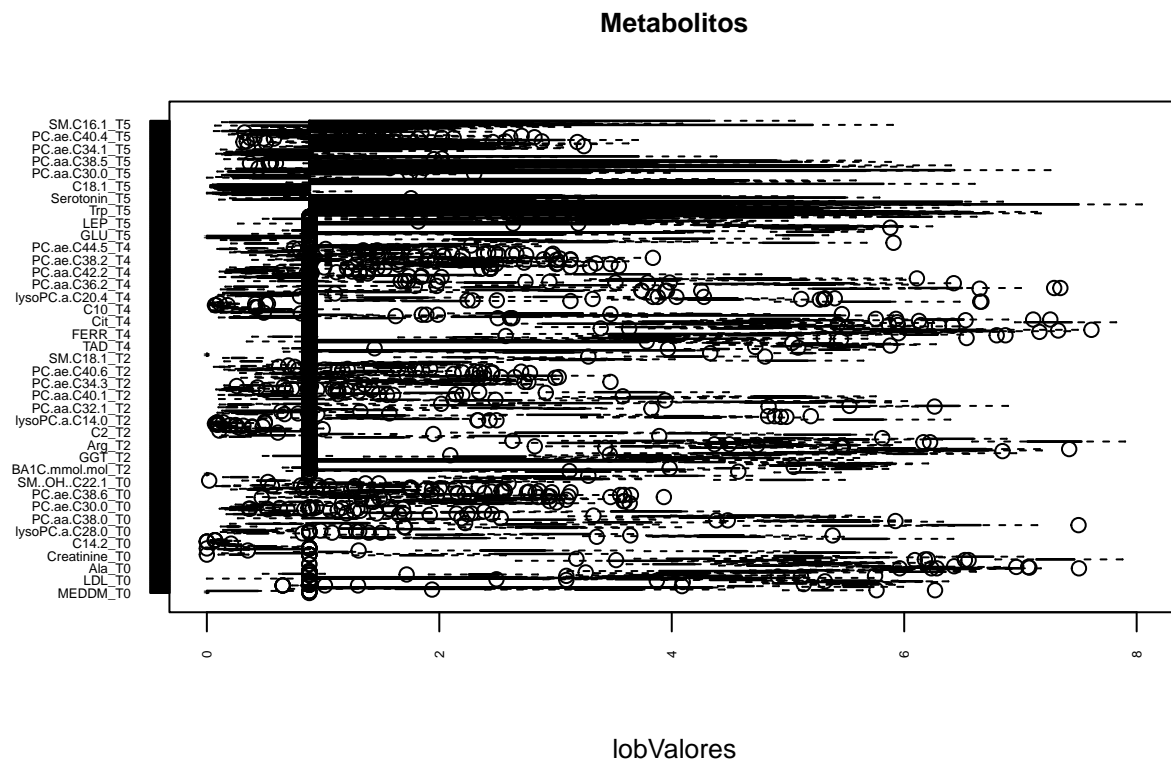
TRANSFORMACIÓN DE LOS DATOS, ESTO NOS DARA UNA MEJOR VIAUALIZACIÓN DE LOS MISMOS.

```
# Transformación de los datos:
# Aplicar la transformación asinh para manejar valores negativos y ceros de forma robusta
asinh_transform <- asinh(assay(sePEC1, "valores_na_fix"))
# Agregar la transformación como un nuevo ensayo en el objeto
assays(sePEC1)$asinh_transform <- asinh_transform
# Mostrar el objeto actualizado
show(sePEC1)
```

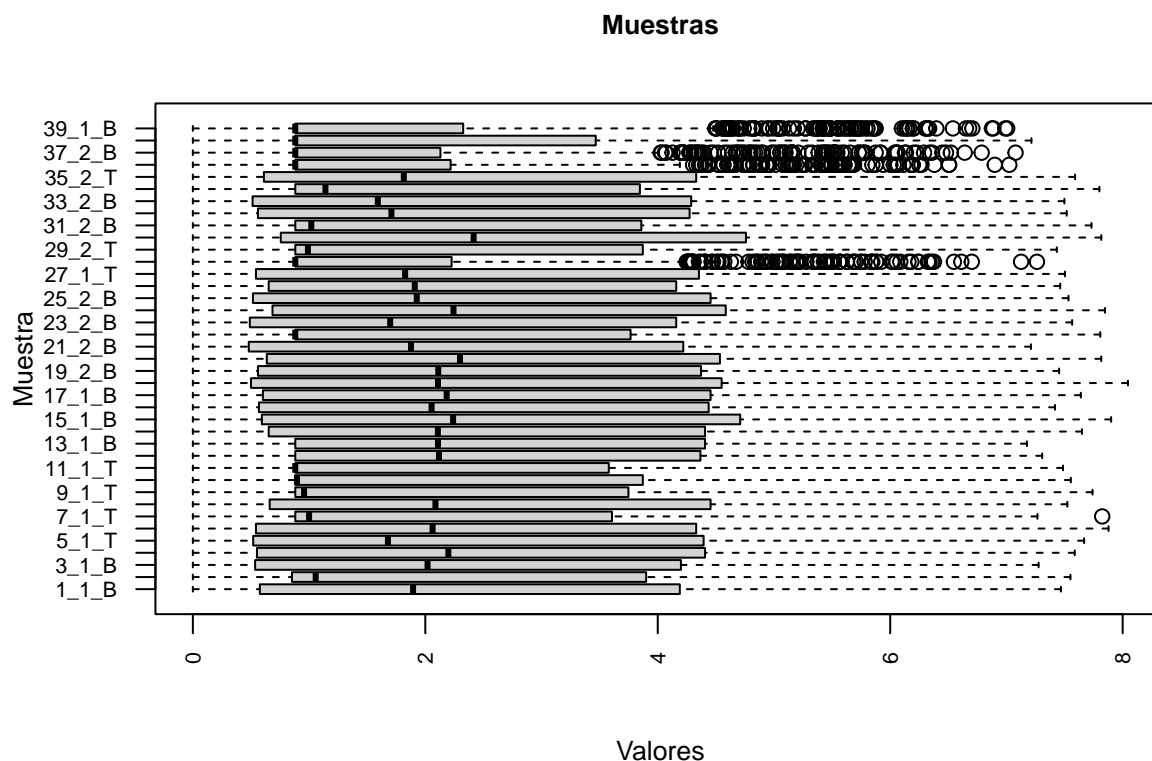
```
## class: SummarizedExperiment
## dim: 39 690
## metadata(1): descripcion
## assays(3): valores valores_na_fix asinh_transform
## rownames(39): 1_1_B 2_2_B ... 38_1_T 39_1_B
## rowData names(5): SUBJECTS SURGERY AGE GENDER Group
## colnames(690): MEDDM_TO MEDCOL_TO ... SM.C24.0_T5 SM.C24.1_T5
## colData names(3): VarName varTpe Description
```

```
# Guardar el objeto SummarizedExperiment preprocesado y transformado
save(sePEC1, file = "sePEC1norm.Rda")
```

```
# Exploración de los datos normalizados:
# Boxplot de los metabolitos usando la transformación asinh
boxplot(assay(sePEC1, "asinh_transform"),
        xlab = "lobValores",
        cex.lab = 0.8,
        horizontal = TRUE,
        cex.axis = 0.4,
        las = 2,
        main = "Metabolitos",
        cex.main = 0.8)
```



```
# Boxplot de las muestras usando la transformación asinh (traspuesto para que cada caja sea una muestra)
boxplot(t(assay(sePEC1, "asinh_transform")),
        ylab = "Muestra",
        xlab = "Valores",
        cex.lab = 0.8,
        horizontal = TRUE,
        cex.axis = 0.7,
        las = 2,
        main = "Muestras",
        cex.main = 0.8)
```



```
# Clustering de las muestras (sin transponer la matriz, ya que filas = muestras)
# Extraer la matriz asinh transformada (filas = muestras, columnas = metabolitos)
datos_cluster <- (assay(sePEC1, "asinh_transform"))

# Escalar los datos para normalizar cada metabolito (columna)
datos_cluster_scaled <- scale(datos_cluster)

# Calcular la matriz de distancias Euclidianas entre muestras
dist_cluster <- dist(datos_cluster_scaled)

# Realizar clustering jerárquico usando el método Ward
hc <- hclust(dist_cluster, method = "ward.D2")

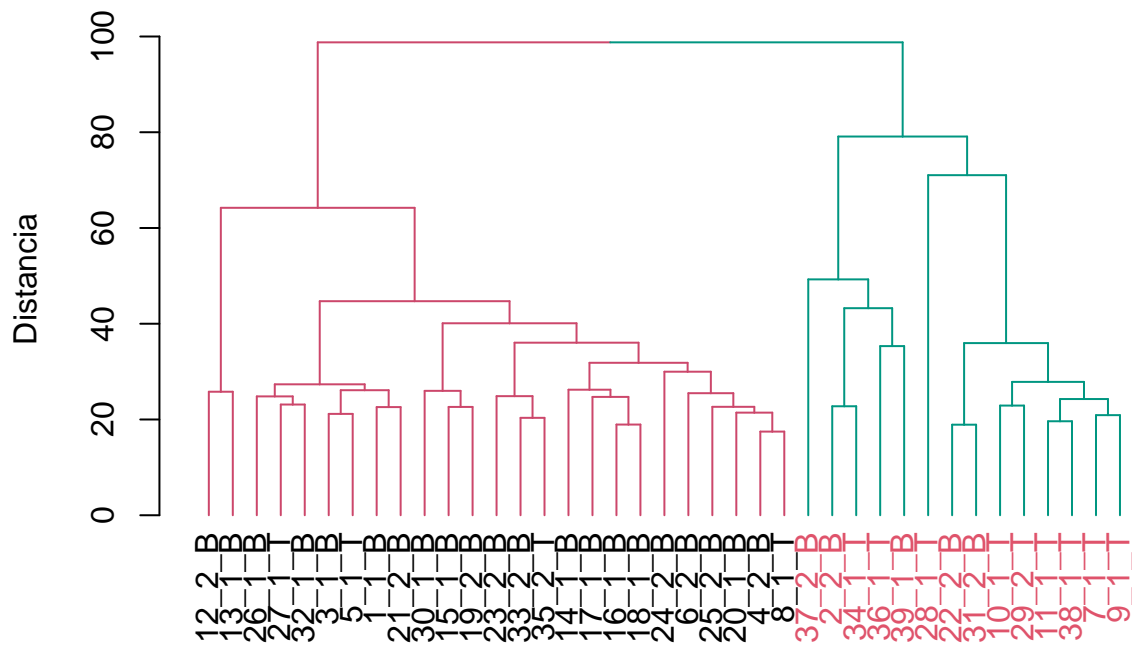
# Convertir el objeto hclust a un dendrograma
dend <- as.dendrogram(hc)

# Colorar las ramas del dendrograma en 2 clusters
dend <- color_branches(dend, k = 2)

# Asignar colores a las etiquetas según el corte de clusters
clusters <- cutree(hc, k = 2)
labels_colors(dend) <- clusters[order.dendrogram(dend)]

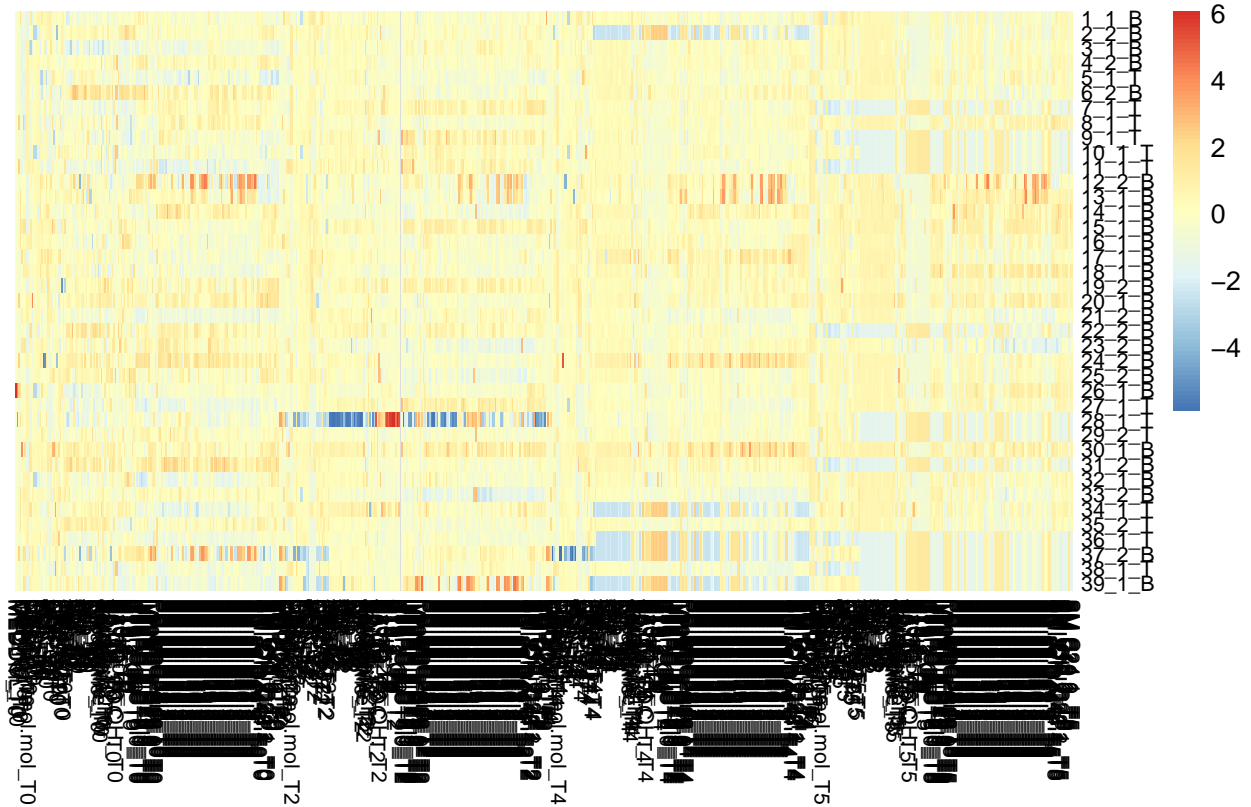
# Dibujar el dendrograma
plot(dend, main = "Dendrograma coloreado de muestras", ylab = "Distancia", cex = 0.7)
```

## Dendrograma coloreado de muestras



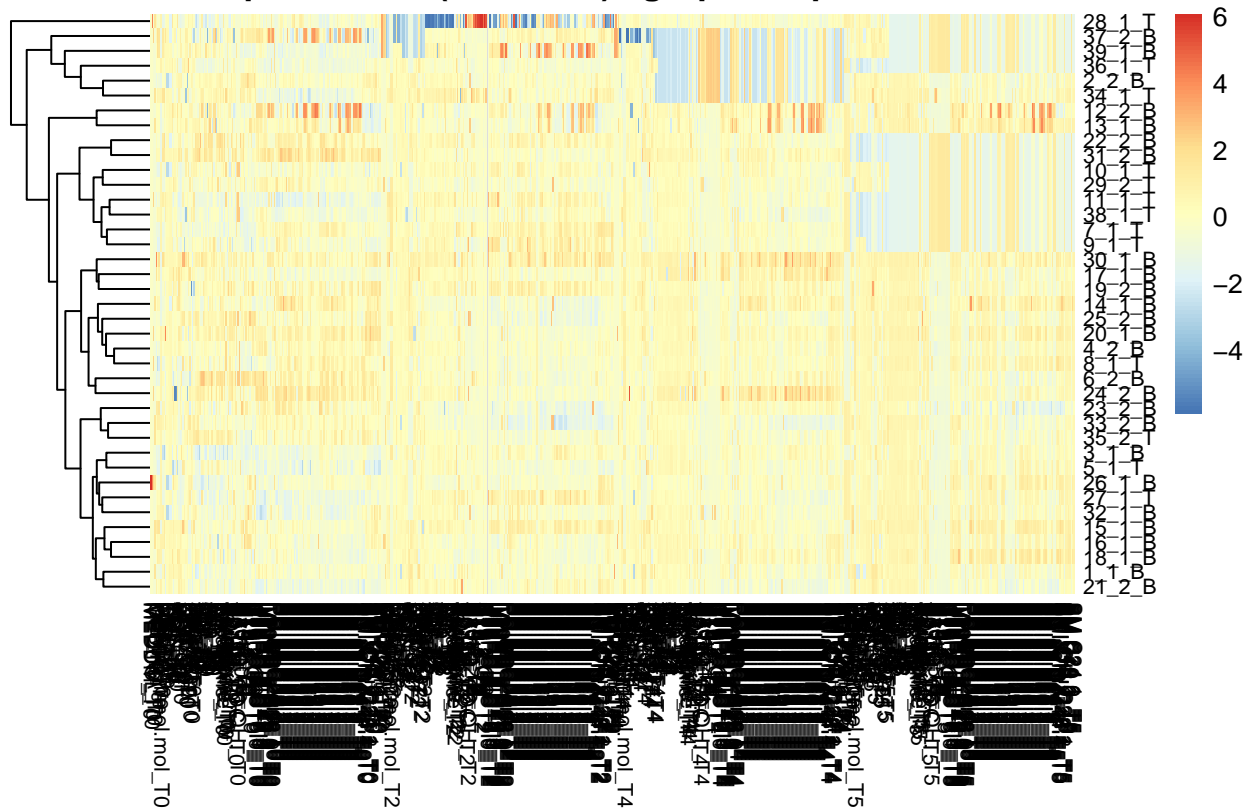
```
# Mapa de calor sin clustering:
# Generar un mapa de calor de la matriz escalada sin aplicar clustering a filas ni columnas, con cluster
pheatmap(datos_cluster_scaled,
  cluster_rows = FALSE,
  cluster_cols = FALSE,
  main = "Mapa de calor (muestras) sin clustering",
  fontsize_row = 8,
  fontsize_col = 8)
```

Mapa de calor (muestras) sin clustering



```
# Mapa de calor agrupando solo por muestras:
# Aplicar clustering solo en las filas (muestras) para visualizar la agrupación de las mismas
pheatmap(datos_cluster_scaled,
          cluster_rows = TRUE,
          cluster_cols = FALSE,
          main = "Mapa de calor (muestras) agrupando por muestras",
          fontsize_row = 8,
          fontsize_col = 8)
```

## Mapa de calor (muestras) agrupando por muestras

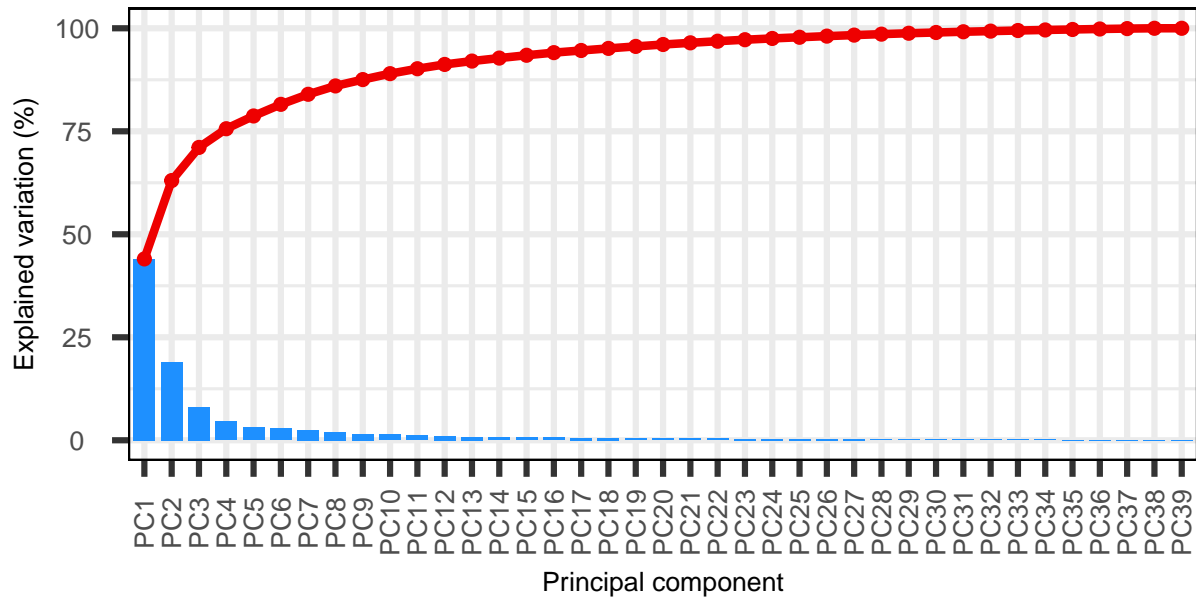


```
# Realizar PCA para analizar la variabilidad de las muestras:
# Se transpone la matriz para que las columnas sean muestras, ya que PCAtools requiere que así sea
pca_res <- pca(t(assay(sePEC1, "asinh_transform")),
              metadata = rowData(sePEC1),
              removeVar = 0.1) # Elimina metabolitos con muy baja variabilidad

## -- removing the lower 10% of variables based on variance

# Generar el screeplot para visualizar el porcentaje de varianza explicado por cada componente
screeplot(pca_res, axisLabSize = 10, titleLabSize = 22)
```

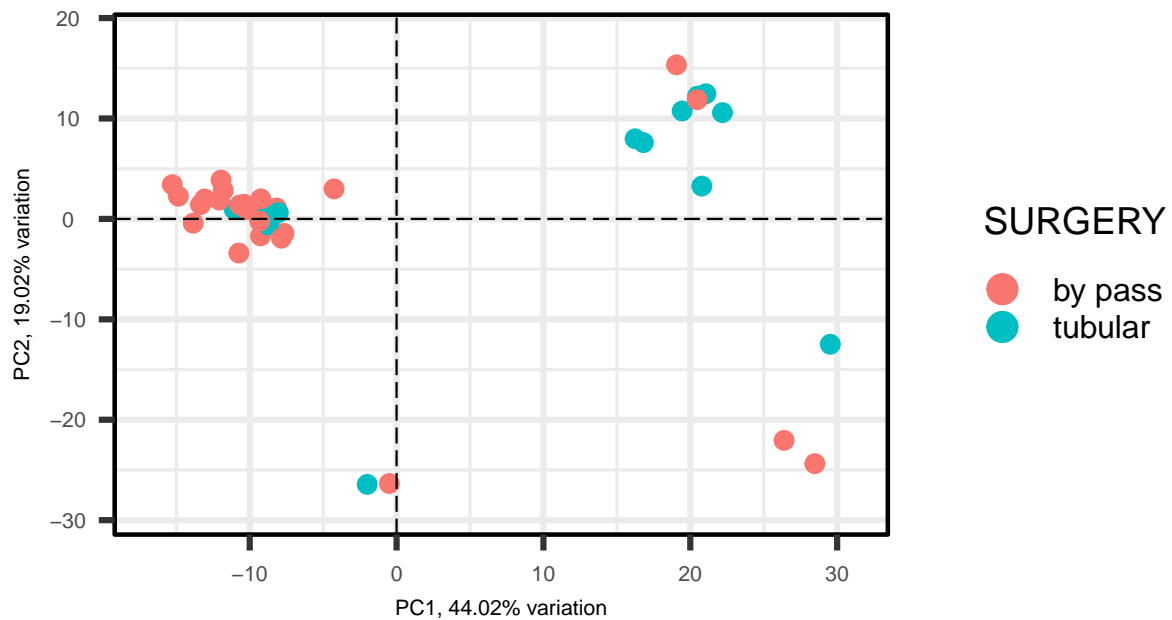
# SCREE plot



```
# Generar el biplot para visualizar la dispersión de las muestras en el espacio de las componentes prin
biplot(pca_res,
  showLoadings = FALSE,      # Cambia a TRUE si deseas ver las flechas de carga de los metabolitos
  colby = "SURGERY",        # Colorear las muestras según la variable SURGERY
  lab = NULL,                # No mostrar etiquetas para evitar saturación
  pointSize = 3,
  axisLabSize = 8,
  title = "PCA de las muestras",
  sizeLoadingsNames = 3,
  hline = 0, vline = 0,
  legendPosition = "right")
```



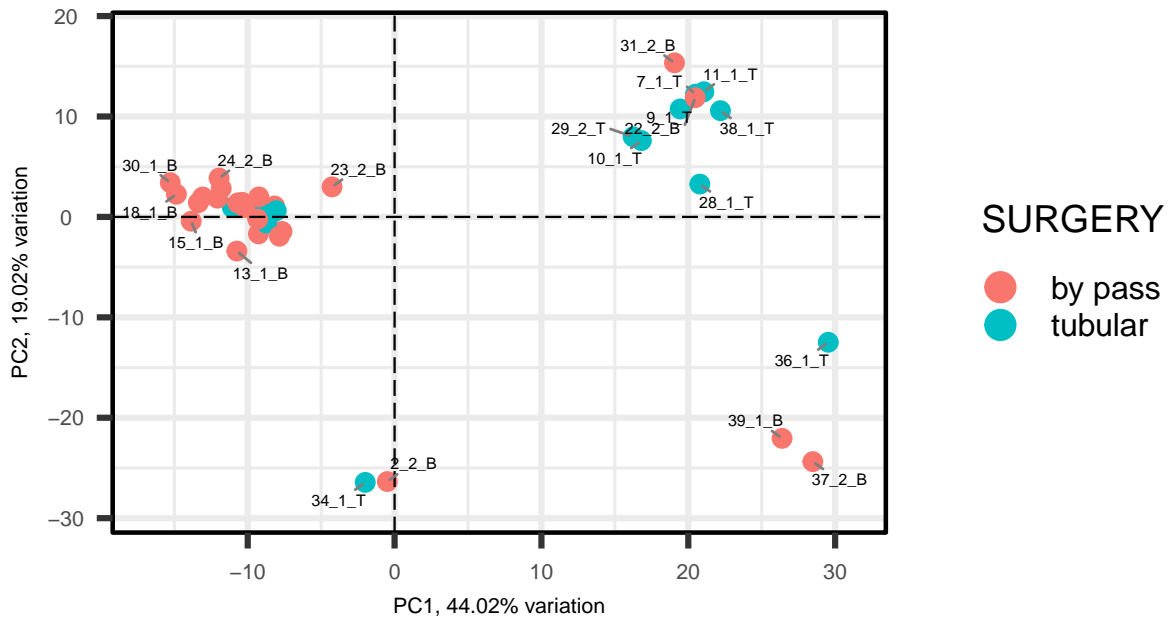
## PCA de las muestras



```
# Generar otro biplot del PCA con ajustes en labSize para refinar la visualización
biplot(pca_res, showLoadings = FALSE, labSize = 2, pointSize = 3, axisLabSize = 8,
       title = "PCA de las muestras", sizeLoadingsNames = 3, colby = "SURGERY",
       hline = 0, vline = 0, legendPosition = "right")
```

```
## Warning: ggrepel: 19 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```

## PCA de las muestras



```
# Visualización de los loadings (contribución de cada metabolito a las componentes)
plotloadings(pca_res, rangeRetain = 0.0001, labSize = 3)
```

```
## -- variables retained:
```

```
## C18.1.OH_T5, C16.2_T5, Gln_T5, Gln_T4, TRANSF_T5, Gln_T2, LEP_T0, TRANSF_T0, LDL_T5
```

```
## Warning: ggrepel: 17 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```

