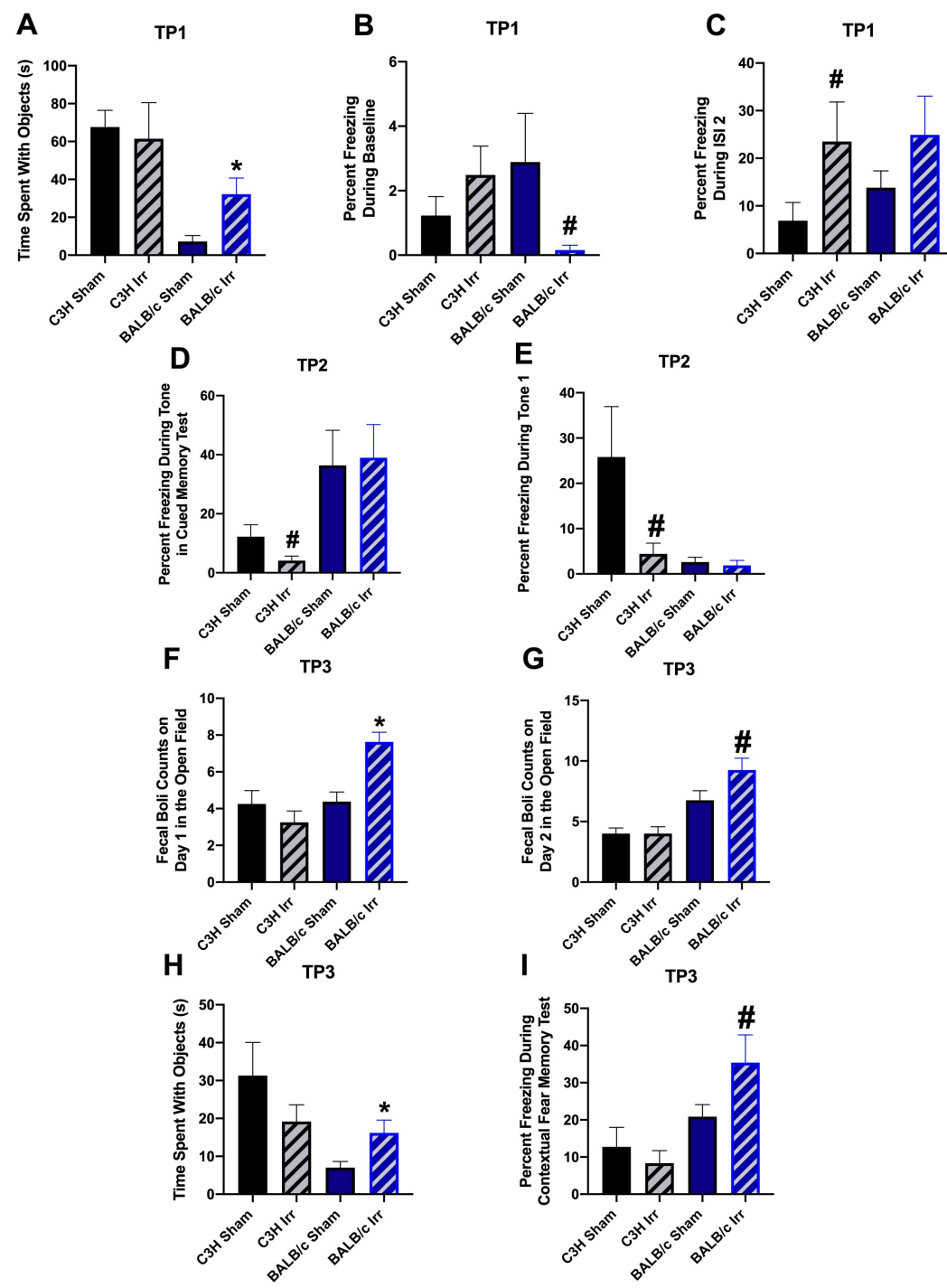
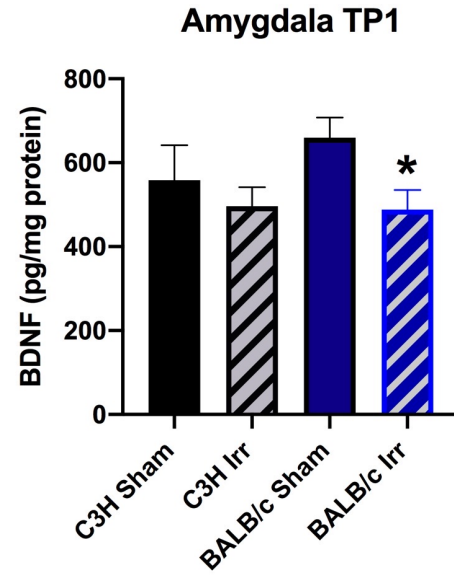


Suppl Fig 1

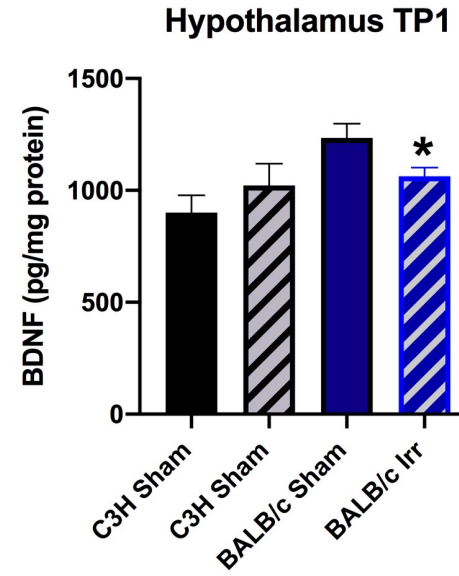


Suppl Fig 2

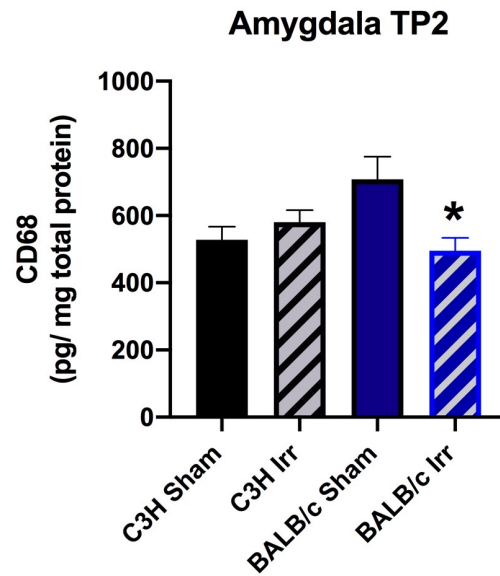
A



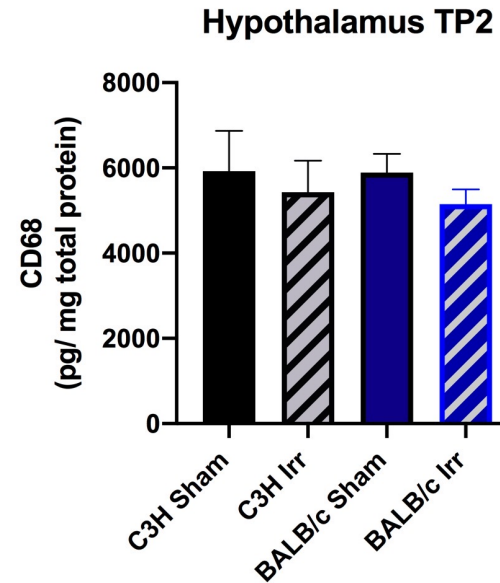
B



C

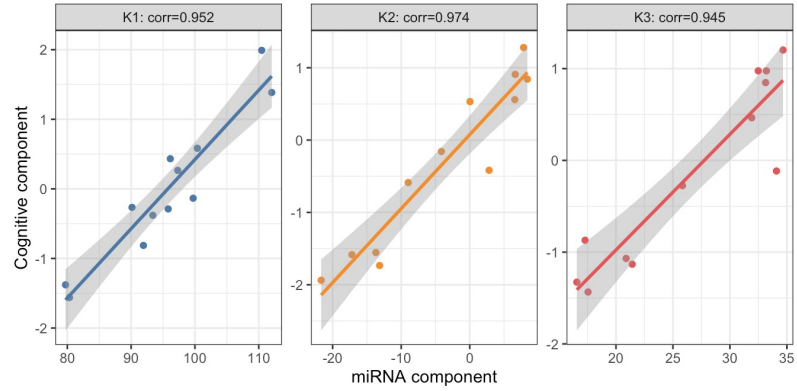


D



Suppl Fig 3 Cognitive vs miRNA – TP2

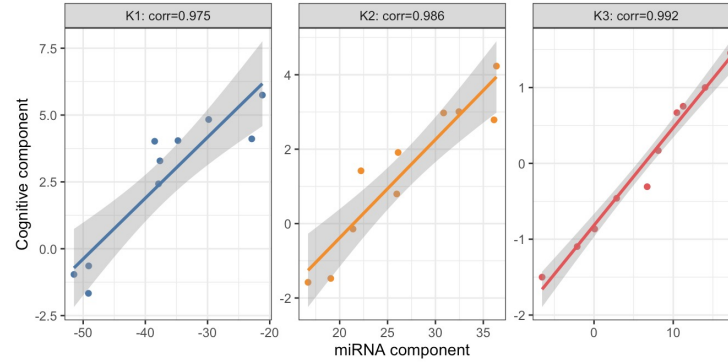
Sparse CCA: miRNA vs Cognitive (TP2 SHAM)



Linear combination

- K1: $-0.853 \cdot \text{train_tone5} + -0.522 \cdot \text{train_tone4}$
- K2: $-0.522 \cdot \text{bin_3_preference_obj_2} + 0.853 \cdot \text{context_total}$
- K3: $-0.522 \cdot \text{bin_1_preference_obj_2} + 0.853 \cdot \text{context_minute4}$

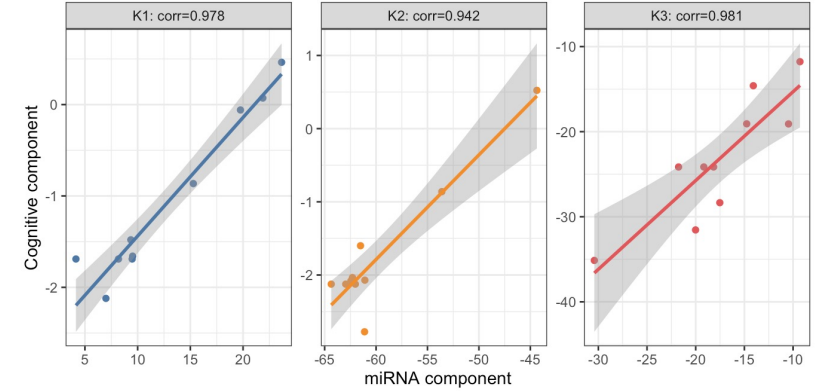
Sparse CCA: miRNA vs Cognitive (TP2 IRR)



Linear combination

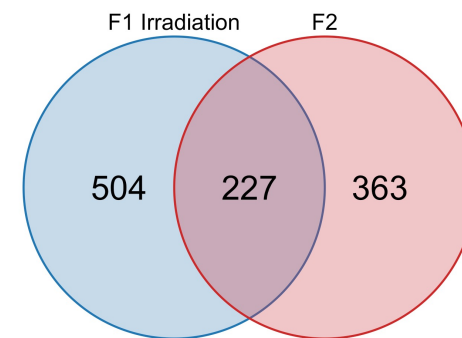
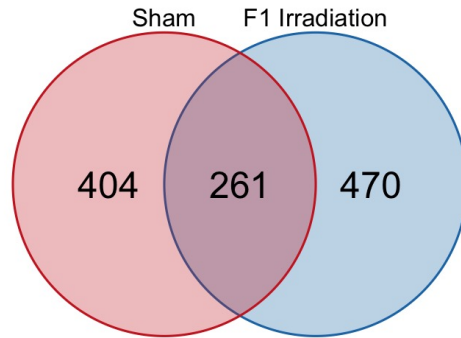
- K1: $-0.901 \cdot \text{tone} + 0.042 \cdot \text{preference_obj_2} + 0.431 \cdot \text{bin_2_preference_obj_2}$
- K2: $0.037 \cdot \text{train_isi4} + 0.44 \cdot \text{train_isi3} + 0.897 \cdot \text{train_tone5}$
- K3: $0.522 \cdot \text{context_minute1} + 0.853 \cdot \text{train_tone4}$

Sparse CCA: miRNA vs Cognitive (TP2 F2)



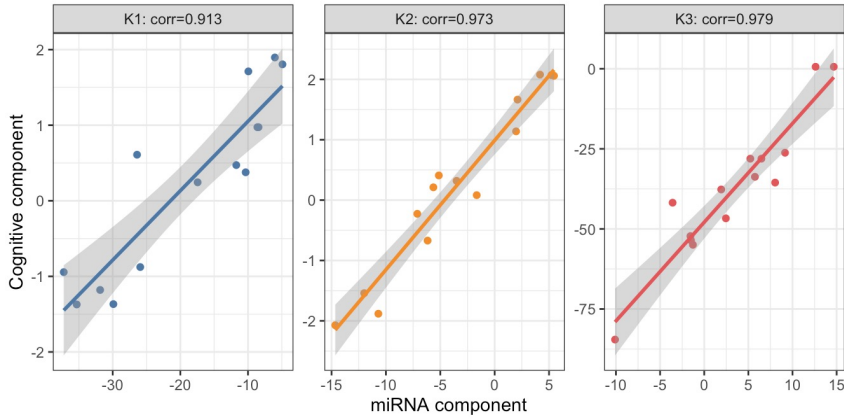
Linear combination

- K1: $-0.938 \cdot \text{train_isi3} + -0.329 \cdot \text{train_isi2} + -0.108 \cdot \text{train_tone4}$
- K2: $-0.853 \cdot \text{context_total} + -0.522 \cdot \text{context_minute5}$
- K3: $-0.929 \cdot \text{train_tone5} + -0.361 \cdot \text{train_isi4} + -0.085 \cdot \text{train_tone4}$

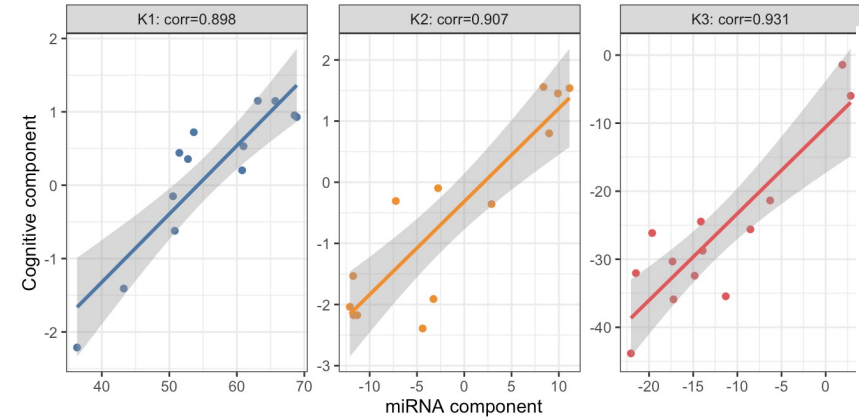


Suppl Fig 4 - Cognitive vs miRNA – TP3

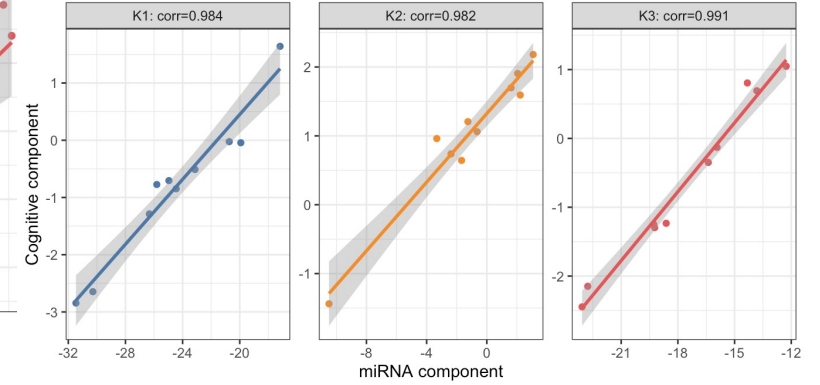
Sparse CCA: miRNA vs Cognitive (TP3 SHAM)



Sparse CCA: miRNA vs Cognitive (TP3 IRR)



Sparse CCA: miRNA vs Cognitive (TP3 F2)



Linear combination

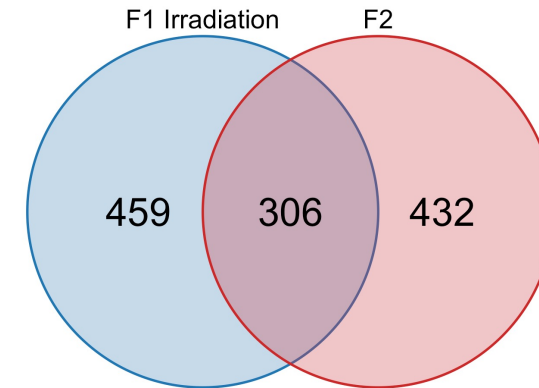
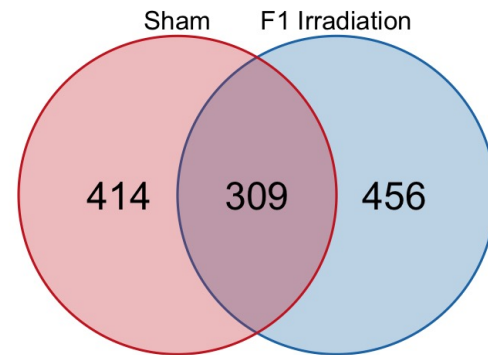
- K1: $-0.229 \cdot \text{context_minute5} + 0.191 \cdot \text{time_with_objects} + 0.954 \cdot \text{bin_1_preference_obj_2}$
- K2: $-0.867 \cdot \text{train_isi2} + -0.498 \cdot \text{train_tone3} + -0.01 \cdot \text{train_isi3}$
- K3: $-0.853 \cdot \text{preference_obj_2} + -0.522 \cdot \text{bin_3_preference_obj_2}$

Linear combination

- K1: $-0.482 \cdot \text{train_tone2} + -0.017 \cdot \text{train_isi2} + 0.876 \cdot \text{bin_2_preference_obj_2}$
- K2: $0.016 \cdot \text{context_minute5} + 0.484 \cdot \text{context_total} + 0.875 \cdot \text{context_minute4}$
- K3: $-0.853 \cdot \text{bin_3_preference_obj_2} + -0.522 \cdot \text{preference_obj_2}$

Linear combination

- K1: $-0.853 \cdot \text{train_tone4} + -0.522 \cdot \text{train_tone3}$
- K2: $0.522 \cdot \text{context_minute4} + 0.853 \cdot \text{context_minute2}$
- K3: $\text{n_2_preference_obj_2}$



Suppl Fig 5 - Cognitive vs miRNA – TP1

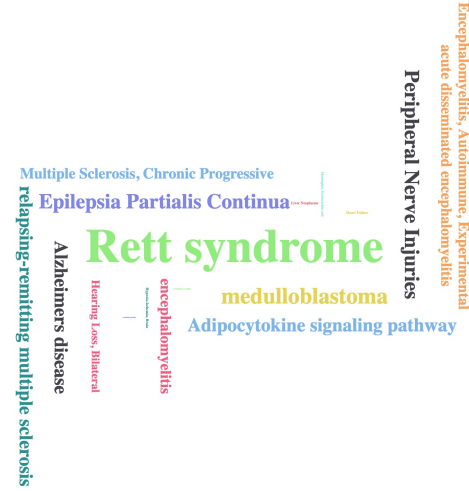
F1 Sham

Wordcloud of categories (top 100 by p-value)



F1 IRR

Wordcloud of categories (top 100 by p-value)



F2 IRR

Wordcloud of categories (top 100 by p-value)



Suppl Fig 6 Cognitive vs miRNA – TP2

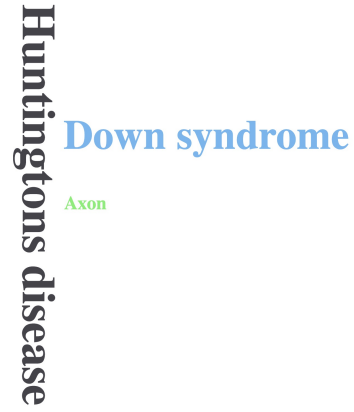
F1 Sham

Wordcloud of categories (top 100 by p-value)



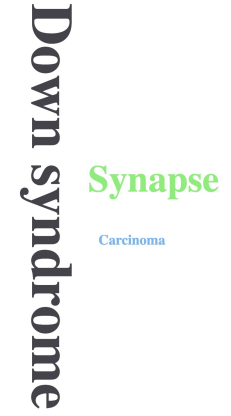
F1 IRR

Wordcloud of categories (top 100 by p-value)



F2 IRR

Wordcloud of categories (top 100 by p-value)



Suppl Fig 7 - Cognitive vs miRNA – TP3

F1 Sham

F1 IRR

F2 IRR

Wordcloud of categories (top 100 by p-value)

Wordcloud of categories (top 100 by p-value)

(None)

Meis2
GAGGUAG

positive regulation of cysteine-type endopeptidase activity involved in apoptotic process GO0043288

DNA-binding transcription activator activity, RNA polymerase II-specific GO0001228

negative regulation of cell growth GO0030308

relapsing-remitting multiple sclerosis
positive regulation of cell differentiation GO0045597

Peripheral Nerve Injuries
Seizures
encephalomyelitis
medulloblastoma
Alzheimers disease
Rett syndrome

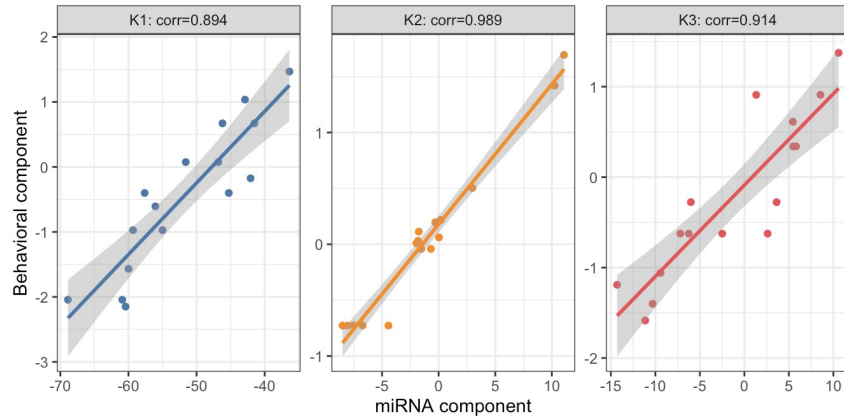
negative regulation of fat cell differentiation GO0045599

Multiple Sclerosis, Chronic, Progressive
Hexahydro-1,3,5-triazine-1,3,5-triazine RDX
acute disseminated encephalomyelitis

sensorineural hearing loss
outflow tract morphogenesis GO0003151
neuroimmune, Experimental
neuro-muscular process controlling balance GO0050885
ventricular septum morphogenesis GO0060412
integral component of postsynaptic density membrane GO0099061
regulation of peptidyl-tyrosine phosphorylation GO0059730
negative regulation of mitotic cell cycle GO0045930

Suppl Fig 8 – Behavioral vs miRNA – TP2

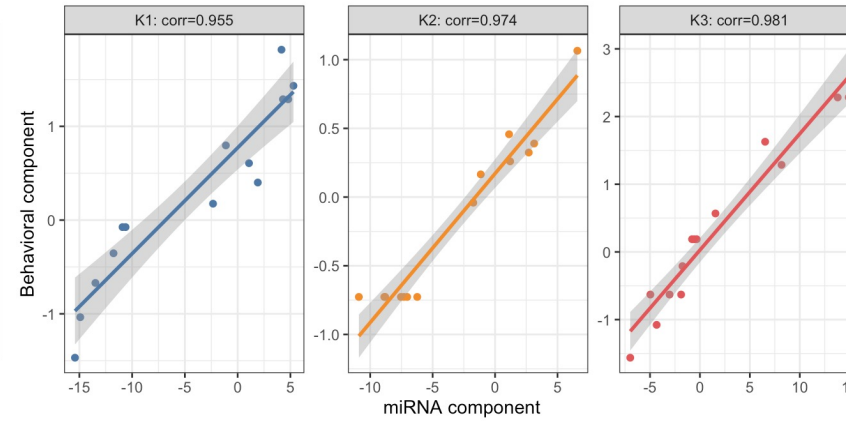
Sparse CCA: miRNA vs Behavioral (TP2 SHAM)



Linear combination

- K1: $-1 \cdot \text{nod2_fecal}$
- K2: $1 \cdot \text{fc_cued_percent_time_frz_baseline}$
- K3: $-1 \cdot \text{nod1_fecal}$

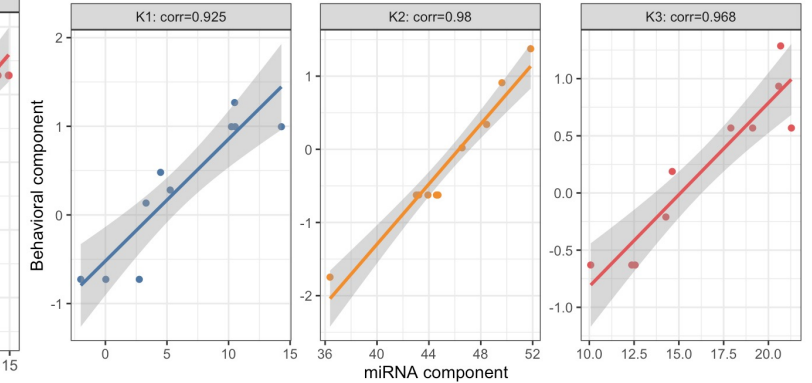
Sparse CCA: miRNA vs Behavioral (TP2 IRR)



Linear combination

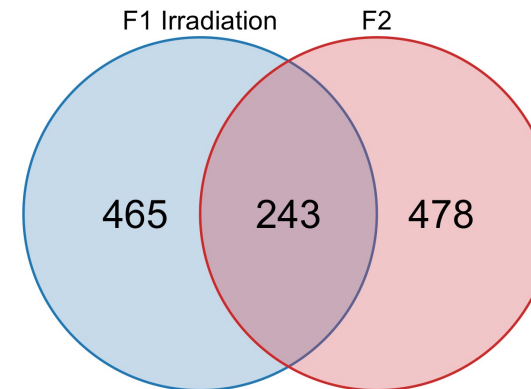
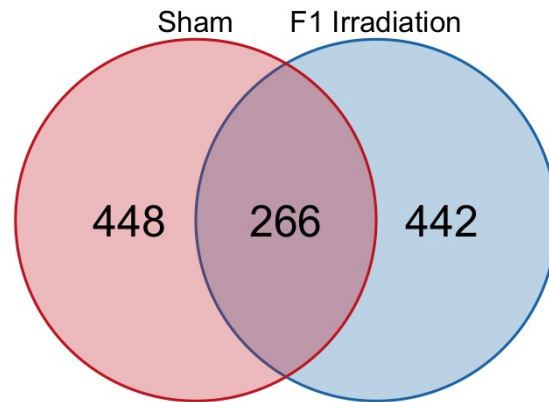
- K1: $1 \cdot \text{nod2_fecal}$
- K2: $1 \cdot \text{fc_cued_percent_time_frz_baseline}$
- K3: $1 \cdot \text{ofd1_fecal}$

Sparse CCA: miRNA vs Behavioral (TP2 F2)



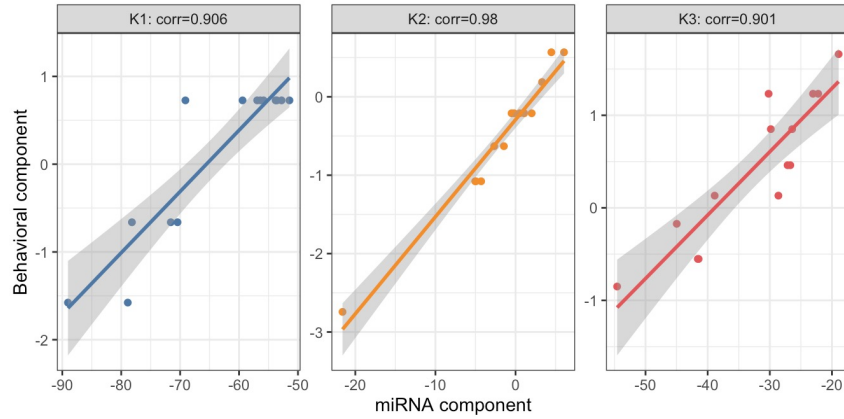
Linear combination

- K1: $1 \cdot \text{fc_cued_percent_time_frz_baseline}$
- K2: $-1 \cdot \text{nod1_fecal}$
- K3: $1 \cdot \text{ofd1_fecal}$



Suppl Fig 9 - Behavioral vs miRNA – TP3

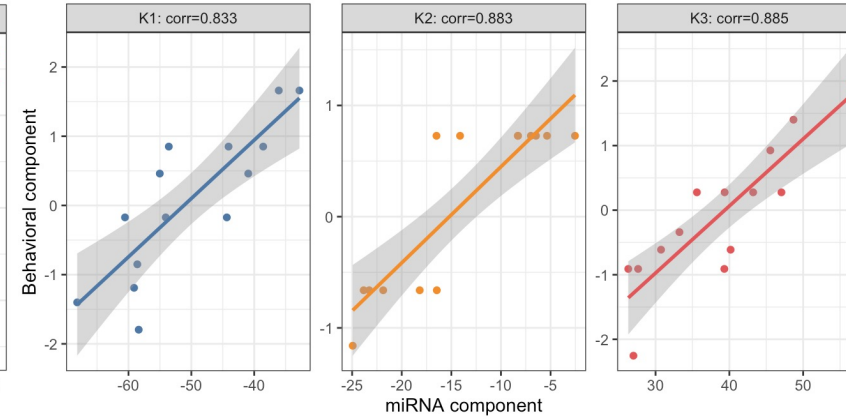
Sparse CCA: miRNA vs Behavioral (TP3 SHAM)



Linear combination

- K1: $-1 \cdot \text{fc_cued_percent_time_frz_baseline}$
- K2: $1 \cdot \text{ofd1_fecal}$
- K3: $-1 \cdot \text{ofd2_fecal}$

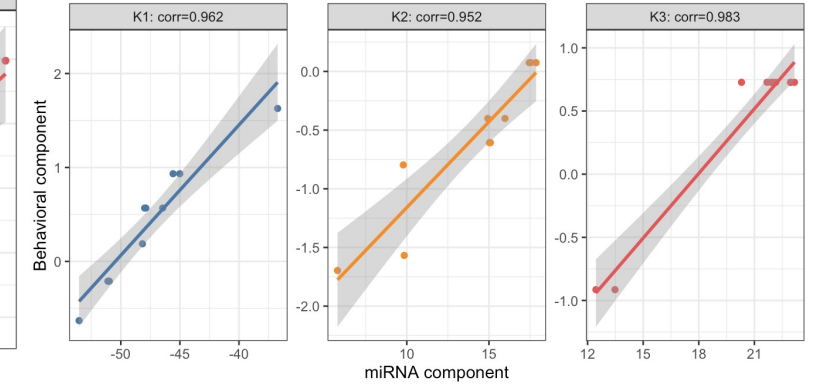
Sparse CCA: miRNA vs Behavioral (TP3 IRR)



Linear combination

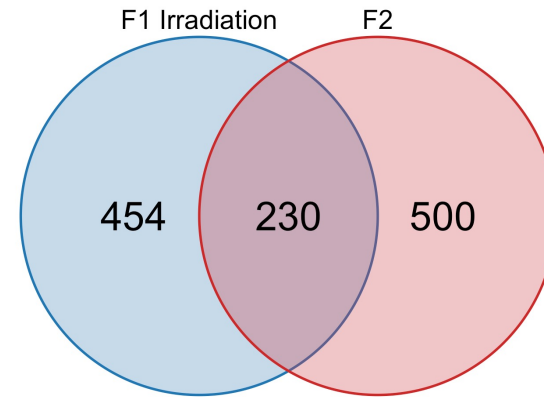
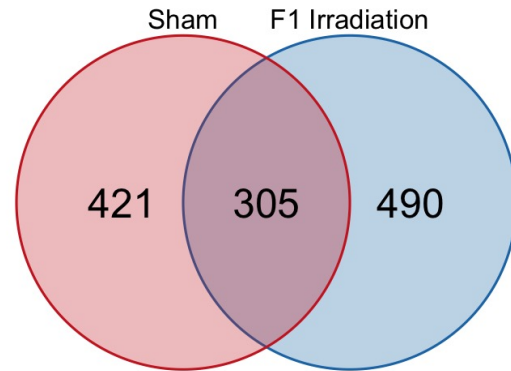
- K1: $-1 \cdot \text{ofd2_fecal}$
- K2: $-1 \cdot \text{fc_cued_percent_time_frz_baseline}$
- K3: $1 \cdot \text{nod1_fecal}$

Sparse CCA: miRNA vs Behavioral (TP3 F2)



Linear combination

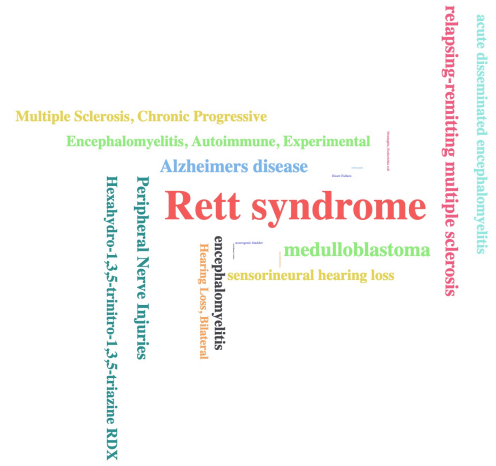
- K1: $1 \cdot \text{ofd1_fecal}$
- K2: $-1 \cdot \text{nod2_fecal}$
- K3: $-1 \cdot \text{fc_cued_percent_time_frz_baseline}$



Suppl Fig 10 Behavioral vs miRNA – TP1

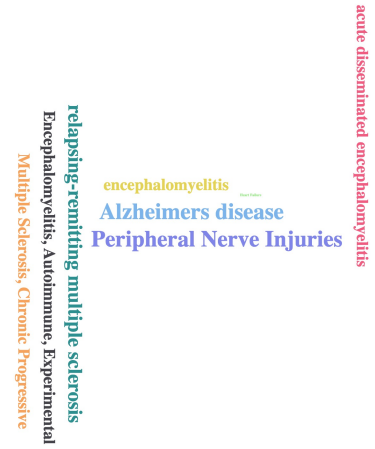
F1 Sham

Wordcloud of categories (top 100 by p-value)



F1 IRR

Wordcloud of categories (top 100 by p-value)



F2 IRR

Wordcloud of categories (top 100 by p-value)

Chromosome 2

Suppl Fig 11 – Behavioral vs miRNA – TP2

F1 Sham

F1 IRR

F2 IRR

(None)

Wordcloud of categories (top 100 by p-value)

Rheumatoid arthritis
Chromosome 12
Citrate cycle TCA cycle
AGE-RAGE signaling pathway in diabetic complications

Wordcloud of categories (top 100 by p-value)

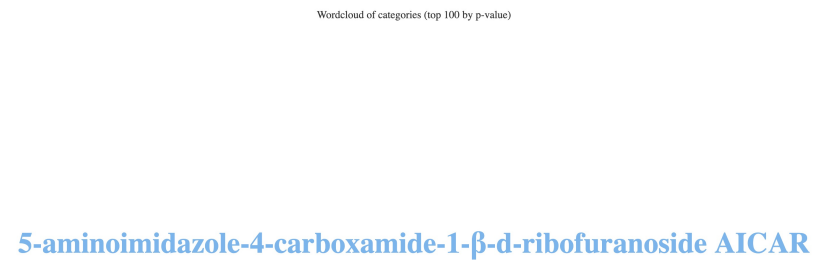
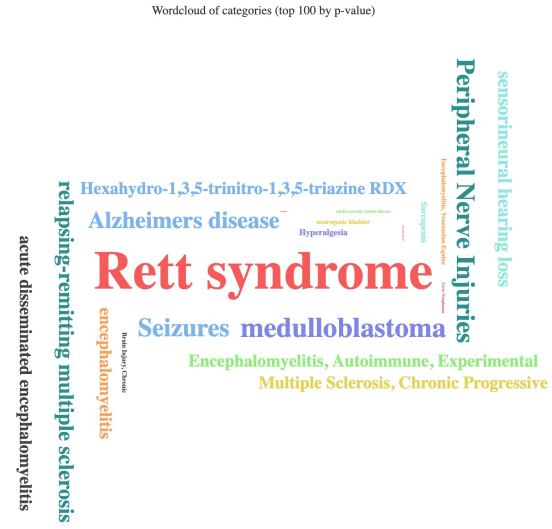
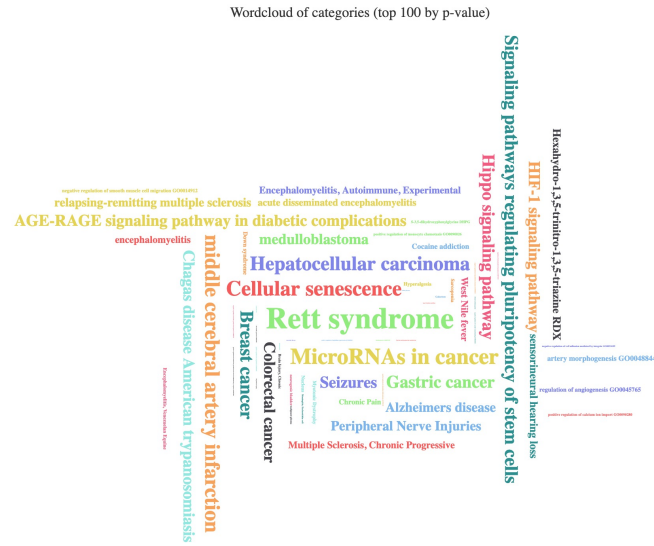
Tamoxifen

Suppl Fig 12 - Behavioral vs miRNA – TP3

F1 Sham

F1 IRR

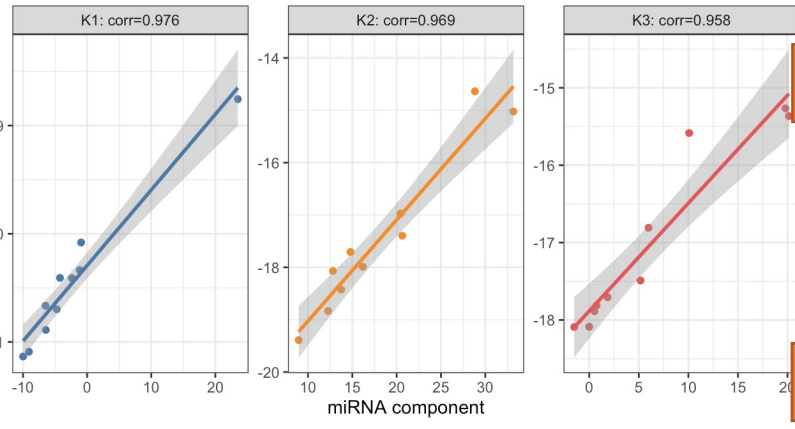
F2 IRR



Suppl Fig 13 Lipidomics vs miRNA – TP1 miRNA enrichment

LIPIDS

Sparse CCA: miRNA vs Lipidomics (TP1 IRR)



Linear combination
 K1: $-1 \times 290.087_A$
 K2: $-1 \times 265.147_H$
 K3: $-1 \times 265.147_A$

290.087 A = fatty acid which can be of multiple carbon length and/or number of double bonds

265.147 H = Micropine (sphingoid base analogue)

265.147 A = Micropine (sphingoid base analogue)

K1
K2
K3

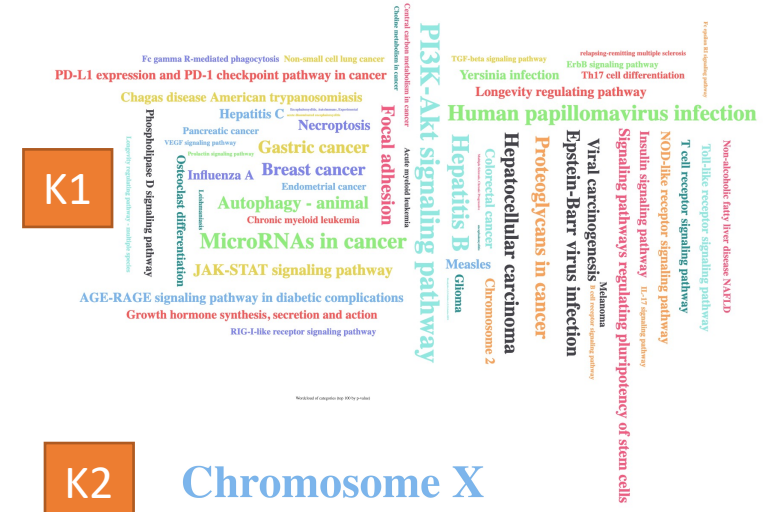
877.291 A = no identification,
 564.533 A = three biological possibilities: a large 34-35 carbon oxidized unsaturated fatty acid, an oxidized diacylglycerol or a branched fatty acid esters of hydroxy fatty acids (FAHFA 18:1 18:0, Delta of 0.0212) are endogenous lipids found in adipose tissue and serum that correlate with insulin sensitivity and are reduced in insulin-resistant humans,
 546.523 A = Most-likely a large 34-35 carbon oxidized unsaturated fatty acid or an oxidized diacylglycerol

K1
K2
K3

1544.847 A = no ID, 290.087 H = fatty acid which can be of multiple carbon length and/or number of double bonds, 493.164 A = no ID

451.305 A = matched mass 451.2699, Delta 0.0351, lysophosphatidylethanolamine (16:0) or Lysophosphatidylcholine (O-14:1) delta 0.0013. LPC is a signal of mitochondrial stress. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2 , 265.147A = Micropine (sphingoid base analogue) , 1281.790 A = No ID

Linear combination
 K1: $-0.72 \times 877.291_A + -0.663 \times 564.533_A + -0.204 \times 546.523_A$
 K2: $-0.807 \times 1544.847_A + -0.539 \times 290.087_H + -0.241 \times 493.165_A$
 K3: $-0.458 \times 451.305_A + -0.289 \times 265.147_A + 0.841 \times 1281.79_A$



K1
K2
K3

Chromosome X

K3 (None)

K1

(None)

K2

Kidney

K3

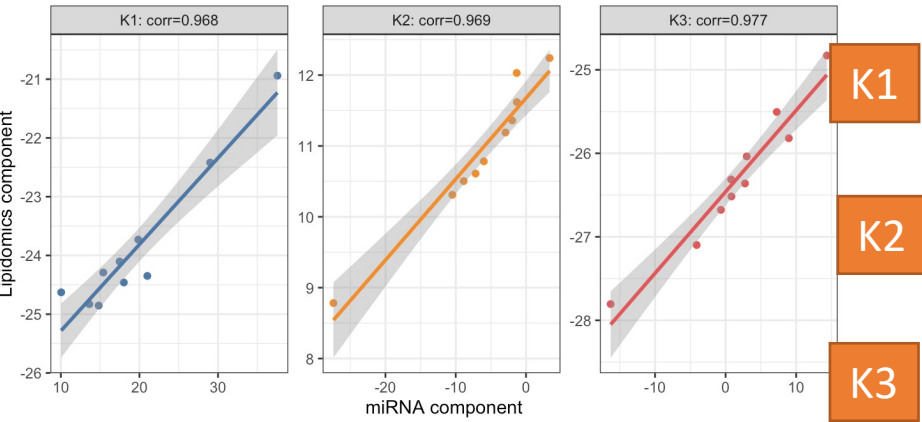
Chromosome 10
Chromosome 8
Chromosome 1

Suppl Fig 14 Lipidomics vs miRNA – TP2

miRNA enrichment

LIPIDS

Sparse CCA: miRNA vs Lipidomics (TP2 IRR)



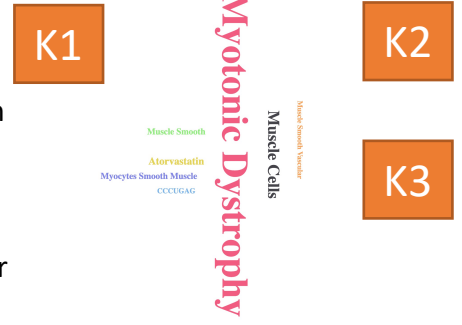
Linear combination

- K1: $-0.923 \times 290.086_A + -0.385 \times 888.642_A$
- K2: $-0.331 \times 581.183_A + 0.034 \times 682.283_A + 0.943 \times 283.264_A$
- K3: $-0.923 \times 710.314_A + -0.385 \times 886.553_A$

290.086 A = fatty acid which can be of multiple carbon length and/or number of double bonds, 888.642 A = Isobars for unsaturated Phosphatidylinositol with 38 carbons in its tail or an unsaturated triacylglycerol (TG) with 55 carbons composing its three fatty acid tails.

581.183 A = no ID, 682.283 A = no ID, 283.264 A = n-acylethanolamine (15:1), (induction of inflammation, precursor of eicosanoids or Delta 0.0235, sphingolipid (m18:1), sphingolipid base analog

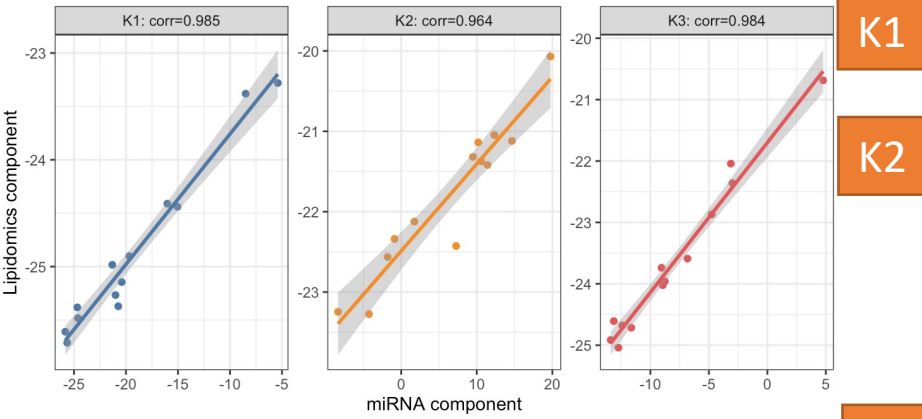
710.314 A = isobars corresponding to either an oxidized Phosphatidylglycerol or oxidized Phosphatidylinositol, 886.553 A = Most hits are for an unsaturated Phosphatidylinositol with 38 carbons in its tail



Glrx2
(None)

Diabetes Mellitus
Insulin Resistance

Sparse CCA: miRNA vs Lipidomics (TP2 SHAM)



Linear combination

- K1: $-0.961 \times 581.183_A + -0.276 \times 1572.899_A$
- K2: $-0.961 \times 581.309_A + -0.276 \times 1253.773_A$
- K3: $-0.961 \times 1544.867_A + -0.276 \times 888.641_A$

581.183 A = no ID, 1572.899 A = several possible isomers of a sulfated globoside

581.309 A = either lysophosphatidylethanolamine (26:6) delta 0.0391 or Lysophosphatidylserine (22:0) delta 0.0603. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2. The lysophospholipids lead to increase eicosanoid production (leukotrienes and prostaglandins), 1253.773 A = no ID



1544.867 A = possibly Ganglioside SB1a (t18:0/26:0), matched mass 1544.83069, another sulfated globoside.

888.641 A = Isobars for unsaturated Phosphatidylinositol with 38 carbons in its tail or an unsaturated triacylglycerol (TG) with 55 carbons composing its three fatty acid tails.

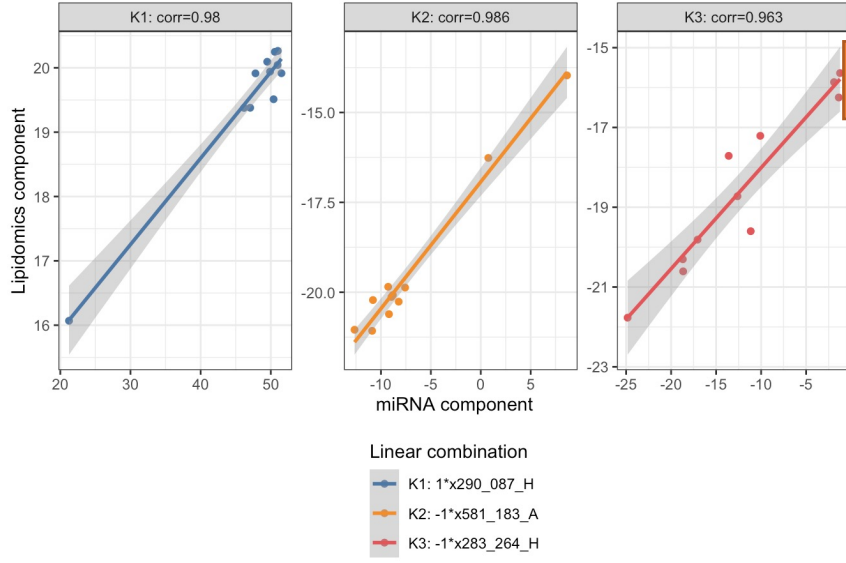
Diabetes Mellitus
Insulin Resistance
Rheumatoid arthritis
Kidney
Muscles

Suppl Fig 15 Lipidomics vs miRNA – TP3

miRNA enrichment

LIPIDS

Sparse CCA: miRNA vs Lipidomics (TP3 IRR)

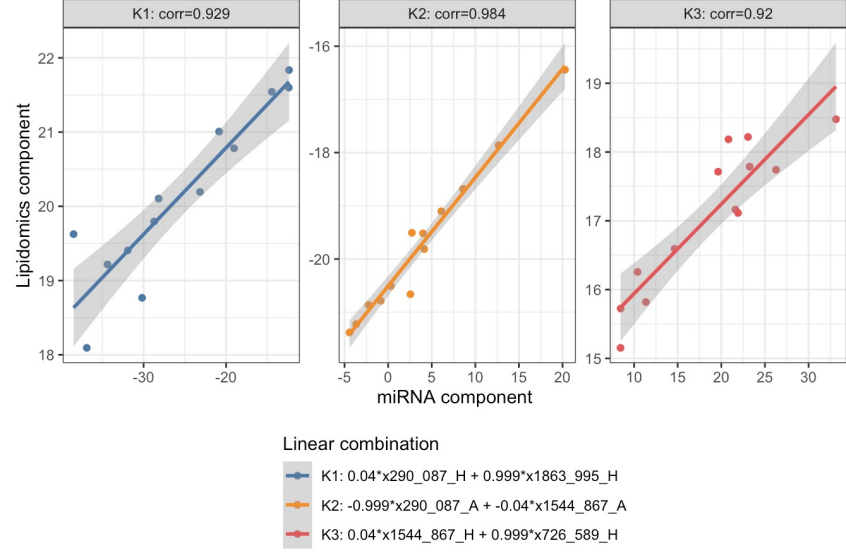


K1 290.087 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

K2 581.183 A = no ID

K3 283.264 H = n-acylethanolamine (15:1), (induction of inflammation, precursor of eicosanoids or Delta 0.0235, sphingolipid (m18:1), sphingolipid base analog

Sparse CCA: miRNA vs Lipidomics (TP3 SHAM)



K1 290.087 H = fatty acid which can be of multiple carbon length and/or number of double bonds. 1863.995 H = no ID

K2 290.087 H = fatty acid which can be of multiple carbon length and/or number of double bonds 1544.867 A = possibly Ganglioside SB1a (t18:0/26:0), matched mass1544.83069, another sulfated globoside.

K3 1544.867 A = possibly Ganglioside SB1a (t18:0/26:0), matched mass1544.83069, another sulfated globoside. 726.589 H = isobars corresponding to either sphingomyelin (d18:2/18:1, delta 0.0214) which makes up the myelin sheath around neurons, diacylglycerol or phosphatidic acid

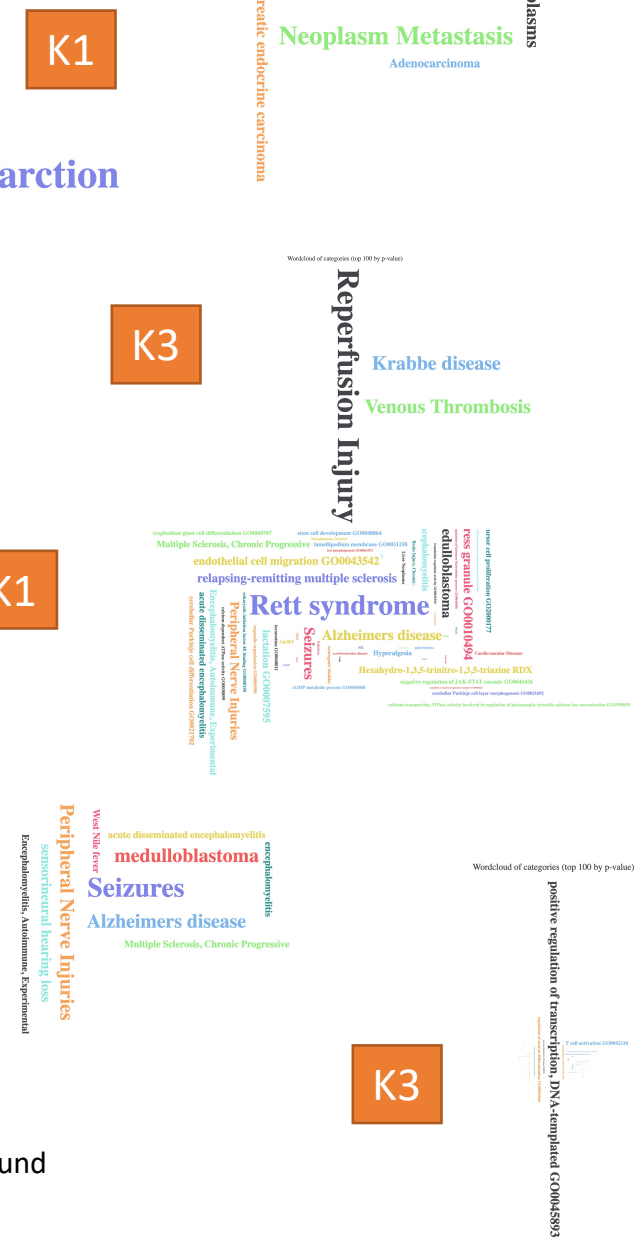
middle cerebral artery infarction

Workload of categories (top 100 by p-value)

Workload of categories (top 100 by p-value)

Workload of categories (top 100 by p-value)

Workload of categories (top 100 by p-value)



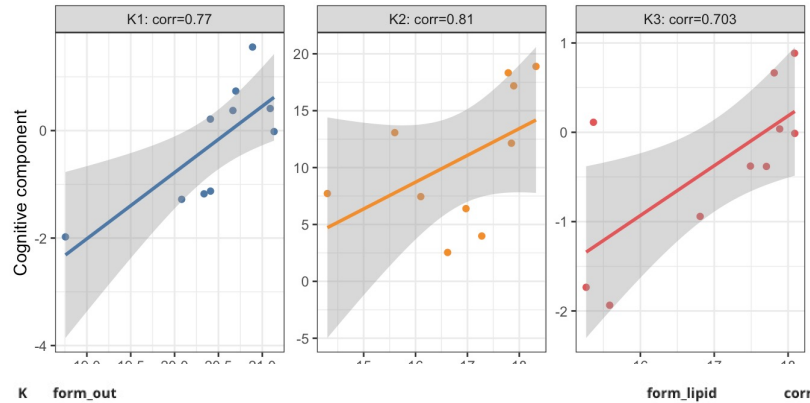
Lung Neoplasms

positive regulation of transcription, DNA-templated

Suppl Fig 16 Cognitive vs lipidomics – TP1

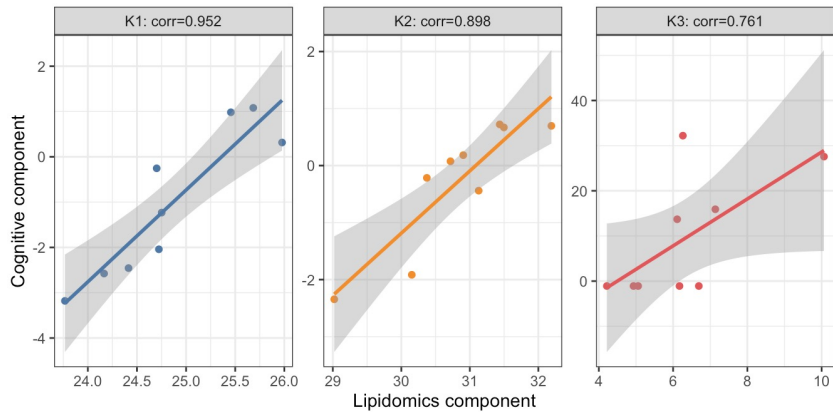
LIPIDS

Sparse CCA: Lipidomics vs Cognitive (TP1 IRR)



K	form_out	form_lipid	corr
V1	K1: $-0.959bin_2_preference_obj_2 + -0.243tone + -0.139context_minute4 + -0.033context_minute5$	1 x290_087_A	0.7697754
V2	K2: $-0.972train_tone1 + 0.054train_isi3 + 0.068train_tone5 + 0.077train_tone4 + 0.204*train_isi4$	1 x290_086_H	0.8096856
V3	K3: $-0.974bin_1_preference_obj_2 + -0.076train_tone2 + -0.009train_tone5 + 0.021context_minute1 + 0.122context_minute4 + 0.173train_tone1$	1 x265_147_A	0.7025606

Sparse CCA: Lipidomics vs Cognitive (TP1 SHAM)



K	form_out	form_lipid	corr
V1	K1: $-0.959bin_2_preference_obj_2 + -0.243tone + -0.139context_minute4 + -0.033context_minute5$	1 x290_087_A	0.7697754
V2	K2: $-0.972train_tone1 + 0.054train_isi3 + 0.068train_tone5 + 0.077train_tone4 + 0.204*train_isi4$	1 x290_086_H	0.8096856
V3	K3: $-0.974bin_1_preference_obj_2 + -0.076train_tone2 + -0.009train_tone5 + 0.021context_minute1 + 0.122context_minute4 + 0.173train_tone1$	1 x265_147_A	0.7025606

K1

290.087 A = a fatty acid which can be of multiple carbon length and/or number of double bonds

K2

290.086 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

K3

265.147 A = Micropine (sphingoid base analogue)

K1

451.305 A = lysophosphatidylethanolamine (16:0) or Lysophosphatidylcholine (O-14:1) delta 0.0013. LPC is a signal of mitochondrial stress. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2

1281.79 A = no ID

1544.847 A = possibly Ganglioside SB1a (t18:0/26:0)

290.087 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

K2

1544.847 A = possibly Ganglioside SB1a (t18:0/26:0)

419.255 A = N-Arachidonoyl Taurine (NAT (18:0)), an arachidonoyl aminoacid, N-Arachidonoyl Taurine is increased after the administration of cannabinoid agonists

886.546 A = Most hits are for an unsaturated Phosphatidylinositol with 38 carbons in its tail

K3

493.165 A = no ID, 581.180 A = no ID

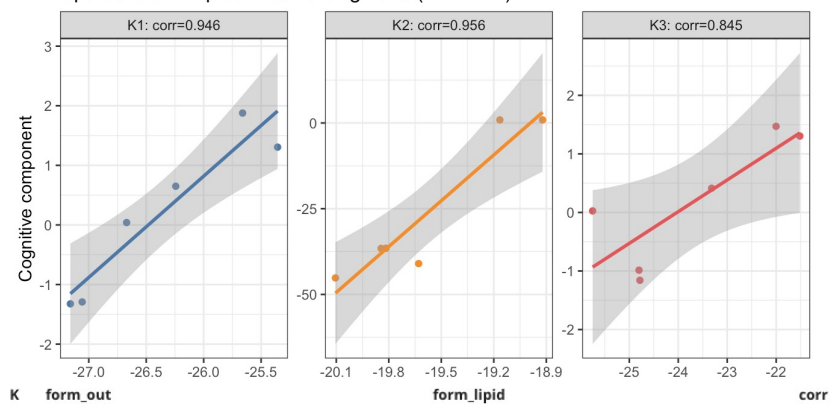
708.574 A = Several isobaric possibilities. The largest number of hits corresponds to a Phosphatidylglycerol (PG) of various carbon chain lengths totaling 31 carbons, next would be a diacylglycerol (20:0/22:0 or 21:0/21:0)

1544.849 A = possibly Ganglioside SB1a (t18:0/26:0)

Suppl Fig 17 Cognitive vs lipidomics – TP2

LIPIDS

Sparse CCA: Lipidomics vs Cognitive (TP2 IRR)



K	form_out	form_lipid	corr
V1	K1: 0.164context_minute5 + 0.259context_minute3 + 0.952*context_total	-0.385 x291_091_A + -0.923 x581_184_A	0.9456560
V2	K2: -0.853bin_2_preference_obj_2 + -0.522preference_obj_2	-0.971 x290_088_A + -0.153 x581_183_A + 0.184 x886_553_A	0.9557277
V3	K3: -0.227bin_3_preference_obj_2 + 0.193train_tone3 + 0.955*train_isi2	-0.385 x1544_867_A + -0.923 x835_283_A	0.8446590

K1

291.091 A = no ID
581.184 A = no ID

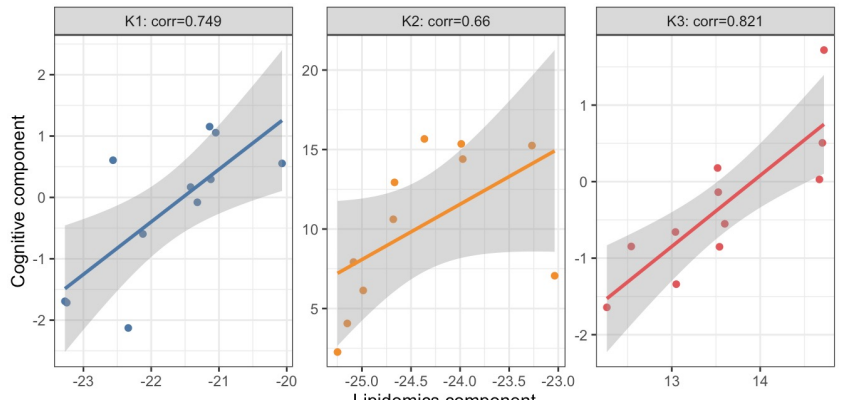
K2

290.088 H = a fatty acid which can be of multiple carbon length and/or number of double bonds
581.183 A = no ID

K3

1544.867 A = possibly Ganglioside SB1a (t18:0/26:0)
835.283 A = CDP-1-hexanoyl-2-(6Z,9Z,12Zoctadecatrienoyl)-sn-glycerol CP1 (cytodine diphosphate lipid), I cannot find any biological activity

Sparse CCA: Lipidomics vs Cognitive (TP2 SHAM)



K	form_out	form_lipid	corr
V1	K1: 0.067context_minute2 + 0.39context_minute3 + 0.919*context_total	-0.276 x1253_773_A + -0.961 x581_309_A	0.7493977
V2	K2: 0.191train_isi4 + 0.23context_minute1 + 0.954*context_minute2	-0.276 x291_091_A + -0.961 x581_183_A	0.6596294
V3	K3: 0.094context_minute4 + 0.146tone + 0.165context_minute5 + 0.971train_tone3	0.961 x290_087_A + -0.276 x419_256_A	0.8207900

K1

1253.773 A = no ID
581.309 A = either lysophosphatidylethanolamine (26:6) delta 0.0391 or Lysophosphatidylserine (22:0) delta 0.0603. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2. The lysophospholipids lead to increase eicosanoid production (leukotrienes and prostaglandins)

K2

291.091 A = no ID
581.183 A = no ID

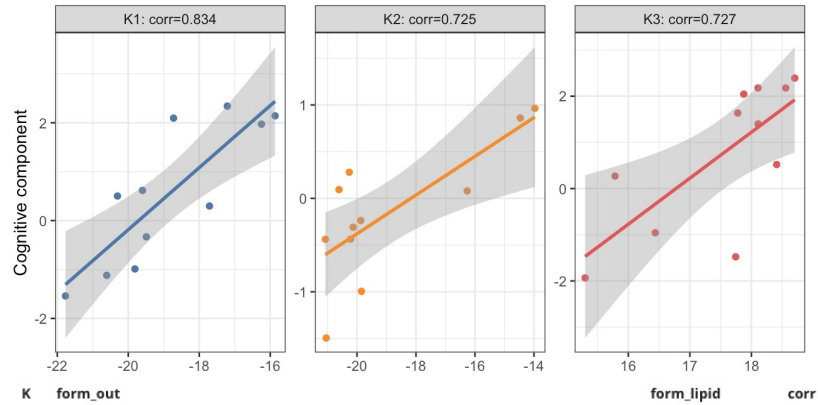
K3

290.087 A = a fatty acid which can be of multiple carbon length and/or number of double bonds
419.256 A = either an acyl carnitine (18:4) matched mass 419.3036, delta 0.0486 or an acyl taurine (20:0) matched mass of 419.3069, delta 0.0519

Suppl Fig 18 Cognitive vs lipidomics – TP3

LIPIDS

Sparse CCA: Lipidomics vs Cognitive (TP3 IRR)



K	form_out	form_lipid	corr
V1	K1: $-0.896\text{context_minute5} + -0.442\text{context_total} + -0.036\text{context_minute3}$	-1 x283_264_H	0.8338296
V2	K2: $-0.081\text{train_tone3} + -0.021\text{train_isi1} + 0.035\text{bin_1_preference_obj_2} + 0.283\text{bin_2_preference_obj_2} + 0.955\text{time_with_objects}$	-1 x581_183_A	0.7248504
V3	K3: $-0.879\text{context_minute1} + -0.476\text{context_total} + -0.019\text{context_minute4}$	1 x888_641_H	0.7268940

K1

283.264 H = Delta0.0129, n-acylethanolamine (15:1), (induction of inflammation, precursor of eicosanoids or Delta 0.0235, sphingolipid (m18:1), sphingolipid base analog

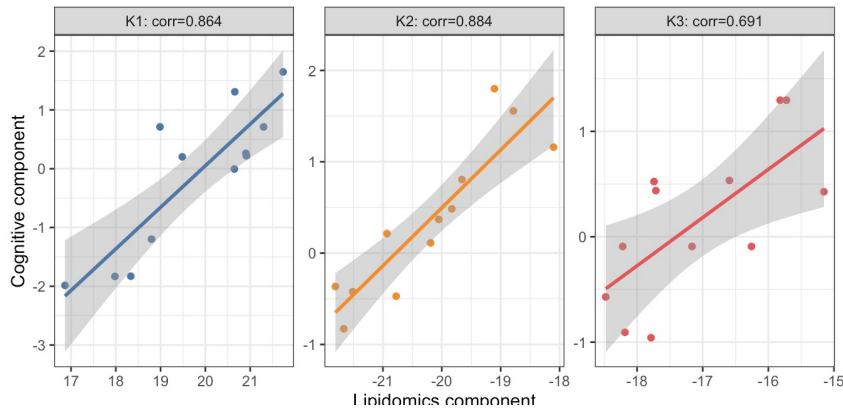
K2

581.183 A = no ID

K3

888.641 H = Isobars for unsaturated Phosphatidylinositol with 38 carbons in its tail or an unsaturated triacylglycerol (TG) with 55 carbons composing its three fatty acid tails.

Sparse CCA: Lipidomics vs Cognitive (TP3 SHAM)



K	form_out	form_lipid	corr
V1	K1: $0.156\text{context_minute2} + 0.268\text{train_isi3} + 0.951\text{context_minute1}$	0.04 x290_087_A + 0.999 x581_183_A	0.8644827
V2	K2: $-0.853\text{train_isi1} + -0.522\text{train_isi2}$	-0.04 x1604_89_H + -0.999 x1863_995_H	0.8844297
V3	K3: $-0.853\text{train_tone1} + 0.522\text{bin_2_preference_obj_2}$	-0.04 x1544_867_H + -0.999 x726_589_H	0.6908343

K1

290.087 A = a fatty acid which can be of multiple carbon length and/or number of double bonds
581.183 A = no ID

K2

1604.89 H = several possible isomers of a sulfated globoside
1863.995 H = no ID

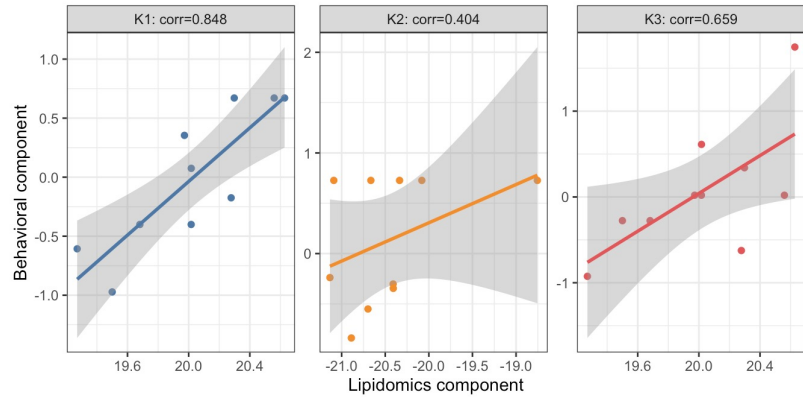
K3

1544.867 H = possibly Ganglioside SB1a (t18:0/26:0)
726.589 H = isobars corresponding to either sphingomyelin (d18:2/18:1, delta 0.0214) which makes up the myelin sheath around neurons, diacylglycerol or phosphatidic acid

Suppl Fig 19 Behavioral vs lipidomics – TP1

LIPIDS

Sparse CCA: Lipidomics vs Behavioral (TP1 IRR)



K	form_out	form_lipid	corr
V1	K1: -1*nod2_fecal	1 x290_087_H	0.8482406
V2	K2: -1*fc_cued_percent_time_frz_baseline	-1 x290_087_A	0.4035642
V3	K3: -1*nod1_fecal	1 x290_087_H	0.6593617

K1

290.087 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

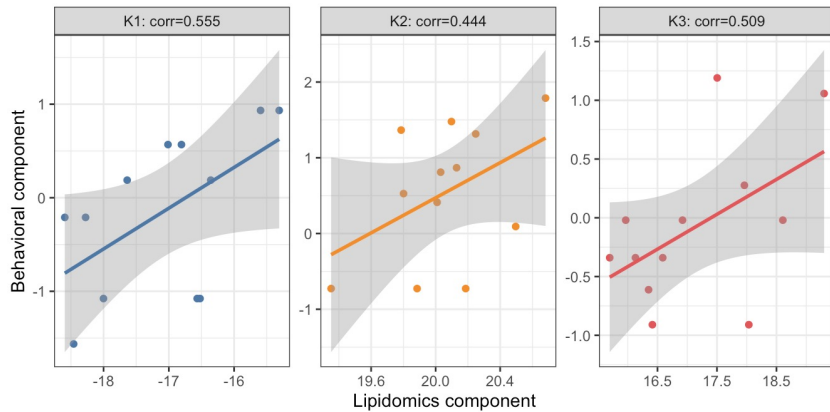
K2

290.087 A = a fatty acid which can be of multiple carbon length and/or number of double bonds

K3

290.087 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

Sparse CCA: Lipidomics vs Behavioral (TP1 SHAM)



K	form_out	form_lipid	corr
V1	K1: 1*ofd1_fecal	-1 x290_086_H	0.5554043
V2	K2: 1*fc_cued_percent_time_frz_baseline	1 x290_087_H	0.4440140
V3	K3: 1*nod1_fecal	1 x265_147_A	0.5085519

K1

290.086 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

K2

290.087 H = a fatty acid which can be of multiple carbon length and/or number of double bonds

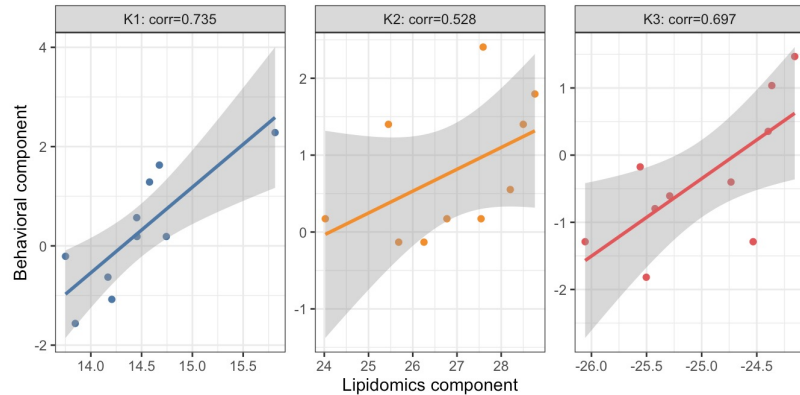
K3

265.147 A = Delta0.0572, Micropine (sphingoid base analogue)

Suppl Fig 20 Behavioral vs lipidomics – TP2

LIPIDS

Sparse CCA: Lipidomics vs Behavioral (TP2 IRR)



K	form_out	form_lipid	corr
V1	K1: 1*ofd1_fecal	-0.152 x1544_867_A + 0.971 x1863_996_A + -0.185 x888_642_A	0.7354057
V2	K2: 1*ofd2_fecal	0.385 x1544_87_A + 0.923 x2127_061_A	0.5280724
V3	K3: -1*nod2_fecal	0.0159 x581_184_A + -0.933 x682_283_A + -0.358 x710_314_A	0.6965808

K1

1544.867 A = possibly Ganglioside SB1a (t18:0/26:0)
1863.996 A = no ID

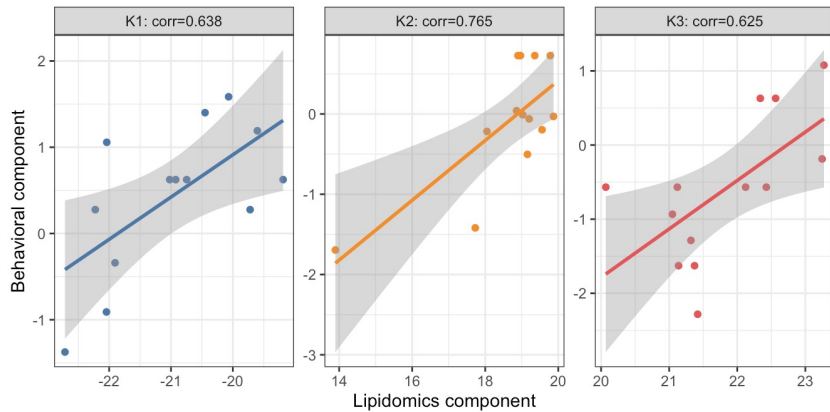
K2

1544.870 A = possibly Ganglioside SB1a (t18:0/26:0)
2127.061 A = Matched mass, 2127.16016 Ganglioside GD1a(NeuGc/NeuGc) (t18:0/36:6(18Z,21Z,24Z,27Z,30Z,33Z), brain ganglioside and it shows the correct mouse sialylation of NeuGc.

K3

581.184 A = no ID
682.283 A = no ID
710.314 A = isobars corresponding to either an oxidized Phosphatidylglycerol or oxidized Phosphatidylinositol

Sparse CCA: Lipidomics vs Behavioral (TP2 SHAM)



K	form_out	form_lipid	corr
V1	K1: 1*nod1_fecal	-0.978 x1253_773_A + -0.0592 x1544_867_A + -0.2 x581_309_A	0.6383476
V2	K2: -1*fc_cued_percent_time_frz_baseline	-0.157 x888_641_A + 0.0975 x1544_867_H + 0.983 x581_183_H	0.7651704
V3	K3: -1*ofd1_fecal	0.276 x1253_773_A + 0.961 x581_309_A	0.6251693

K1

1253.773 A = no ID
1544.867 A = possibly Ganglioside SB1a (t18:0/26:0)
581.309 A = either lysophosphatidylethanolamine (26:6) delta 0.0391 or Lysophosphatidylserine (22:0) delta 0.0603. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2. The lysophospholipids lead to increase eicosanoid production (leukotrienes and prostaglandins)

K2

888.641 A = Isobars for unsaturated Phosphatidylinositol with 38 carbons in its tail or an unsaturated triacylglycerol (TG) with 55 carbons composing its three fatty acid tails.
1544.867 H = possibly Ganglioside SB1a (t18:0/26:0)
581.183 H = no ID

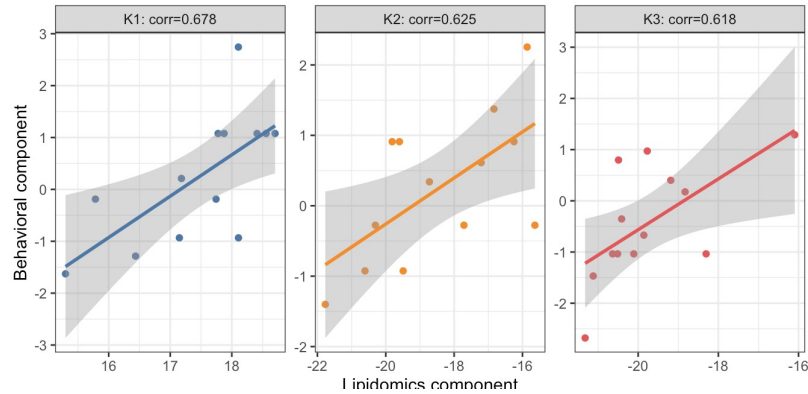
K3

1253.773 A = no ID
581.309 A = either lysophosphatidylethanolamine (26:6) delta 0.0391 or Lysophosphatidylserine (22:0) delta 0.0603. Both compounds are derived from their precursors by the enzymatic action of phospholipase A2. The lysophospholipids lead to increase eicosanoid production (leukotrienes and prostaglandins)

Suppl Fig 21 Behavioral vs lipidomics – TP3

LIPIDS

Sparse CCA: Lipidomics vs Behavioral (TP3 IRR)



K	form_out	form_lipid	corr
V1	K1: -1*ofd1_fecal	1 x888_641_H	0.6780741
V2	K2: -1*nod1_fecal	-1 x283_264_H	0.6246149
V3	K3: 1*nod2_fecal	-1 x581_183_H	0.6177454

K1

888.641 H = Isobars for unsaturated Phosphatidylinositol with 38 carbons in its tail or an unsaturated triacylglycerol (TG) with 55 carbons composing its three fatty acid tails.

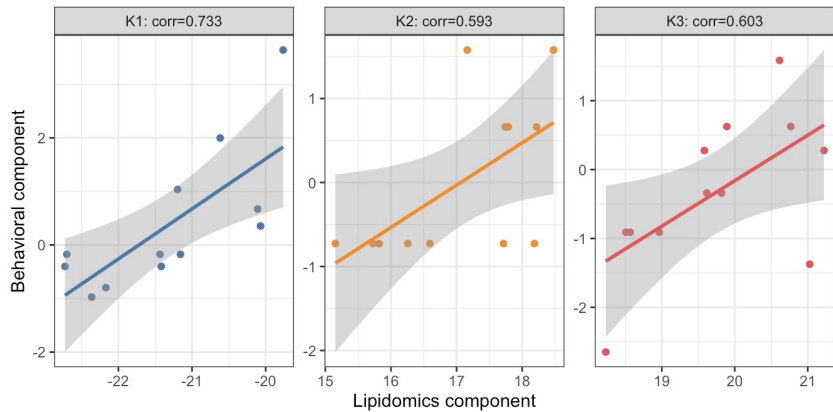
K2

283.264 H = Delta0.0129, n-acylethanolamine (15:1), (induction of inflammation, precursor of eicosanoids or Delta 0.0235, sphingolipid (m18:1), sphingolipid base analog

K3

581.183 H = no ID

Sparse CCA: Lipidomics vs Behavioral (TP3 SHAM)



K	form_out	form_lipid	corr
V1	K1: -1*nod2_fecal	-0.04 x1544_867_A + -0.999 x1835_964_A	0.7329386
V2	K2: 1*fc_cued_percent_time_frz_baseline	0.04 x1544_867_H + 0.999 x726_589_H	0.5932461
V3	K3: 1*nod1_fecal	0.999 x1835_964_A + -0.04 x1863_995_H	0.6027099

K1

1544.867 A = possibly Ganglioside SB1a (t18:0/26:0)
1835.964 A = no ID

K2

1544.867 H = possibly Ganglioside SB1a (t18:0/26:0)
726.589 H = isobars corresponding to either sphingomyelin (d18:2/18:1, delta 0.0214) which makes up the myelin sheath around neurons, diacylglycerol or phosphatidic acid

K3

1835.964 A = no ID
1863.995 H = no ID

Suppl. Fig 22

