

S2: Neuroimaging preprocessing and interpreting results

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fMRPrep

Results included in this manuscript come from preprocessing performed using *fMRIPrep* 23.0.2 (@fmrip1; @fmrip2; RRID:SCR_016216), which is based on *Nipype* 1.8.6 (@nipype1; @nipype2; RRID:SCR_002502).

Preprocessing of B0 inhomogeneity mappings

A total of 2 fieldmaps were found available within the input BIDS structure for this particular subject. A *B0*-nonuniformity map (or *fieldmap*) was estimated based on two (or more) echo-planar imaging (EPI) references with `topup` (@topup; FSL 6.0.5.1:57b01774).

Anatomical data preprocessing

A total of 2 T1-weighted (T1w) images were found within the input BIDS dataset. All of them were corrected for intensity non-uniformity (INU) with `N4BiasFieldCorrection` [@n4], distributed with ANTs 2.3.3 [@ants; RRID:SCR_004757]. The T1w-reference was then skull-stripped with a *Nipype* implementation of the `antsBrainExtraction.sh` workflow (from ANTs), using OASIS30ANTs as target template. Brain tissue segmentation of cerebrospinal fluid (CSF), white-matter (WM) and gray-matter (GM) was performed on the brain-extracted T1w using `fast` [FSL 6.0.5.1:57b01774; RRID:SCR_002823; @fsl_fast]. An anatomical T1w-reference map was computed after registration of 2 T1w images (after INU-correction) using `mri_robust_template` [FreeSurfer 7.3.2, @fs_template]. Brain surfaces were reconstructed using `recon-all` [FreeSurfer 7.3.2; RRID:SCR_001847, @fs_reconall], and the brain mask estimated previously was refined with a custom variation of the method to reconcile ANTs-derived and FreeSurfer-derived segmentations of the cortical gray-matter of Mindboggle [RRID:SCR_002438, @mindboggle]. Volume-based spatial normalization to two standard spaces (MNI152NLin6Asym, MNI152NLin2009cAsym) was performed through nonlinear registration with `antsRegistration` (ANTs 2.3.3), using brain-extracted versions of both T1w reference and the T1w template. The following templates were selected for spatial normalization and accessed with *TemplateFlow* [23.0.0, @templateflow]: *FSL's MNI ICBM 152 non-linear 6th Generation Asymmetric Average Brain Stereotaxic Registration Model* [@mni152nlin6asym; RRID:SCR_002823; TemplateFlow ID: MNI152NLin6Asym], *ICBM 152 Nonlinear Asymmetrical template version 2009c* [@mni152nlin2009casym; RRID:SCR_008796; TemplateFlow ID: MNI152NLin2009cAsym].

Functional data preprocessing

For each of the 2 BOLD runs found per subject (across all tasks and sessions), the following preprocessing was performed. First, a reference volume and its skull-stripped version were generated using a custom methodology of *fMRIPrep*. Head-motion parameters with respect to the BOLD reference (transformation matrices, and six corresponding rotation and translation parameters) are estimated before any spatiotemporal filtering using `mcflirt` [FSL 6.0.5.1:57b01774, @mcflirt]. The estimated *fieldmap* was then aligned with rigid-registration to the target EPI (echo-planar imaging) reference run. The field coefficients were mapped on to the reference EPI using the transform. BOLD runs were slice-time corrected to 1.18s (0.5 of slice acquisition range 0s-2.37s) using `3dTshift` from AFNI [@afni; RRID:SCR_005927]. The BOLD reference

was then co-registered to the T1w reference using **bbregister** (FreeSurfer) which implements boundary-based registration [bbr]. Co-registration was configured with six degrees of freedom. Several confounding time-series were calculated based on the *preprocessed BOLD*: framewise displacement (FD), DVARS and three region-wise global signals. FD was computed using two formulations following Power (absolute sum of relative motions, @power_fd_dvars) and Jenkinson (relative root mean square displacement between affines, @mcflirt). FD and DVARS are calculated for each functional run, both using their implementations in *Nipype* [following the definitions by @power_fd_dvars]. The three global signals are extracted within the CSF, the WM, and the whole-brain masks. Additionally, a set of physiological regressors were extracted to allow for component-based noise correction [*CompCor*, @compcor]. Principal components are estimated after high-pass filtering the *preprocessed BOLD* time-series (using a discrete cosine filter with 128s cut-off) for the two *CompCor* variants: temporal (tCompCor) and anatomical (aCompCor). tCompCor components are then calculated from the top 2% variable voxels within the brain mask. For aCompCor, three probabilistic masks (CSF, WM and combined CSF+WM) are generated in anatomical space. The implementation differs from that of Behzadi et al. in that instead of eroding the masks by 2 pixels on BOLD space, a mask of pixels that likely contain a volume fraction of GM is subtracted from the aCompCor masks. This mask is obtained by dilating a GM mask extracted from the FreeSurfer’s *aseg* segmentation, and it ensures components are not extracted from voxels containing a minimal fraction of GM. Finally, these masks are resampled into BOLD space and binarized by thresholding at 0.99 (as in the original implementation). Components are also calculated separately within the WM and CSF masks. For each *CompCor* decomposition, the k components with the largest singular values are retained, such that the retained components’ time series are sufficient to explain 50 percent of variance across the nuisance mask (CSF, WM, combined, or temporal). The remaining components are dropped from consideration. The head-motion estimates calculated in the correction step were also placed within the corresponding confounds file. The confound time series derived from head motion estimates and global signals were expanded with the inclusion of temporal derivatives and quadratic terms for each [confound_satterthwaite_2013]. Frames that exceeded a threshold of 0.5 mm FD or 1.5 standardized DVARS were annotated as motion outliers. Additional nuisance timeseries are calculated by means of principal components analysis of the signal found within a thin band (*crown*) of voxels around the edge of the brain, as proposed by [patriat_improved_2017]. The BOLD time-series were resampled into standard space, generating a *preprocessed BOLD run in MNI152NLin6Asym space*. First, a reference volume and its skull-stripped version were generated using a custom methodology of *fMRIPrep*. Automatic removal of motion artifacts using independent component analysis [ICA-AROMA, @aroma] was performed on the *preprocessed BOLD on MNI space* time-series after removal of non-steady state volumes and spatial smoothing with an isotropic, Gaussian kernel of 6mm FWHM (full-width half-maximum). Corresponding “non-aggressively” denoised runs were produced after such smoothing. Additionally, the “aggressive” noise-regressors were collected and placed in the corresponding confounds file. All resamplings can be performed with a *single interpolation step* by composing all the pertinent transformations (i.e. head-motion transform matrices, susceptibility distortion correction when available, and co-registrations to anatomical and output spaces). Gridded (volumetric) resamplings were performed using **antsApplyTransforms** (ANTs), configured with Lanczos interpolation to minimize the smoothing effects of other kernels [lanczos]. Non-gridded (surface) resamplings were performed using **mri_vol2surf** (FreeSurfer).

Many internal operations of *fMRIPrep* use *Nilearn* 0.9.1 [nilearn, RRID:SCR_001362], mostly within the functional processing workflow. For more details of the pipeline, see the section corresponding to workflows in *fMRIPrep*’s documentation.

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FSL analysis

Regions of interest

We created two masks containing regions of interest, one only containing the bilateral fusiform gyrus, the other additionally containing the following regions: ACC_pre_L, ACC_pre_R, ACC_sub_L, ACC_sub_R, ACC_sup_L, ACC_sup_R, Amygdala_L, Amygdala_R, Insula_L, Insula_R, Precuneus_L, Precuneus_R, SupraMarginal_R and Temporal_Rup_R. All regions were extracted from the AAL3 atlas.

The ROI mask only containing the fusiform gyri was used to assess the colour prediction errors in the comparison group, as well as group differences in neural correlates of colour prediction errors. The other ROI mask was used to evaluate all other hypotheses, including emotion prediction error and prediction strength in the comparison group as well as the pooled sample and group differences in neural correlates of emotion prediction errors.

Combine FSL output

```
# get one type of input from each contrast
ls.files = dir(pattern = '*.MNI-AAL.csv', path = "./results_sig")

for (file in ls.files) {
  contrast = gsub("_MNI-AAL.csv", "", file)
  type     = substr(contrast, nchar(contrast)-5, nchar(contrast)-5)
  maxima   = read_csv(file.path("results_sig", file), show_col_types = F)
  if (nrow(maxima) == 0) next
  summary  = read_delim(file.path("results_sig",
                                paste0(contrast, '_cluster-summary.txt')),
                        show_col_types = F)
  output   = read_delim(file.path("results_sig",
                                paste0(contrast, '_randomise_output_all.txt')),
                        show_col_types = F)
```

```

relinfo =
  merge(
    output %>% select(`Cluster Index`, Voxels),
    maxima %>% select(`Cluster Index`, `Value`, MNIx, MNIy, MNIZ, AALname)
  ) %>%
  mutate(
    H = if_else(MNIx >= 0, "R", "L")
  ) %>%
  rename(
    `Cluster size` = "Voxels",
    "Region" = "AALname",
    "x" = "MNIx",
    "y" = "MNIy",
    "z" = "MNIZ"
  ) %>%
  arrange(desc(`Cluster Index`), desc(Value)) %>%
  relocate(`Cluster Index`, Region, `Cluster size`, H)
colnames(relinfo)[colnames(relinfo) == "Value"] = paste0(type, "-value")

write_csv(relinfo, file = file.path("results_sig", paste0(contrast, '.csv')))
}

```

Hypothesis-guided ROI analysis

```

# COMP: same areas as Stefanics et al. (2019), Neuroimage

read_csv(file.path("results_sig", 'hgf_ctr_eps_c_ROI_fstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'COMP: colour prediction error')

```

Table 1: COMP: colour prediction error

Cluster Index	Region	Cluster size	H	f-value	x	y	z
1	Fusiform gyrus	241	R	24.3	30	-70	-10
1	Fusiform gyrus	241	R	23.1	32	-60	-14
1	Fusiform gyrus	241	R	22.9	28	-60	-16
1	Fusiform gyrus	241	R	20.8	30	-64	-16
1	Fusiform gyrus	241	R	17.8	28	-52	-18
1	Fusiform gyrus	241	R	14.2	32	-78	-6

```

read_csv(file.path("results_sig", 'hgf_ctr_mu_e_ROI_fstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'COMP: emotion prediction strength')

```

Table 2: COMP: emotion prediction strength

Cluster Index	Region	Cluster size	H	f-value	x	y	z
1	Precuneus	3	R	26	6	-76	52

pooled: same areas as Stefanics et al. (2019), Neuroimage

```
read_csv(file.path("results_sig", 'hgf_all_eps_c_ROI_fstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'Pooled: colour prediction error')
```

Table 3: Pooled: colour prediction error

Cluster Index	Region	Cluster size	H	f-value	x	y	z
7	Fusiform gyrus	230	R	39.8	32	-60	-16
7	Fusiform gyrus	230	R	35.9	28	-70	-12
7	Fusiform gyrus	230	R	24.5	34	-74	-14
6	Superior temporal gyrus	58	R	19.2	50	-40	22
5	Insula	57	R	23.3	32	24	-4
5	Insula	57	R	22.3	42	26	-4
5	Insula	57	R	16.1	42	22	-10
4	Anterior cingulate cortex, supracallosal	47	R	22.0	8	34	24
3	Fusiform gyrus	28	L	32.1	-28	-56	-16
2	Superior temporal gyrus	15	R	17.9	52	-6	-14
1	Superior temporal gyrus	2	R	13.9	50	-18	-8

```
read_csv(file.path("results_sig", 'hgf_all_mu_c_ROI_fstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'Pooled: colour prediction strength')
```

Table 4: Pooled: colour prediction strength

Cluster Index	Region	Cluster size	H	f-value	x	y	z
7	Precuneus	2401	L	30.5	-8	-70	40
7	Precuneus	2401	R	28.0	12	-46	42
7	Precuneus	2401	R	27.7	8	-50	42
7	Precuneus	2401	R	26.8	4	-56	50
7	Precuneus	2401	R	25.2	10	-50	46
7	Precuneus	2401	R	24.1	2	-62	48
6	SupraMarginal gyrus	553	R	25.5	58	-44	36
6	SupraMarginal gyrus	553	R	24.4	58	-46	44
6	Superior temporal gyrus	553	R	22.9	48	-40	10
6	SupraMarginal gyrus	553	R	21.9	52	-44	38
6	SupraMarginal gyrus	553	R	21.2	52	-40	44
6	Superior temporal gyrus	553	R	20.4	58	-50	18
5	Anterior cingulate cortex, supracallosal	254	R	22.4	10	24	26
5	Anterior cingulate cortex, pregenual	254	R	20.9	8	40	16
5	Anterior cingulate cortex, pregenual	254	R	15.1	8	46	14
4	Insula	171	L	23.3	-28	22	4
4	Insula	171	L	22.4	-32	20	-8
4	Insula	171	L	21.2	-28	26	-4
4	Insula	171	L	16.8	-36	16	-2
3	Insula	119	R	26.9	32	24	-4
3	Insula	119	R	24.2	38	26	-4
3	Insula	119	R	22.1	42	20	-8
3	Insula	119	R	14.6	44	22	0
2	Precuneus	63	R	13.1	20	-54	20
2	Precuneus	63	R	11.9	14	-54	18

Cluster Index	Region	Cluster size	H	f-value	x	y	z
1	Precuneus	3	R	12.5	4	-46	14

```
read_csv(file.path("results_sig", 'hgf_all_mu_e_ROI_fstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'Pooled: emotion prediction strength')
```

Table 5: Pooled: emotion prediction strength

Cluster Index	Region	Cluster size	H	f-value	x	y	z
4	Precuneus	124	R	23.9	8	-78	56
4	Precuneus	124	R	23.6	6	-74	52
4	Precuneus	124	R	18.2	16	-70	48
3	Fusiform gyrus	86	R	30.1	32	-52	-20
3	Fusiform gyrus	86	R	21.5	28	-52	-14
3	Fusiform gyrus	86	R	20.4	32	-62	-18
3	Fusiform gyrus	86	R	17.9	30	-62	-14
2	Fusiform gyrus	62	L	24.7	-30	-64	-16
2	Fusiform gyrus	62	L	22.8	-34	-60	-18
2	Fusiform gyrus	62	L	20.4	-34	-54	-18
2	Fusiform gyrus	62	L	17.9	-34	-54	-22
1	Precuneus	2	R	13.2	14	-74	48

Neural adaptation

```
read_csv(file.path("results_sig", 'smp_adapt_neg_ROI_tstat1.csv'), show_col_types = F) %>%
  kable(., caption = 'ALL: repetition suppression')
```

Table 6: ALL: repetition suppression

Cluster Index	Region	Cluster size	H	t-value	x	y	z
3	Fusiform gyrus	55	R	4.36	28	-80	-16
3	Fusiform gyrus	55	R	4.24	36	-76	-16
2	Fusiform gyrus	27	R	4.62	38	-56	-22
1	Fusiform gyrus	12	R	4.16	32	-56	-14

Plotting

Plot the participants' activation in clusters larger than 100 voxels to visualise the effects.

```
# custom colour palette
custom.col = c("#009E73", "#D55E00", "#0058b2", "#CC79A7")

# load in the extracted activation
df.act = read_csv(file.path("fMRI_data", "grp_use-sorted.csv"),
  show_col_types = F) %>%
  mutate(
    diagnosis = fct_recode(diagnosis,
      "COMP" = "CTR")
  ) %>%
  select(diagnosis) %>%
```

```

mutate(
  # load zstats for eps-c
  `colour PE-rFG` = scan(file.path("fMRI_data", "eps_c_C7_meants.txt")),
  `colour PE-rSTS` = scan(file.path("fMRI_data", "eps_c_C6_meants.txt")),
  `colour PE-rINS` = scan(file.path("fMRI_data", "eps_c_C5_meants.txt")),
  `colour PE-rACC` = scan(file.path("fMRI_data", "eps_c_C4_meants.txt")),
  # load zstats for mu-z
  `colour PS-rINS` = scan(file.path("fMRI_data", "mu_c_C3_meants.txt")),
  `colour PS-lINS` = scan(file.path("fMRI_data", "mu_c_C4_meants.txt")),
  `colour PS-rACC` = scan(file.path("fMRI_data", "mu_c_C5_meants.txt")),
  `colour PS-rSMG` = scan(file.path("fMRI_data", "mu_c_C6_meants.txt")),
  `colour PS-PRC` = scan(file.path("fMRI_data", "mu_c_C7_meants.txt")),
  # load zstats for mu-e
  `emotion PS-rPRC` = scan(file.path("fMRI_data", "mu_e_C4_meants.txt")),
  `emotion PS-rFG` = scan(file.path("fMRI_data", "mu_e_C3_meants.txt")),
  `emotion PS-lFG` = scan(file.path("fMRI_data", "mu_e_C2_meants.txt")),
  # load zstat for neural adaptation
  `RS-rFG` = scan(file.path("fMRI_data", "adapt_meants.txt"))
) %>%
pivot_longer(cols = -diagnosis, names_to = c("parameter", "region"),
              names_sep = "-", values_to = "activation")

# plot
df.act %>%
  ggplot(aes(region, activation, fill = diagnosis, colour = diagnosis)) + #
  geom_rain(rain.side = 'r',
boxplot.args = list(color = "black", outlier.shape = NA, show.legend = FALSE, alpha = .8),
violin.args = list(color = "black", outlier.shape = NA, alpha = .6),
boxplot.args.pos = list(
  position = ggpp::position_dodgenudge(x = 0, width = 0.3), width = 0.3
),
point.args = list(show_guide = FALSE, alpha = .5, size = 0.5),
violin.args.pos = list(
  width = 0.6, position = position_nudge(x = 0.16)),
point.args.pos = list(position = ggpp::position_dodgenudge(x = -0.25, width = 0.1))) +
  scale_fill_manual(values = custom.col) +
  scale_color_manual(values = custom.col) +
  labs(title = "Neural correlates", x = "", y = "z-stat") +
  facet_grid(. ~ parameter, scales = "free", space = "free") +
  geom_hline(yintercept = 0) +
  theme_bw() +
  theme(legend.position = "bottom",
        plot.title = element_text(hjust = 0.5),
        legend.direction = "horizontal",
        text = element_text(size = 12, family = "mono", face = "bold")
  )

```

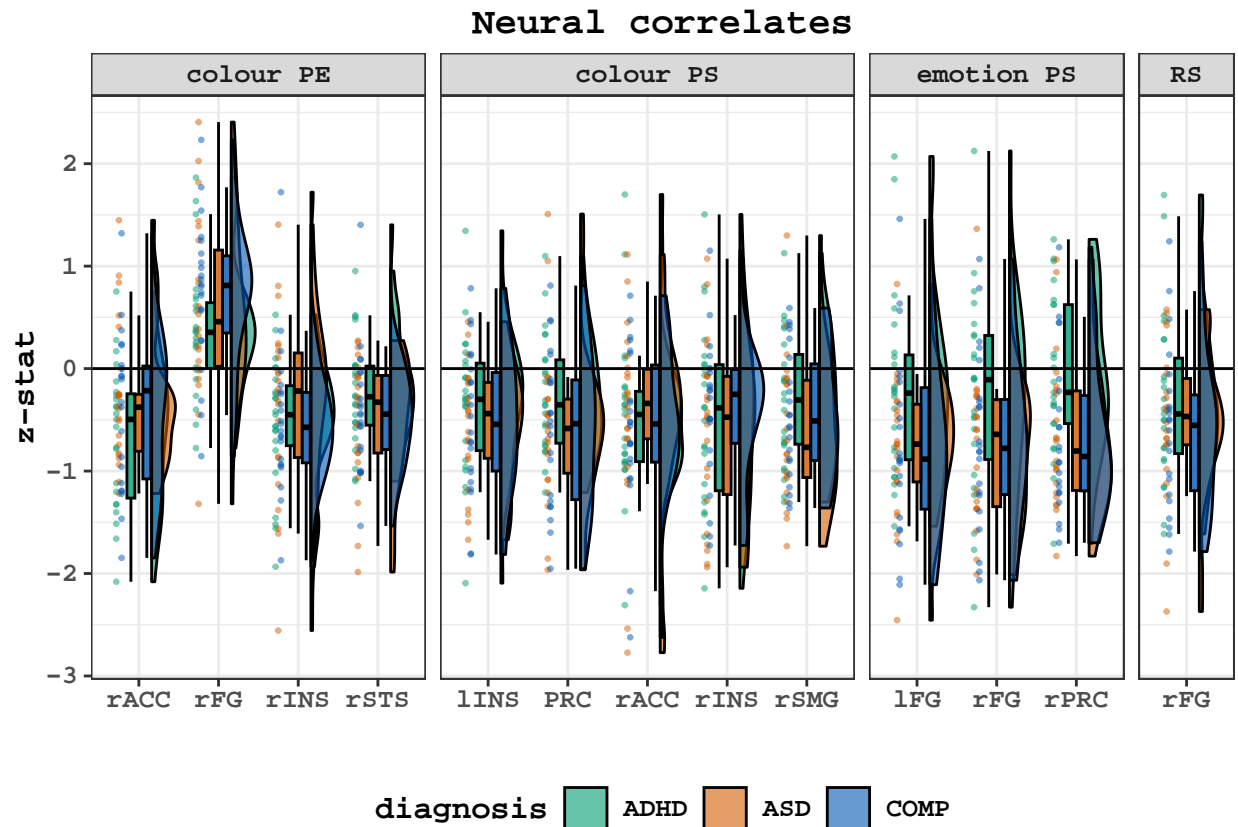
```

## Warning: The `show_guide` argument of `layer()` is deprecated as of ggplot2 2.0.0.
## i Please use the `show.legend` argument instead.
## i The deprecated feature was likely used in the gggrain package.
##   Please report the issue at <https://github.com/njudd/gggrain/issues>.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.

```



```
## Warning in (function (mapping = NULL, data = NULL, stat = "half_ydensity", :
## Ignoring unknown parameters: `outlier.shape`
```



```
ggsave("neural_zstat.pdf",
  units = "mm", width = 270, height = 100, dpi = 300)
```

```
# check normal distribution
df.act %>% group_by(diagnosis, parameter, region) %>%
  shapiro_test(activation) %>%
  arrange(region, parameter)
```

```
## # A tibble: 39 x 6
##   diagnosis parameter region variable statistic      p
##   <fct>      <chr>      <chr> <chr>      <dbl> <dbl>
## 1 ADHD      colour PS    PRC    activation  0.970 0.699
## 2 ASD      colour PS    PRC    activation  0.924 0.0915
## 3 COMP      colour PS    PRC    activation  0.974 0.811
## 4 ADHD      emotion PS   lFG    activation  0.920 0.0656
## 5 ASD      emotion PS   lFG    activation  0.975 0.821
## 6 COMP      emotion PS   lFG    activation  0.963 0.545
## 7 ADHD      colour PS    lINS    activation  0.961 0.488
## 8 ASD      colour PS    lINS    activation  0.965 0.594
## 9 COMP      colour PS    lINS    activation  0.979 0.901
## 10 ADHD     colour PE    rACC    activation  0.979 0.892
## # i 29 more rows
```

```
# not: colour PE - rACC, rINS, but most are
df.act = df.act %>%
```

```

mutate(
  param_region = paste0(parameter, '_', region)
)

# compute bayes factor using anovas
bf.log = c()
comb = c()
for (c in unique(df.act$param_region)) {
  df.small = df.act %>% filter(param_region == c)
  aov = anovaBF(activation ~ diagnosis, data = df.small)
  comb = c(comb, c)
  bf.log = c(bf.log, aov@bayesFactor$bf)
}

# apply multiple comparison correction after Westfall (1997)
# as described by de Jong (2019)
m = 6 # output of ceil(max(roots([1, -1, -26]))) in MATLAB
c = 0.5^(2/m);
podds = exp(bf.log) * ((1-c)/c)
bf.cor = c()
for (i in 1:length(bf.log)) {
  ph1 = podds[i]/(1 + podds[i])
  bf.cor = c(bf.cor, log(ph1/(1 - ph1)))
}

# put everything into a dataframe
df.aov = data.frame(comb, bf.log, bf.cor) %>%
  separate(comb, into = c("parameter", "region"), sep = "_") %>%
  mutate(
    interpretation = interpret_bf(bf.cor, log = T)
  )

kable(df.aov %>% arrange(bf.cor))

```

parameter	region	bf.log	bf.cor	interpretation
colour PS	rACC	-1.9853210	-3.3326983	strong evidence against
colour PE	rINS	-1.8599635	-3.2073408	strong evidence against
colour PS	rINS	-1.8258148	-3.1731921	strong evidence against
colour PS	lINS	-1.5348511	-2.8822284	strong evidence against
RS	rFG	-1.5018543	-2.8492316	strong evidence against
colour PS	rSMG	-1.2851827	-2.6325601	strong evidence against
colour PE	rSTS	-1.2690302	-2.6164076	strong evidence against
colour PE	rFG	-1.1409374	-2.4883147	strong evidence against
colour PS	PRC	-0.8845863	-2.2319636	moderate evidence against
colour PE	rACC	-0.8614937	-2.2088711	moderate evidence against
emotion PS	rFG	-0.4132379	-1.7606152	moderate evidence against
emotion PS	lFG	0.3435591	-1.0038183	anecdotal evidence against
emotion PS	rPRC	1.2601849	-0.0871925	anecdotal evidence against