Supplementary Material

Method

fMRI task

A Sternberg type working memory task divided into verbal and spatial working memory components was adapted from Thomason et al. (2009). Each trial began with a central fixation cross displayed for 400 ms. In the verbal task participants were presented with an array of capital letters, two in the low load condition and six in the high load condition for a duration of 500 ms. After a 3000 ms delay a single letter in lower case was presented for 1500 ms and participants indicated by button-press whether the letter was present in the previously shown array. In the verbal control condition only one type of letter was shown, two in the low and six in the high load condition and the 3000 ms delay was shortened to a 100 ms delay. Only consonants were used and letters were not repeated if they appeared in the previous two trials. In the spatial task either one or five black dots were presented randomly across 52 possible locations arranged on four invisible circles around fixation. After a 3000 ms delay a probe appeared in the form of a circle that matched or did not match the location of one of the previously displayed dots. Participants needed to indicate whether the location of the probe matched the location of the dot on the screen. As in the verbal task, the control condition only had a 100 ms delay and all but one circle were greyed out. Locations were not repeated over three consecutive trials. Control tasks were designed to match experimental conditions on as many elements as possible (motor response, decision making, visual stimuli, luminance) except for the working memory component. For both, verbal and spatial conditions, probes matched the target 50% of the time. The total duration of the experimental and control trials were matched. For each task, a total of 64 trials (32 experimental, 32 control) were presented in 16 blocks of four trials. Blocks alternated between experimental and control conditions in a pseudorandom fashion. Each condition was repeated four times. Total trial length was 5400

ms, which equates to a block length of 21.6 s together with an inter-block interval of 3000 ms resulting in a total scan time of 7 min and 10 s for each task. For the purpose of the current analysis, we combined high and low load conditions to maximize the number of trials to be used in the MVPA analysis. The task was programmed and presented using Presentation Software Version 14.2 (Neurobehavioral Systems, Berkeley). Stimuli were displayed using Helvetica font (size: 45 pt) in black on a white background. The order of presentation of verbal and spatial tasks in the scanner was counterbalanced across participants. All young people were allowed to practice sample trials of the task on a Toshiba laptop before entering the scanner. The scripts for the tasks can be downloaded from our OSF repository: https://osf.io/a5349/.

MVPA Signal Detection Metrics: (Accuracy, Sensitivity, Specificity, ROC, AUC)

The linear SVM classifier generates signal detection metrics from a confusion matrix that can be used to evaluate performance of the classification model (Zhu et al., 2010). An example confusion matrix and corresponding relevant metrics (e.g., classification accuracy, sensitivity, specificity) is illustrated in Supplement Figure 1a. Importantly, these metrics can be utilized to facilitate quantitative comparison of model performance between networks and groups via a receiver operating characteristic (ROC) curve and area under the ROC curve (AUC). These computations for each metric are detailed in the subsequent paragraphs.

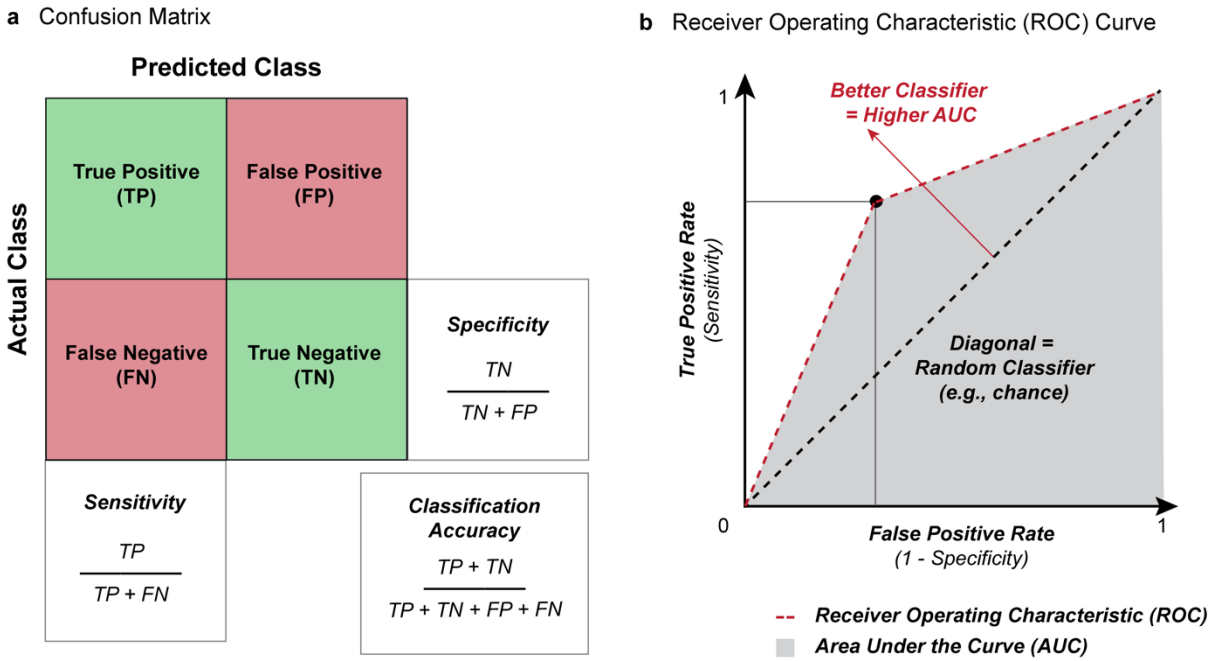

Figure S1: a) Illustration of confusion matrix that summarizes the performance of the classification model, as well as computations for relevant signal detection metrics (e.g., classification accuracy, sensitivity and specificity). b) Illustration of an empirical receiver operating characteristic (ROC) curve that is generated from the true positive rate (sensitivity) and false positive rate (1-specificity). The area under the ROC curve (AUC) can be computed from this empirical ROC function.

For each network within each group, we evaluated ***classification accuracy***, which refers to the proportion of correctly classified observations (i.e., both true positives [TP] and true negatives [TN] divided by all observations including true positives [TP], true negatives [TN], false positives [FP] and false negatives [FN]), a commonly used metric for linear SVM model comparison. Critically, because we used leave-one-subject-out cross validation, we were able to estimate the average accurate performance of the classifier across subjects within each group for each network. The equation for computing classification accuracy is shown below.

$$Classification\ Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

Another relevant metric we computed is the model's ***sensitivity***, which refers to the proportion of true positive assessments (e.g., true positive rate) correctly identified by the

model. In other words, the sensitivity reflects how good the model is at correctly detecting the true positives in the data (e.g., correctly classifying a subject's verbal working memory beta estimate as a verbal working memory beta estimate), such that a higher value decreases the likelihood of false positive results.

$$Sensitivity = \frac{TP}{TP + FN}$$

Next, we also computed the model's ***specificity*****,** which refers to the proportion of true negative assessments (i.e., true negative rate) correctly identified by the model. In other words, the specificity reflects the degree to which the model correctly detecting true negatives in the data (e.g., correctly classifying a subject's verbal working memory beta estimate as not a spatial working memory beta estimate), such that higher value decreases the likelihood of false negative results.

$$Specificity \ = \frac{TN}{TN + FP}$$

Finally, as both specificity and sensitivity measures provide important complementary information about the classifier performance, we combined both measures into a receiver operating characteristic (**ROC**) curve to evaluate and compare the diagnostic ability of the classifier between networks and between groups. Specifically, the ROC curve encompasses both the ***false positive rate*** (1-specificity) and ***true positive rate*** (sensitivity), and the area under the ROC curve (also known as **AUC**) reflects an aggregate measure of classifier performance across all possible classification thresholds (See Supp Figure 1b). Critically, we can compute an **AUC** measure for classifier performance for each network, which allows for a quantitative comparison of which networks are better for differentiating between verbal and spatial working memory in each group as well as comparison of classifier performance between groups.

Results

Table S1: Mean (SD) for task performance measures for each group for the verbal and spatial task. Accuracy refers to the number of correct trials (out of 28 total trials per experimental and control condition), reaction times are presented in milliseconds (ms).

	Accuracy (Number of Correct Trials)				**Reaction Times (ms)**			
	Experimental		**Control**		**Experimental**		**Control**	
	Spatial	**Verbal**	**Spatial**	**Verbal**	**Spatial**	**Verbal**	**Spatial**	**Verbal**
TD	25.22	25.53	30.67	31.00	1112	1059	914	872
(n=19)	(2.90)	(3.86)	(1.75)	(1.33)	(328)	(253)	(308)	(301)
PDD	23.62	23.19	29.94	30.56	1305	1132	906	823
(n=16)	(4.54)	(2.64)	(2.29)	(2.10)	(659)	(472)	(331)	(205)
ADHD	23.95	23.40	30.20	29.95	1157	1043	892	853
(n=20)	(4.41)	(3.59)	(2.02)	(2.26)	(544)	(190)	(170)	(191)

Head Motion

To test for effects of head motion between the task conditions within each group, we conducted t-tests for the Euclidean norm of the motion parameters (enorm) between spatial vs. verbal stimulus material in both working memory conditions and control conditions. In the working memory conditions, head motion did not differ between the verbal and spatial working memory task components (PDD $t(15)=1.70$, $p=0.110$; ADHD $t(19)=-.02$, $p=0.981$; TD $t(18)=-.23$, $p=0.822$). In the control conditions, head motion also did not differ between the two tasks (PDD $t(15)=1.45$, $p=0.167$; ADHD $t(19)=0.44$, $p=0.665$; TD $t(18)=-1.31$, $p=0.207$). All means and standard deviations of the enorm by condition are listed in Table S2.

Table S2: Mean (SD) of the Euclidean norm of head motion for the verbal and spatial task for each group.

	Experimental		**Control**	
	Spatial	**Verbal**	**Spatial**	**Verbal**
TD (n=19)	.119 (.227)	.124 (.254)	.110 (.119)	.124 (.230)
PDD (n=16)	.157 (.275)	.119 (.167)	.161 (.254)	.135 (.169)
ADHD (n=20)	.208 (.361)	.205 (.358)	.210 (.376)	.200 (.342)

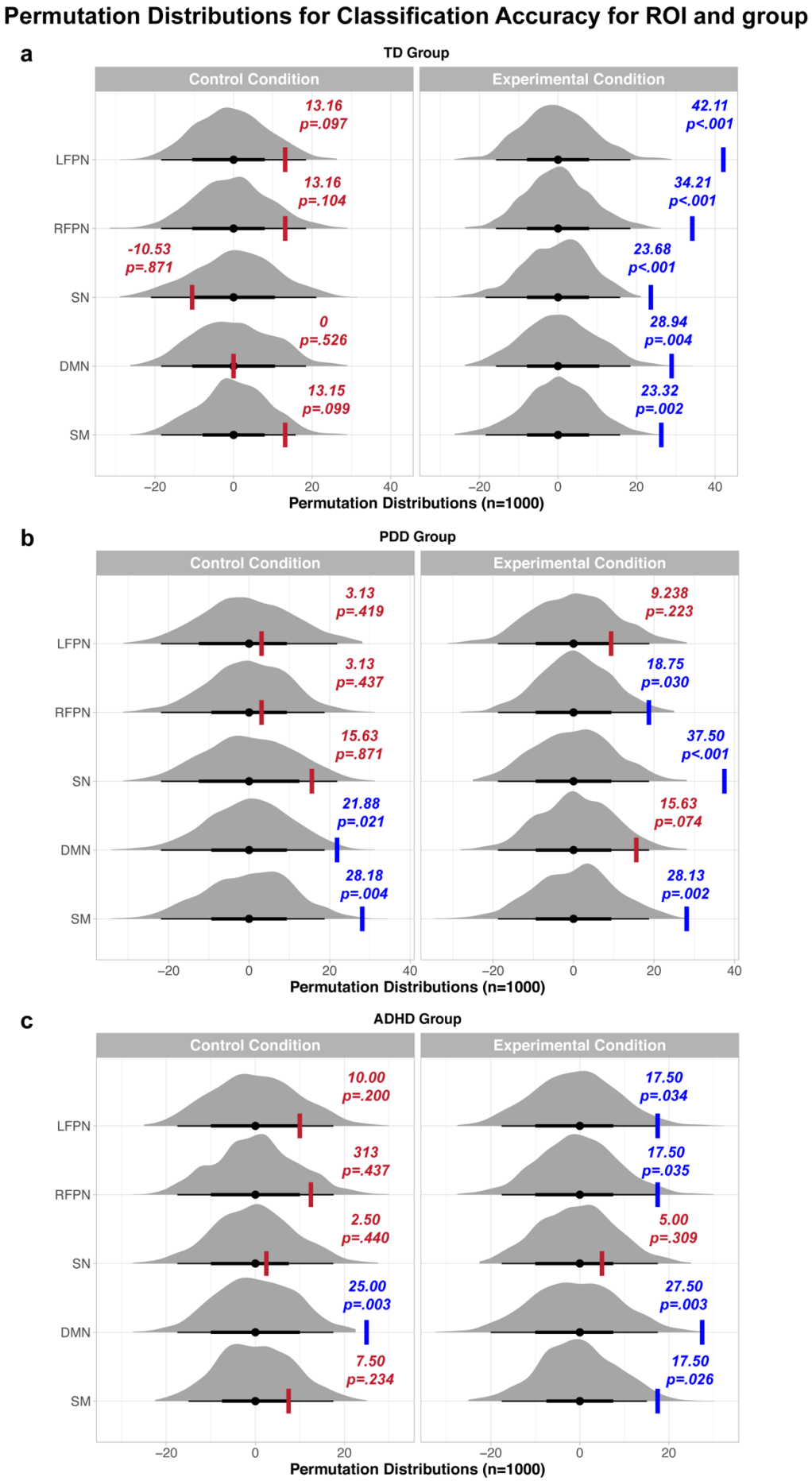
Permutation Distributions for Classification Accuracy for ROI and group
a
TD Group
Control Condition
Experimental Condition
LFPN
RFPN
SN
DMN
SM
13.16 p=.097
13.16 p=.104
-10.53 p=.871
0 p=.526
13.15 p=.099
42.11 p<.001
34.21 p<.001
23.68 p<.001
28.94 p=.004
23.32 p=.002
−20 0 20 40
Permutation Distributions (n=1000)
b
PDD Group
Control Condition
Experimental Condition
LFPN
RFPN
SN
DMN
SM
3.13 p=.419
3.13 p=.437
15.63 p=.871
21.88 p=.021
28.18 p=.004
9.238 p=.223
18.75 p=.030
37.50 p<.001
15.63 p=.074
28.13 p=.002
−20 0 20 40
Permutation Distributions (n=1000)
c
ADHD Group
Control Condition
Experimental Condition
LFPN
RFPN
SN
DMN
SM
10.00 p=.200
313 p=.437
2.50 p=.440
25.00 p=.003
7.50 p=.234
17.50 p=.034
17.50 p=.035
5.00 p=.309
27.50 p=.003
17.50 p=.026
−20 0 20
Permutation Distributions (n=1000)

Figure S2: Permutation Distributions (n=1000) to compute p-values (1-tailed, right side) for classification accuracies for each ROI network, condition, and group. The blue and red bars indicate the significant and non-significant cross-validated classification accuracies (threshold is $p<.05$) from the SVM, respectively.

Table S3: Signal Detection Metrics for each ROI network, condition, and group.

		Experimental Condition			Control Condition		
	Metric	**TD**	**ADHD**	**PDD**	**TD**	**ADHD**	**PDD**
Left Frontoparietal	*AUC*	97.51	73.50	66.02	73.96	68.75	57.42
	Sensitivity	89.47	75.00	50.00	89.47	75.00	50.00
	Specificity	94.74	60.00	68.75	73.68	55.00	62.5
Right Frontoparietal	*AUC*	85.32	65.25	73.83	57.62	56.50	48.44
	Sensitivity	78.95	60.00	68.75	52.63	60.00	43.75
	Specificity	89.47	75.00	68.75	73.68	65.00	62.50
Salience	*AUC*	77.84	56.50	93.75	42.11	52.00	71.09
	Sensitivity	73.68	50.00	81.25	36.84	55.00	68.75
	Specificity	73.68	60.00	93.75	42.11	50.00	62.50
Default Mode	*AUC*	84.49	84.00	74.22	57.62	80.00	76.17
	Sensitivity	73.68	75.00	68.75	52.63	70.00	62.50
	Specificity	84.21	80.00	62.50	47.37	80.00	81.25
Sensorimotor	*AUC*	80.61	68.25	83.59	61.50	49.25	78.52
	Sensitivity	73.68	70.00	75.00	63.16	50.00	81.25
	Specificity	78.95	65.00	81.25	63.16	65.00	75.00

Whole Brain Univariate Results for Spatial and Verbal Working Memory Tasks

In order to verify that the fMRI task reliably activated key working memory related regions, we averaged whole-brain activations for spatial and verbal working memory experimental conditions for each group. In accordance with predictions, the tasks significantly activate regions in the frontoparietal network and deactivate midline regions associated with the DMN in each group. Peak voxels for each cluster are shown in Table S4.

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Table S4: MNI Coordinates of significant peak activations for both spatial and verbal working memory tasks. Signification clusters were thresholded at p<.001 and cluster corrected with a threshold of $\alpha = .01$. Asterisk(*) denotes significant negative activation.

Contrast	Cluster	Voxels	X	Y	Z	Stat
TD						
Verbal Task						
Positive	Dorsal Anterior Cingulate Cortex	593	5	-11	53	6.61
	Left Anterior Insula	416	44	-20	8	5.96
	Left Precentral Cortex	385	38	29	62	6.09
	Right Inferior Temporal Cortex	376	-44	68	-2	5.04
	Left Inferior Temporal Cortex	300	47	77	-2	5.28
	Left Superior Parietal Lobule	222	26	74	44	5.49
	Left Dorsolateral Prefrontal Cortex	218	44	-11	32	4.98
	Right Anterior Insula	169	-35	-26	2	5.31
	Right Superior Parietal Lobule	129	-32	65	56	4.77
	Right Cerebellum	85	-11	71	-23	5.77
Negative	Left Posterior Cingulate*	164	14	59	17	-5.53
	Ventromedial Frontal Cortex*	113	8	-56	-2	-5.33
	Left Precuneus*	64	41	77	35	-4.54
	Left Parahippocampal Cortex*	41	32	41	-8	-4.89
Spatial Task						
Positive	Bilateral Inferior Parietal Cortex	1986	44	44	41	6.15
	Dorsal Anterior Cingulate Cortex	109	-2	-23	41	6.18
	Left Inferior Temporal Cortex	440	47	74	-5	5.40
	Right Inferior Temporal Cortex	182	-50	59	-11	4.79
	Left Precentral Cortex	175	32	5	56	5.86
	Left Anterior Insula	146	32	-26	-5	5.74
	Right Anterior Insula	136	-32	-26	-5	6.46
	Left Cerebellum	128	8	74	-20	5.64
	Right Cerebellum	74	-32	50	-32	5.07
	Right Middle Frontal Gyrus	65	-35	-44	32	4.47
	Left Thalamus	54	11	17	8	5.26
	Left Putamen	40	23	-14	-2	4.83
	Left Cuneus	33	14	71	5	3.83
	Left Dorsolateral Prefrontal Cortex	30	47	-8	29	4.05
	Left Caudate	29	17	2	17	4.39
	Right Caudate	28	-14	-20	2	4.04
Negative	Ventromedial Frontal Cortex*	532	5	-53	-14	-5.50
	Posterior Cingulate Cortex*	515	8	53	32	-5.86
	Left Angular Gyrus*	164	47	68	32	-5.30
	Left Orbitofrontal Cortex*	66	38	-35	-11	-4.62
	Left Inferior Frontal Cortex*	53	56	-32	2	-4.80
	Left Superior Frontal Cortex*	41	14	-47	47	-4.78
ADHD						
Verbal Task						
Positive	Left Precentral Cortex	160	35	23	68	4.87
	Dorsal Anterior Cingulate Cortex	131	8	-11	50	4.89
	Left Inferior Temporal Cortex	85	44	65	-11	5.64
	Left Dorsolateral Prefrontal Cortex	64	53	-11	32	4.67
	Left Inferior Parietal Cortex	32	47	47	47	4.27
	Right Inferior Temporal Cortex	24	-50	77	-8	4.25
Negative	Left Posterior Cingulate Cortex*	161	8	53	32	-5.68
	Right Posterior Cingulate Cortex*	80	-14	59	20	-5.08
	Left Parahippocampal Cortex*	31	29	44	-8	-4.49

Spatial Task						
Positive	Bilateral Inferior Parietal Cortex	1851	38	26	59	5.73
	Dorsal Anterior Cingulate Cortex	376	5	-11	50	5.40
	Right Middle Frontal Gyrus	90	-29	2	62	4.41
	Right Dorsolateral Prefrontal cortex	86	-47	-14	32	4.91
	Right Inferior Temporal Cortex	71	-56	62	-11	4.44
	Left Inferior Temporal Cortex	71	53	68	-5	4.72
	Left Precentral Cortex	59	44	2	38	4.71
	Left Anterior Insula	57	32	-26	5	4.91
	Right Dorsolateral Prefrontal Cortex	54	-41	-38	35	4.69
	Right Anterior Insula	50	-35	-26	-2	5.61
	Left Cerebellum	30	11	77	-26	4.34
	Right Visual Cortex	26	-32	95	5	4.10
Negative	Ventromedial Frontal Cortex*	129	-2	-56	-8	-4.77
	Left Posterior Cingulate Cortex*	55	5	50	14	-4.74
	Left Posterior Cingulate Cortex*	44	-2	44	32	-4.51
PDD						
Verbal Task						
Positive	Left Inferior Parietal Cortex	419	29	56	47	4.99
	Dorsal Anterior Cingulate Cortex	246	-2	-20	47	4.82
	Right Inferior Parietal Cortex	156	-32	71	38	3.80
	Left Inferior Temporal Cortex	138	41	65	-11	4.83
	Left Anterior Insula	97	35	-20	11	5.34
	Right Anterior Insula	91	-35	-23	8	4.90
	Right Inferior Temporal Cortex	86	-50	68	2	4.72
	Left Cerebellum	76	38	71	-32	4.78
	Right Cerebellum	71	-29	68	-26	5.11
	Left Dorsolateral Prefrontal Cortex	61	50	-5	38	4.77
	Right Dorsolateral Prefrontal Cortex	45	-41	-47	20	4.04
	Right Occipital Cortex	42	-41	92	-2	4.65
	Mid Cerebellum	31	-11	71	-26	4.90
	Left Thalamus	28	14	14	5	4.63
Negative	Posterior Cingulate Cortex*	321	-8	53	20	-5.10
	Ventromedial Prefrontal Cortex*	174	2	-41	-5	-4.79
	Left Superior Frontal Cortex*	74	20	-50	41	-4.62
	Right Orbitofrontal Cortex*	28	-38	-38	-11	-4.59
	Right Superior Frontal Cortex*	28	-23	-35	44	-4.61
	Left Parahippocampal Cortex*	26	32	35	-14	-4.32
	Right Parahippocampal Cortex*	24	-26	45	-14	-4.08
Spatial Task						
Positive	Left Inferior Parietal Cortex	521	50	44	53	5.80
	Right Inferior Parietal Cortex	436	-38	56	56	5.69
	Right Dorsolateral Prefrontal Cortex	273	-50	-11	41	4.76
	Dorsal Anterior Cingulate Cortex	148	-5	-11	53	4.98
	Left Precentral Cortex	90	29	5	62	5.19
	Left Precentral Cortex	50	50	-5	38	4.90
	Right Superior Frontal Cortex	45	-26	-2	59	4.16
Negative	Left Posterior Cingulate Cortex*	65	11	50	32	-3.98

NN1 for activation $p < .001$ for all images, cluster corrected at $p<.01$

References

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