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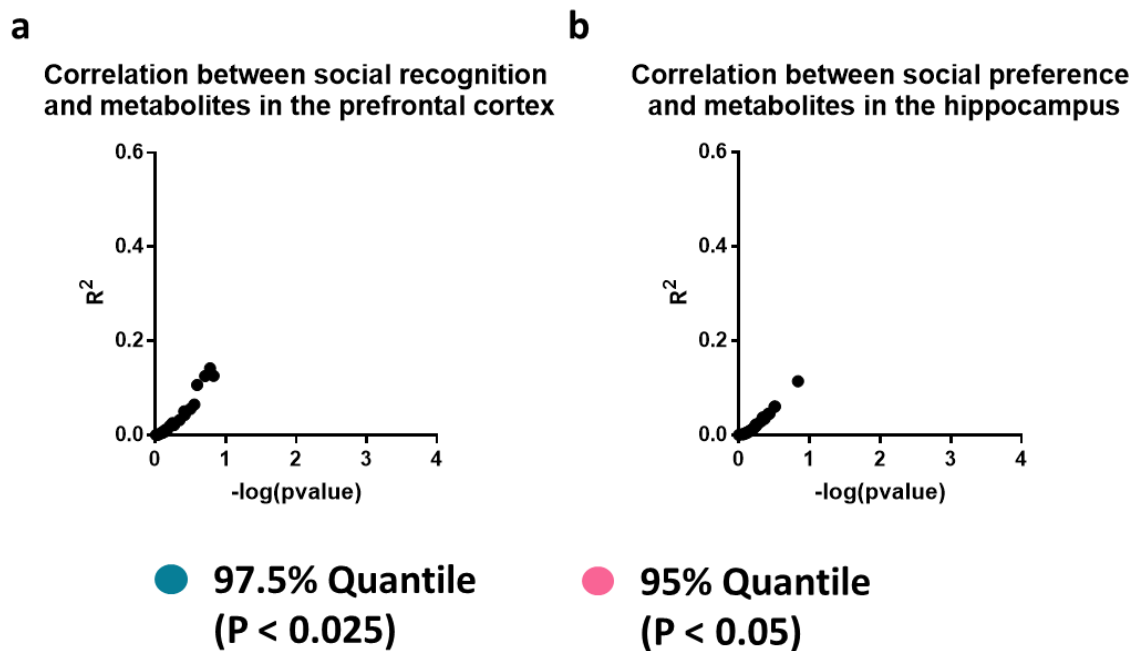
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Table S1. Total metabolites in the prefrontal cortex

PFC	Ab	Ala	Asp	Asp	Cr	Cr	Pcr	Pcr	GABA	GABA	Glc	Glc	Gln	Gln	Glu	Glu	Grc	Grc	Rh	Rh	Gsh	Gsh	Ins	Ins	Lac	Lac	Naa	Naa	NaaG	NaaG	So1b	So1b	Tau	Tau		
	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD	%SD			
WT1	1.196	81	5.331	26	1.838	116	12.991	16	2.375	52	2.058	47	6.186	18	14.332	8	2.832	7	0	999	4.563	13	9.973	10	0	999	8.881	9	0.38	66	0	999	23.41	5		
WT2	1.874	36	3.838	25	0	999	9.697	6	2.133	41	0.122	489	6.897	14	12.904	7	1.748	28	0.545	8	4.54	10	4.862	12	0	999	7.658	8	0.245	198	0	999	14.58	5		
WT3	1.245	38	7.247	19	5.654	18	8.482	13	3.235	28	0.515	159	5.448	16	18.247	4	0.606	91	2.427	24	4.41	11	11.537	7	0	999	10.878	6	0.79	69	0	999	23.742	4		
WT4	2.411	22	7.973	19	2.968	39	10.139	13	3.939	21	0.70	100	8.153	9	17.92	4	1.429	31	1.165	47	4.844	8	8.819	6	1.531	36	10.02	5	1.395	33	0	999	18.073	3		
WT5	2.832	19	7.167	14	5.81	14	7.158	11	4.736	16	1.08	64	6.507	12	17.464	4	1.089	38	1.745	25	4.96	9	11.007	6	0	999	10.612	5	1.148	35	0	999	21.888	3		
WT6	2.154	25	8.722	13	4.027	36	8.915	18	4.403	19	0	999	9.114	9	18.068	4	1.689	27	1.594	30	5.213	8	9.317	6	0	999	10.917	6	0.644	112	0	999	19.416	3		
WT7	1.981	38	8.553	13	7.413	11	5.292	12	4.195	20	0.88	88	4.776	16	18.288	4	1.332	52	1.805	36	5.166	8	10.248	5	0	999	10.658	5	1.347	35	0	999	26.258	3		
WT8	2.188	27	8.224	13	0.348	394	13.376	12	5.225	16	0	999	5.866	13	16.968	4	1.48	43	1.326	38	5.166	11	10.942	5	0	999	11.428	5	0.758	63	0	999	28.258	3		
WT9	1.523	35	7.107	18	4.472	28	8.832	15	4.508	20	0.28	473	4.868	18	18.684	5	1.188	43	1.738	31	4.412	11	10.783	6	2.182	28	11.452	6	0.333	171	0	999	23.975	3		
KO1	0.842	187	5.722	18	5.648	20	5.868	21	3.927	23	0.542	125	5.328	9	13.684	6	1.601	31	1.065	48	5.018	10	6.82	9	0	999	8.652	6	0.13	999	16.977	4				
KO2	1.683	42	6.213	16	3.091	39	7.366	17	3.668	21	0.78	94	4.313	16	13.608	6	1.277	38	1.045	50	4.62	10	8.382	7	0	999	8.833	6	0	999	20.382	4				
KO3	2.196	30	7.896	15	5.665	22	6.43	19	4.232	21	0.78	94	4.313	20	17.281	5	1.583	30	1.343	38	4.388	10	8.195	7	0	999	10.975	6	0.793	740	0	999	21.384	4		
KO4	3.337	15	6.889	16	3.043	33	9.837	11	2.513	32	0.285	247	4.728	16	13.605	6	0.606	77	1.724	28	4.821	9	10.58	6	0	999	10.073	5	0	999	21.997	3				
KO5	2.095	28	8.028	13	5.152	23	7.888	15	5.244	15	0.875	84	5.417	14	18.129	4	1.697	25	1.8	25	4.816	8	9.747	6	0	999	11.908	6	1.108	416	0	999	21.146	3		
KO6	2.905	24	9.145	14	1.412	129	13.512	13	5.244	19	1.588	63	3.883	21	20.621	4	1.038	48	2.305	20	0.33	52	4.823	8	12.109	6	0	999	12.227	5	1.177	418	0	999	28.66	3
KO7	1.75	30	6.888	16	5.102	17	6.712	13	5.718	13	1.146	61	4.791	16	16.638	5	2.261	27	1.438	32	4.823	8	9.795	6	0	999	11.061	5	0.345	43	0	999	20.591	4		
KO8	1.396	37	7.516	13	3.124	30	8.375	13	4.726	18	0.183	396	5.555	13	16.582	4	1.466	28	1.194	31	4.651	8	8.44	7	0	999	9.797	5	0.355	115	0	999	21.382	4		
KO9	2.774	23	8.032	13	1.71	89	10.152	15	5.603	15	0	999	5.695	14	16.67	5	1.46	31	1.565	39	4.448	10	8.748	7	8.5	8	12.718	5	0.355	115	0	999	21.753	4		
KO10	2.051	36	6.795	17	4.471	24	7.445	15	5.205	16	0.196	381	9.495	9	13.5	6	1.598	31	1.275	47	5.677	10	6.518	10	0	999	11.37	5	0	999	19.8	5				
KO11	1.941	32	8.684	12	4.121	26	7.378	16	6.293	12	0.3	223	8.997	9	17.984	4	1.508	24	1.117	47	4.386	9	7.153	7	3.238	19	11.997	4	0.7	61	0	999	17.807	4		

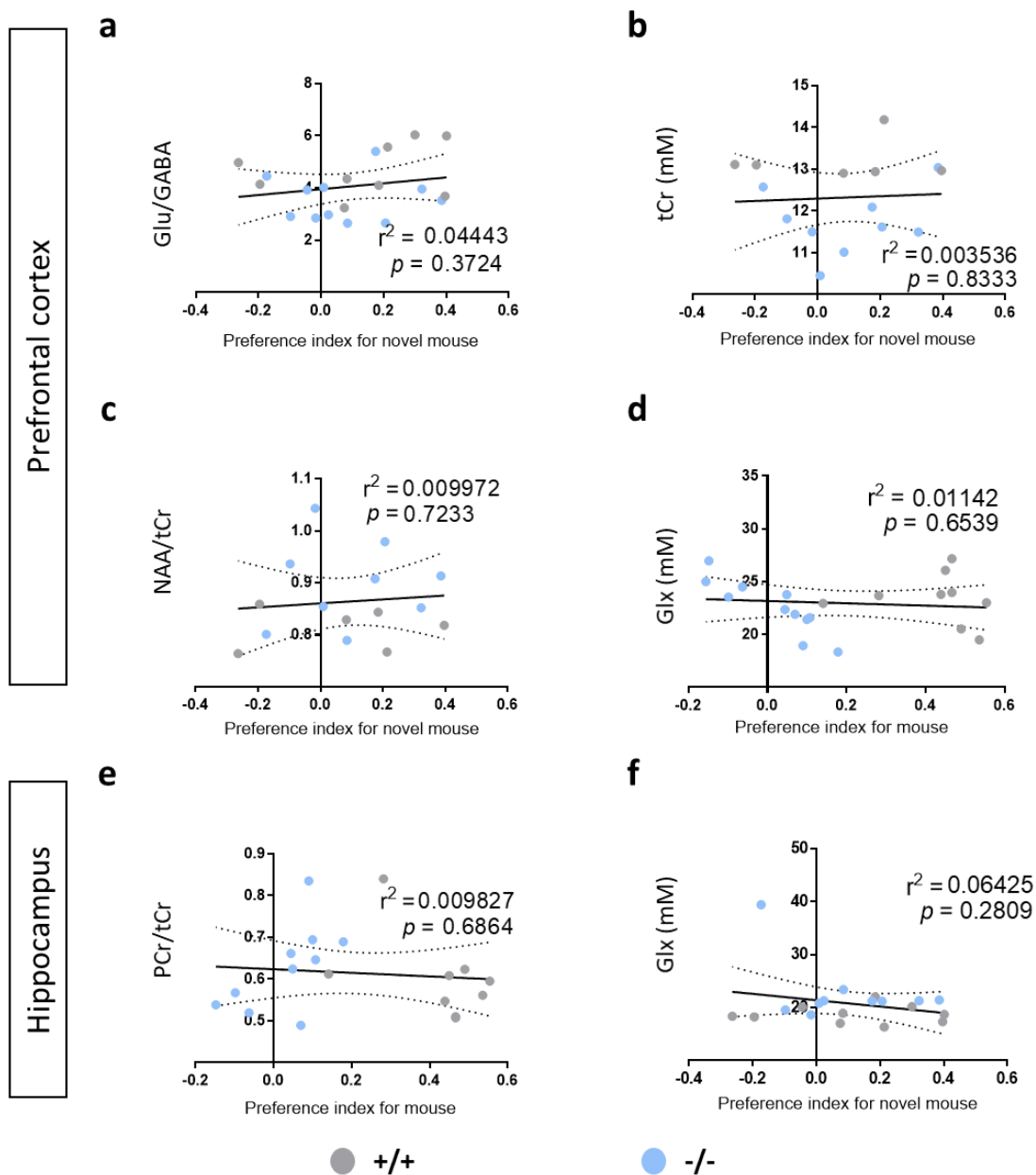
Table S2. Total metabolites in the hippocampus

HPC	Area	Area %SD	Area	Area %SD	Cr	Cr %SD	Cr	Cr %SD	P _{Cr}	P _{Cr} %SD	GABA	GABA %SD	Glc	Glc %SD	Gln	Gln %SD	Glu	Glu %SD	GPC	GPC %SD	GPC	GPC %SD	PCh	PCh %SD	GSH	GSH %SD	Ins	Ins %SD	Ins	Ins %SD	Lac	Lac %SD	NAA	NAA %SD	NAA	NAA %SD	NAG	NAG %SD	Soylio	Soylio %SD	Tau	Tau %SD
W171	1.738	37	5335	17	5335	19	8674	8	4137	3	348	18	0.898	71	444	17	15.714	5	0.564	59	0.352	26	3.935	12	7.881	7	0	399	8.745	7	2.095	18	0	399	18.924	3						
W172	1.539	32	4.711	17	5335	14	8.918	11	3.48	14	1.17	18	1.118	37	6.701	10	12.031	5	0.417	72	1.171	28	4.032	13	3.04	5	0	399	5.513	7	1.74	21	0	399	18.773	4						
W173	2.207	24	3.218	27	5335	19	9.218	14	41.21	14	1.21	28	18.18	54	6.084	10	11.868	6	0.358	59	0.899	57	4.442	8	4.825	2	0	399	7.158	7	1.578	24	0	399	18.584	4						
W174	1.548	34	4.505	17	4.897	19	7.525	13	2.4	13	2.4	19	0.752	64	4.899	4	1.628	5	0.443	59	1.385	23	4.242	8	6.397	0	0	614	7.925	6	1.578	15.985	3									
W175	1.479	31	5.614	17	7.119	12	7.241	13	4.465	13	4.465	12	0.324	142	8.292	8	13.829	3	0.443	74	1.585	23	3.071	8	6.118	0	0.827	36	8.255	5	1.94	19.823	3									
W177	2.545	22	5.715	13	6.031	19	8.232	12	3.192	12	3.192	22	0.824	79	4.951	15	14.597	5	0.833	47	1.25	20	4.071	11	9.795	0	2.295	20	8.257	5	1.99	16.662	3									
W178	3.359	16	6.073	18	3.283	19	8.232	13	3.15	13	3.15	22	0.39	88	4.433	13	14.593	5	0.677	22	0.977	25	4.374	8	5.023	0	0	399	10.219	5	2.048	4.6	0	399	15.535	3						
W179	2.007	23	7.182	12	4.231	17	13.052	12	5.197	12	5.197	19	0.522	108	6.424	19	13.748	4	0.425	27	1.976	19	4.594	8	5.023	0	2.787	18	7.665	5	2.048	4.6	0	399	15.542	3						
KO1	2.057	18	8.57	12	2.728	12	11.152	9	3.867	9	3.867	20	0.785	81	5.912	14	13.748	4	0.784	59	1.27	37	4.874	8	5.023	0	1.828	44	9.618	5	2.048	4.6	0	399	20.577	3						
KO2	1.419	38	7.347	14	6.128	14	11.152	12	3.086	12	3.086	25	0.785	99	4.524	17	16.248	4	0.784	59	1.27	37	4.874	8	5.023	0	1.828	44	9.618	5	2.048	4.6	0	399	20.577	3						
KO3	3.368	32	4.585	14	10.21	23	2.575	12	6.895	12	6.895	22	2.015	66	8.144	17	30.702	4	0.783	69	3.085	23	6.318	9	6.143	0	2.826	124	8.879	5	2.048	4.6	0	399	20.577	3						
KO4	1.139	24	4.585	14	6.772	9	8.272	9	3.697	9	3.697	19	0.272	245	6.708	14	14.87	5	0.557	67	1.385	23	4.218	11	9.453	0	1.585	28	8.825	5	1.448	5.1	0	399	21.232	3						
KO5	1.139	24	4.585	14	6.772	9	8.272	9	3.697	9	3.697	19	0.272	245	6.708	14	14.87	5	0.557	67	1.385	23	4.218	11	9.453	0	1.585	28	8.825	5	1.448	5.1	0	399	21.232	3						
KO6	1.038	29	4.041	16	3.308	28	8.234	13	2.618	13	2.618	19	1.388	28	6.061	11	13.071	3	1.882	42	1.219	24	4.412	9	8.103	0	2.105	34	4.412	6	3.29	13.944	3									
KO8	1.491	29	4.041	16	3.308	28	8.234	13	2.618	13	2.618	19	1.388	28	6.061	11	13.071	3	1.882	42	1.219	24	4.412	9	8.103	0	2.105	34	4.412	6	3.29	13.944	3									
KO9	1.491	29	4.041	16	3.308	28	8.234	13	2.618	13	2.618	19	1.388	28	6.061	11	13.071	3	1.882	42	1.219	24	4.412	9	8.103	0	2.105	34	4.412	6	3.29	13.944	3									
KO10	2.01	23	4.242	21	3.751	18	11.819	10	2.465	10	2.465	29	0.828	58	3.022	19	11.819	3	0.514	43	1.445	26	4.427	8	3.281	0	2.105	34	4.412	6	3.29	13.944	3									
KO11	1.207	23	4.154	17	4.592	11	5.742	9	2.412	9	2.412	17	0.827	77	6.171	9	11.924	3	0.842	30	0.465	73	3.44	9	4.897	0	0	399	6.704	6	1.603	17	0	399	12.478	4						



Supplementary figure 1. Volcano plot showing significant Pearson's correlation between metabolites and rodent sociability

Correlation between mice social preference index for novel mouse or social preference index for mouse and metabolites in the prefrontal cortex (**a**) and hippocampus (**b**) was calculated, respectively. Metabolites with a significant correlation was colored as pink or cyan depending on the quantile of actual Pearson's coefficient from the permuted values, 95% or 97.5% respectively.



Supplementary figure 2. Other linear regression analyses between metabolites and rodent sociability

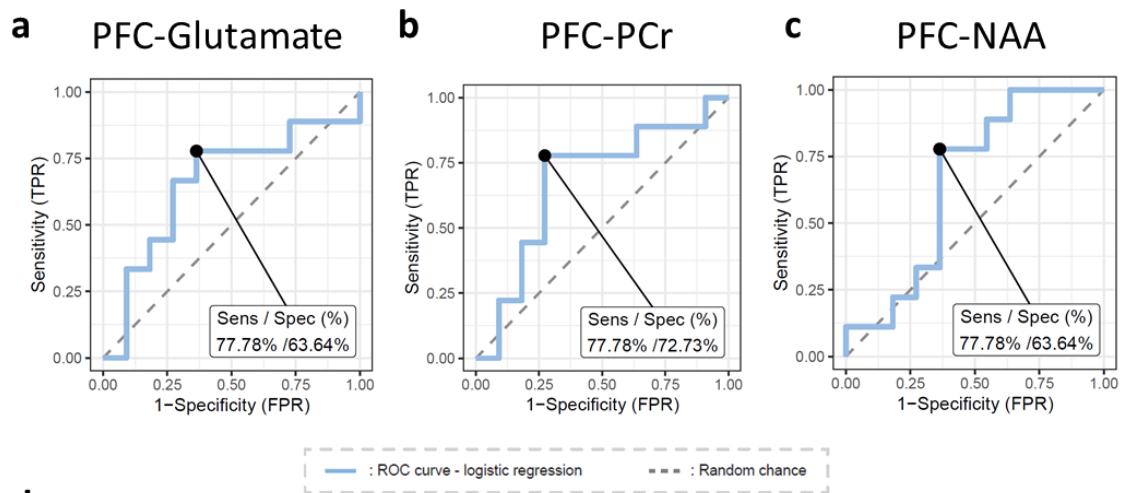
(a-c) Correlation between mice social preference index for novel mouse and each of the significantly altered metabolites in the prefrontal cortex was calculated.

(d) Correlation between mice social preference index and Glx, a metabolite significantly altered in the hippocampus was calculated.

(e) Correlation between mice social preference index and PCr/tCr ratio in hippocampus was calculated.

(f) Correlation between mice social preference index for novel mouse and Glx level in hippocampus was calculated.

Each linear regression line is shown with 95% confidence bands (two dotted lines). The degree of significant correlation (p) and goodness of fit (r^2) were written in each figure.



d

	Glu	PCr	NAA
AUC	0.657	0.677	0.657
(95% CI)	0.409-0.904	0.433-0.92	0.409-0.904
Youden Index	0.414	0.505	0.414
Cut-off(log-odds)	-0.156	-0.262	-0.329

Supplementary figure 3. ROC curve analyses of the prefrontal metabolites

(a-c) ROC curve analyses of glutamate (Glu), phosphocreatine (pCr), and N-acetylaspartate (NAA) in the prefrontal cortex. Each metabolic substrate is not precise enough to predict the genotype. (d) A table describe a detail information for each ROC analysis.