

Supplementary Table 1. 144 anatomical regions and Abbreviations from JHU-MNI atlas (Level 4)

Regions	Abbreviations
SUPERIOR FRONTAL GYRUS left	SFG_L
SUPERIOR FRONTAL GYRUS right	SFG_R
MIDDLE FRONTAL GYRUS left	MFG_L
MIDDLE FRONTAL GYRUS right	MFG_R
INFERIOR FRONTAL GYRUS left	IFG_L
INFERIOR FRONTAL GYRUS right	IFG_R
ORBITAL GYRUS left	OG_L
ORBITAL GYRUS right	OG_R
GYRUS RECTUS left	RG_L
GYRUS RECTUS right	RG_R
POSTCENTRAL GYRUS left	PoCG_L
POSTCENTRAL GYRUS right	PoCG_R
PRECENTRAL GYRUS left	PrCG_L
PRECENTRAL GYRUS right	PrCG_R
SUPERIOR PARIETAL GYRUS left	SPG_L
SUPERIOR PARIETAL GYRUS right	SPG_R
SUPRAMARGINAL GYRUS	SMG_L
SUPRAMARGINAL GYRUS right	SMG_R
ANGULAR GYRUS left	AG_L
ANGULAR GYRUS right	AG_R
PRE-CUNEUS left	PrCu_L
PRE-CUNEUS right	PrCu_R
SUPERIOR TEMPORAL GYRUS left	STG_L
SUPERIOR TEMPORAL GYRUS right	STG_R
MIDDLE TEMPORAL GYRUS left	MTG_L
MIDDLE TEMPORAL GYRUS right	MTG_R
INFERIOR TEMPORAL GYRUS left	ITG_L
INFERIOR TEMPORAL GYRUS right	ITG_R
PARAHIPPOCAMPAL GYRUS left	PHG_L
PARAHIPPOCAMPAL GYRUS right	PHG_R
FUSIFORM GYRUS left	FuG_L
FUSIFORM GYRUS right	FuG_R
SUPERIOR OCCIPITAL GYRUS left	SOG_L
SUPERIOR OCCIPITAL GYRUS right	SOG_R
MIDDLE OCCIPITAL GYRUS left	MOG_L
MIDDLE OCCIPITAL GYRUS right	MOG_R
INFERIOR OCCIPITAL GYRUS left	IOG_L
INFERIOR OCCIPITAL GYRUS right	IOG_R
CUNEUS left	Cu_L
CUNEUS right	Cu_R
LINGUAL GYRUS left	LG_L
LINGUAL GYRUS right	LG_R
POSTERIOR CINGULATE GYRUS left	PCG_L
POSTERIOR CINGULATE GYRUS right	PCG_R

INSULAR left	Insula_L
INSULAR right	Insula_R
AMYGDALA left	Amyg_L
AMYGDALA right	Amyg_R
HIPPOCAMPUS left	Hippo_L
HIPPOCAMPUS right	Hippo_R
CAUDATE NUCLEUS left	Caud_L
CAUDATE NUCLEUS right	Caud_R
PUTAMEN left	Put_L
PUTAMEN right	Put_R
GLOBUS PALLIDUS left	GP_L
GLOBUS PALLIDUS right	GP_R
THALAMUS left	Thalamus_L
THALAMUS right	Thalamus_R
Basal Forebrain left	BasalForebrain_L
Basal Forebrain right	BasalForebrain_R
Nucleus accumbens left	NucAccumbens_L
Nucleus accumbens right	NucAccumbens_R
MIDBRAIN left	midbrain_L
MIDBRAIN right	midbrain_R
Cerebellum left	Cerebellum_L
Cerebellum right	Cerebellum_R
PONS left	Pons_L
PONS right	Pons_R
MEDULLA left	Medulla_L
MEDULLA right	Medulla_R
Anterior Deep Periventricular White Matter left	ant_DPWM_L
Anterior Deep Periventricular White Matter right	ant_DPWM_R
Posterior Deep Periventricular White Matter left	post_DPWM_L
Posterior Deep Periventricular White Matter right	post_DPWM_R
Genu of corpus callosum left	GCC_L
Genu of corpus callosum right	GCC_R
Body of corpus callosum left	BCC_L
Body of corpus callosum right	BCC_R
Splenium of corpus callosum left	SCC_L
Splenium of corpus callosum right	SCC_R
Tapetum left	Tapetum_L
Tapetum right	Tapetum_R
Anterior limb of internal capsule left	ALIC_L
Anterior limb of internal capsule right	ALIC_R
Posterior limb of internal capsule left	PLIC_L
Posterior limb of internal capsule right	PLIC_R
Inferior Deep Periventricular White Matter left	inf_DPWM_L
Inferior Deep Periventricular White Matter right	inf_DPWM_R
Cingulum (cingulate gyrus) left	CGC_L
Cingulum (cingulate gyrus) right	CGC_R
Cingulum (hippocampus) left	CGH_L
Cingulum (hippocampus) right	CGH_R

Fornix/Stria terminalis left	Fx/ST_L
Fornix/Stria terminalis right	Fx/ST_R
Fornix (column and body of fornix) left	Fx_L
Fornix (column and body of fornix) right	Fx_R
Peripheral Parietal White Matter left	PeripheralParietalWM_L
Peripheral Parietal White Matter right	PeripheralParietalWM_R
Anterior Lateral Ventricle left	AnteriorLateralVentricle_L
Anterior Lateral Ventricle right	AnteriorLateralVentricle_R
Posterior Lateral Ventricle left	PosteriorLateralVentricle_L
Posterior Lateral Ventricle right	PosteriorLateralVentricle_R
Inferior Lateral Ventricle left	InferiorLateralVentricle_L
Inferior Lateral Ventricle right	InferiorLateralVentricle_R
III ventricle	III_ventricle
Anterior periventricular white matter cap left	PVWa_L
Anterior periventricular white matter cap right	PVWa_R
Posterior periventricular white matter cap left	PVWp_L
Posterior periventricular white matter cap right	PVWp_R
Peripheral Frontal White Matter left	PeripheralFrontalWM_L
Peripheral Frontal White Matter right	PeripheralFrontalWM_R
Peripheral Temporal White Matter left	PeripheralTemporalWM_L
Peripheral Temporal White Matter right	PeripheralTemporalWM_R
Peripheral Occipital White Matter left	PeripheralOccipitalWM_L
Peripheral Occipital White Matter right	PeripheralOccipitalWM_R
Peripheral Cingulate White Matter left	PeripheralCingulateWM_L
Peripheral Cingulate White Matter right	PeripheralCingulateWM_R
Cerebellum white matter left	CerebellumWM_R
Cerebellum white matter right	CerebellumWM_L
Frontal sulcus left	FrontSul_L
Frontal sulcus right	FrontSul_R
Central sulcus left	CentralSul_L
Central sulcus right	CentralSul_R
Sylvian frontal sulcus left	SylFrontSul_L
Sylvian frontal sulcus right	SylFrontSul_R
Sylvian temporal sulcus left	SylTempSul_L
Sylvian temporal sulcus right	SylTempSul_R
Sylvian parietal sulcus left	SylParieSul_L
Sylvian parietal sulcus right	SylParieSul_R
Parietal sulcus left	ParietSul_L
Parietal sulcus right	ParietSul_R
Cingulate sulcus left	CinguSul_L
Cingulate sulcus right	CinguSul_R
Occipital sulcus left	OcciptSul_L
Occipital sulcus right	OcciptSul_R
Temporal sulcus left	TempSul_L
Temporal sulcus right	TempSul_R
Caudate_tail_L	Caudate_tail_L
Caudate_tail_R	Caudate_tail_R
IV ventricle	IV_ventricle

Anterior external cranial space left	ECSAnterior_L
Posterior external cranial space right	ECSAnterior_R
Anterior external cranial space left	ECSPosterior_L
Posterior external cranial space right	ECSPosterior_R

Supplementary Table 2. Postmortem and in vivo regional values of FA and χ values

Regions	Postmortem FA		In Vivo FA		Postmortem χ		In Vivo χ	
	No. of Pixels	Mean Value	No. of Pixels	Mean Value	No. of Pixels	Mean Value (ppb)	No. of Pixels	Mean Value (ppb)
SFG_L	193044	0.16	232104	0.18	213737	1.97	213680	4.89
SFG_R	NA	NA	247280	0.19	NA	NA	227984	3.88
MFG_L	175071	0.17	217136	0.19	195330	2.21	195192	3.82
MFG_R	NA	NA	213704	0.19	NA	NA	210384	3.92
IFG_L	80965	0.15	90264	0.18	83242	1.92	83312	2.97
IFG_R	NA	NA	87600	0.18	NA	NA	81480	2.56
OG_L	70268	0.17	83864	0.16	85232	1.82	85232	3.14
OG_R	NA	NA	78224	0.16	NA	NA	81456	3.28
RG_L	38456	0.11	49032	0.16	48496	0.88	48584	4.95
RG_R	NA	NA	54744	0.16	NA	NA	54816	5.62
PoCG_L	89922	0.16	98280	0.18	96453	3.85	95840	4.25
PoCG_R	NA	NA	86416	0.17	NA	NA	91680	3.27
PrCG_L	115623	0.19	107008	0.21	93943	5.36	93816	7.54
PrCG_R	NA	NA	135880	0.22	NA	NA	112528	8.02
SPG_L	64976	0.18	67016	0.19	58168	3.62	58168	4.29
SPG_R	NA	NA	54312	0.20	NA	NA	40576	4.29
SMG_L	48179	0.15	85008	0.20	77208	4.06	77208	4.46
SMG_R	NA	NA	86368	0.20	NA	NA	73592	3.55
AG_L	87607	0.16	63064	0.19	63537	2.64	63112	4.25
AG_R	NA	NA	106608	0.20	NA	NA	103520	3.28
PrCu_L	67177	0.17	78768	0.20	79320	4.23	78696	3.28
PrCu_R	NA	NA	75448	0.21	NA	NA	77576	2.85
STG_L	116676	0.14	149920	0.19	134827	3.08	135880	3.56
STG_R	NA	NA	141232	0.18	NA	NA	128056	2.57

MTG_L	107465	0.15	141936	0.20	127798	2.78	128264	3.40
MTG_R	NA	NA	143696	0.19	NA	NA	119936	2.85
ITG_L	65768	0.16	88840	0.16	95303	2.33	94680	4.42
ITG_R	NA	NA	100216	0.15	NA	NA	99400	3.95
PHG_L	12312	0.14	11576	0.16	12352	37.38	12352	5.03
PHG_R	NA	NA	15160	0.15	NA	NA	14976	4.53
FuG_L	86556	0.14	127288	0.15	142881	0.65	141896	2.72
FuG_R	NA	NA	109816	0.16	NA	NA	108480	2.86
SOG_L	18997	0.18	28688	0.20	27864	2.71	26920	2.37
SOG_R	NA	NA	24680	0.20	NA	NA	25704	2.44
MOG_L	113006	0.16	129208	0.20	131790	3.20	132552	3.52
MOG_R	NA	NA	121320	0.20	NA	NA	126784	4.90
IOG_L	29719	0.17	32464	0.17	34824	3.74	34824	5.04
IOG_R	NA	NA	34904	0.18	NA	NA	37280	5.10
Cu_L	55425	0.18	62584	0.22	72323	4.12	72016	4.42
Cu_R	NA	NA	54304	0.21	NA	NA	62528	4.05
LG_L	39945	0.15	67512	0.17	82562	1.82	82712	4.73
LG_R	NA	NA	63704	0.17	NA	NA	72176	4.59
PCG_L	109277	0.16	151336	0.19	139845	1.33	140816	2.42
PCG_R	NA	NA	141952	0.21	NA	NA	131008	2.59
Insula_L	77743	0.15	61040	0.19	62034	0.83	60232	1.96
Insula_R	NA	NA	65320	0.20	NA	NA	62864	1.95
Amyg_L	7368	0.12	14392	0.21	14768	-24.61	14768	-6.34
Amyg_R	NA	NA	15856	0.20	NA	NA	17160	-0.24
Hippo_L	22416	0.18	30232	0.22	29968	-13.12	29968	2.45
Hippo_R	NA	NA	29744	0.21	NA	NA	28904	2.26
Caud_L	31633	0.25	29560	0.21	30368	12.70	30152	34.90
Caud_R	NA	NA	29528	0.19	NA	NA	31120	33.30
Put_L	33807	0.21	39424	0.22	37409	61.60	37314	51.40
Put_R	NA	NA	38016	0.20	NA	NA	36624	49.20
GP_L	6949	0.28	12624	0.28	12393	152.30	11716	119.80

GP_R	NA	NA	12408	0.28	NA	NA	12296	117.90
Thalamus_L	21991	0.21	50984	0.28	55226	-1.63	54816	-4.83
Thalamus_R	NA	NA	52840	0.27	NA	NA	52856	3.34
BasalForebrain_L	12970	0.26	21688	0.31	22312	20.60	22312	5.36
BasalForebrain_R	NA	NA	22192	0.31	NA	NA	24016	5.55
NucAccumbens_L	1836	0.15	5048	0.19	2672	1.11	2672	11.00
NucAccumbens_R	NA	NA	5640	0.20	NA	NA	4392	4.27
midbrain_L	23608	0.38	41936	0.44	41680	19.20	41680	-0.52
midbrain_R	NA	NA	42328	0.43	NA	NA	41688	0.17
Cerebellum_L	250360	0.17	491280	0.22	375864	0.66	375864	-3.66
Cerebellum_R	NA	NA	472056	0.19	NA	NA	421840	-2.58
Pons_L	40488	0.41	67856	0.44	67704	-0.55	67704	-11.20
Pons_R	NA	NA	73680	0.44	NA	NA	75232	-10.84
Medulla_L	1344	0.19	16760	0.34	10680	-0.86	10680	-4.70
Medulla_R	NA	NA	19560	0.36	NA	NA	12576	-3.60
ant_DPWM_L	164414	0.25	232248	0.43	222317	-21.78	222832	-16.43
ant_DPWM_R	NA	NA	235536	0.44	NA	NA	221568	-15.95
post_DPWM_L	40059	0.22	42160	0.45	42521	-21.74	41976	-21.50
post_DPWM_R	NA	NA	35200	0.49	NA	NA	37000	-18.07
GCC_L	18073	0.40	21992	0.64	21988	-5.20	21912	-14.60
GCC_R	NA	NA	21480	0.66	NA	NA	22480	-14.80
BCC_L	24936	0.39	28600	0.64	30204	-4.36	29864	-26.85
BCC_R	NA	NA	27824	0.64	NA	NA	29584	-29.82
SCC_L	41236	0.30	45160	0.61	45980	-4.07	46320	-21.12
SCC_R	NA	NA	46904	0.63	NA	NA	48600	-19.55
Tapetum_L	1311	0.31	1632	0.39	1488	-15.11	1544	2.13
Tapetum_R	NA	NA	1176	0.27	NA	NA	1008	25.50
ALIC_L	6316	0.25	19376	0.47	20986	35.70	20687	19.60
ALIC_R	NA	NA	19624	0.48	NA	NA	19768	8.14
PLIC_L	3882	0.29	25808	0.53	29434	-17.27	29127	-15.49
PLIC_R	NA	NA	26216	0.52	NA	NA	28912	-22.20

inf_DPWM_L	80231	0.39	169112	0.49	173082	-11.74	173668	-14.81
inf_DPWM_R	NA	NA	142760	0.50	NA	NA	144440	-14.98
CGC_L	11745	0.39	23336	0.45	21692	3.75	21608	-2.73
CGC_R	NA	NA	24888	0.44	NA	NA	23984	-6.00
CGH_L	2822	0.27	12624	0.37	12244	-5.90	12344	16.50
CGH_R	NA	NA	12592	0.41	NA	NA	13576	11.90
Fx/ST_L	6640	0.11	11728	0.41	11148	-0.30	11208	-0.55
Fx/ST_R	NA	NA	11312	0.47	NA	NA	11360	3.96
Fx_L	2334	0.27	4136	0.46	4456	-2.68	4400	-16.91
Fx_R	NA	NA	5128	0.50	NA	NA	5008	-27.05
PeripheralParietalWM_L	158096	0.18	291576	0.41	275990	1.41	273280	-1.51
PeripheralParietalWM_R	NA	NA	293432	0.41	NA	NA	264344	-2.83
AnteriorLateralVentricle_L	79315	0.18	33392	0.21	34218	0.78	34472	9.30
AnteriorLateralVentricle_R	NA	NA	30024	0.21	NA	NA	30984	4.19
PosteriorLateralVentricle_L	32645	0.14	11960	0.29	15555	-5.30	14712	12.30
PosteriorLateralVentricle_R	NA	NA	8736	0.20	NA	NA	9992	7.19
InferiorLateralVentricle_L	7343	0.10	4048	0.25	5312	-12.28	5312	1.43
InferiorLateralVentricle_R	NA	NA	7424	0.25	NA	NA	9040	7.15
III_ventricle	18316	0.20	12472	0.27	10758	6.46	10808	-16.98
PVWa_L	8997	0.22	5120	0.28	4400	4.89	4448	-2.50
PVWa_R	NA	NA	5608	0.24	NA	NA	6264	-1.83
PVWp_L	3940	0.27	3016	0.32	3178	1.26	3248	25.40
PVWp_R	NA	NA	2824	0.34	NA	NA	2472	40.50
PeripheralFrontalWM_L	232218	0.25	419280	0.40	355450	-3.01	357432	0.74
PeripheralFrontalWM_R	NA	NA	438960	0.39	NA	NA	366536	-0.64
PeripheralTemporalWM_L	141510	0.27	210488	0.38	180730	-0.82	180000	1.40
PeripheralTemporalWM_R	NA	NA	223816	0.38	NA	NA	168064	1.35
PeripheralOccipitalWM_L	76792	0.30	209536	0.37	208333	-1.57	210464	-6.02
PeripheralOccipitalWM_R	NA	NA	214272	0.39	NA	NA	212736	-7.25
PeripheralCingulateWM_L	9240	0.38	34056	0.41	30568	-2.85	30840	2.58
PeripheralCingulateWM_R	NA	NA	25512	0.40	NA	NA	23808	8.60

CerebellumWM_R	NA	NA	100160	0.38	NA	NA	71112	9.75
CerebellumWM_L	21392	0.10	95080	0.39	30096	-6.37	30096	3.00
FrontSul_L	237688	0.12	154392	0.14	159347	2.04	159736	-1.27
FrontSul_R	NA	NA	105448	0.14	NA	NA	132976	1.42
CentralSul_L	30240	0.12	20200	0.15	24520	9.45	24520	3.78
CentralSul_R	NA	NA	18400	0.16	NA	NA	23104	4.86
SylFrontSul_L	34328	0.11	12848	0.17	21307	2.71	21456	-4.66
SylFrontSul_R	NA	NA	9904	0.17	NA	NA	25144	-8.74
SylTempSul_L	29678	0.08	26152	0.19	29560	8.65	30088	-1.35
SylTempSul_R	NA	NA	19048	0.18	NA	NA	29784	-9.98
SylParieSul_L	8731	0.15	3504	0.19	3144	-0.69	3144	-2.22
SylParieSul_R	NA	NA	1704	0.16	NA	NA	1688	-5.63
ParietSul_L	134652	0.08	74976	0.16	83256	5.98	83256	0.00
ParietSul_R	NA	NA	73512	0.15	NA	NA	86432	0.67
CinguSul_L	28884	0.20	24152	0.17	29304	2.14	29304	9.76
CinguSul_R	NA	NA	23160	0.18	NA	NA	32568	5.42
OcciptSul_L	58472	0.14	13392	0.17	18090	3.92	18208	2.50
OcciptSul_R	NA	NA	14240	0.20	NA	NA	18128	-1.80
TempSul_L	23304	0.08	9248	0.20	10500	0.43	10536	-7.89
TempSul_R	NA	NA	9400	0.20	NA	NA	14120	-12.46
Caudate_tail_L	3528	0.20	2896	0.27	2768	-16.04	2768	-4.19
Caudate_tail_R	NA	NA	3128	0.31	NA	NA	2808	-3.49
IV_ventricle	10768	0.19	14240	0.22	13640	-5.49	13640	30.80
ECSAnterior_L	72565	0.14	20008	0.10	1624	-0.77	1624	-11.92
ECSAnterior_R	NA	NA	15096	0.11	NA	NA	800	3.68
ECSPosterior_L	68943	0.14	12032	0.12	240	0.25	240	7.28
ECSPosterior_R	NA	NA	6224	0.12	NA	NA	56	-3.80

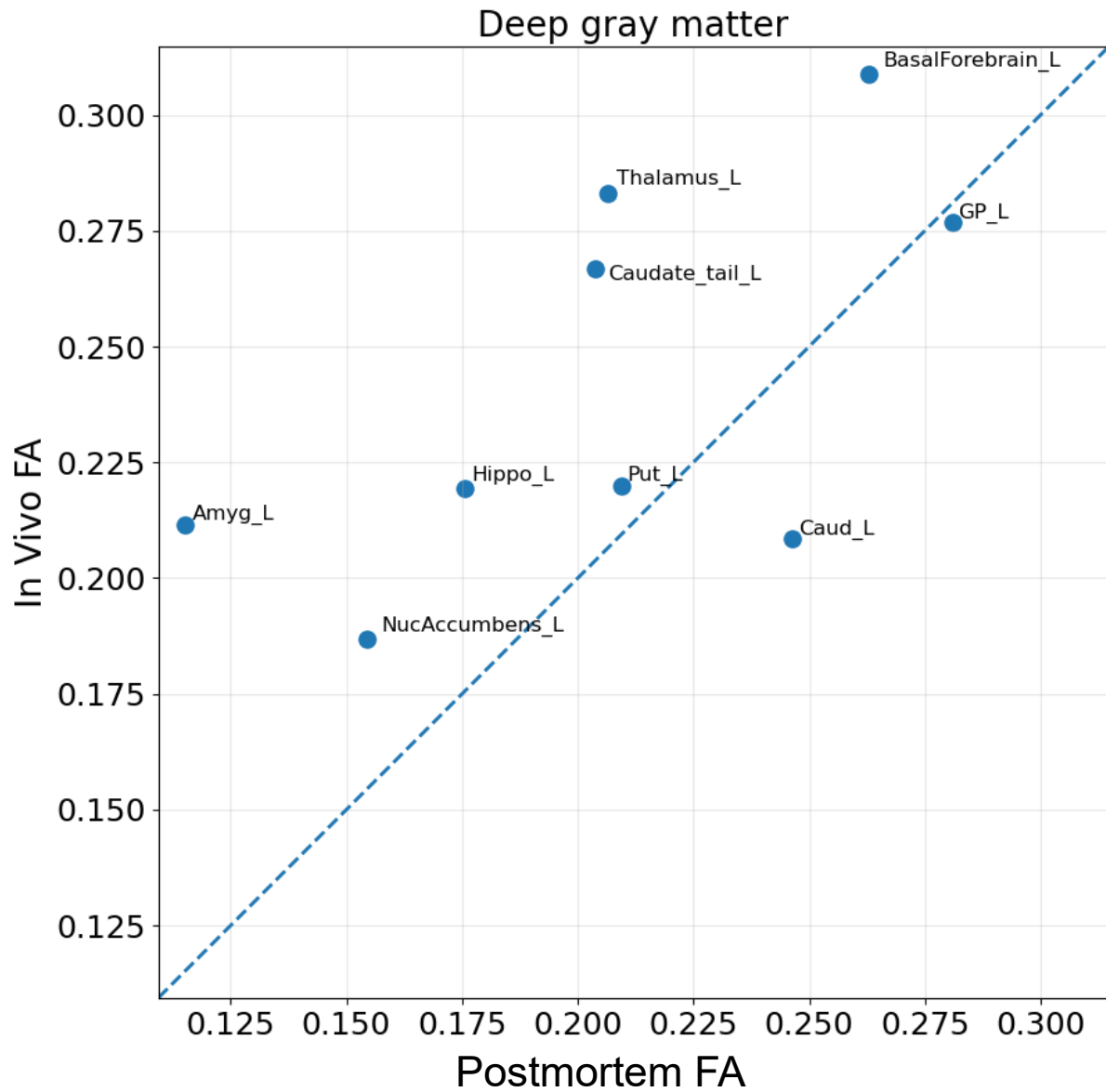
Supplementary Table 3: Equipment explanation

Equipment	Explanations
FreeCAD (ver. 0.21.0, 2023)	Free and open-source software for 3D modeling and design
Ultimaker 2 Extended+ B.V.	3D extruder printer used to create large-scale objects
Cura (ver. 5.4.0)	Open-source slicing software used to prepare the models for printing
1-gallon, wide-mouth, plastic bucket	To fix the brain sample in plentiful 10% phosphate-buffered formalin solution
Chemical-resistant gloves and lab coats	Chemical-resistant gloves and other protective clothing should be worn
Face shields	Face shields should always be worn while handling formalin solutions
100 ml syringe	To pour Fomblin™ into the container from the top holes
27-gauge needle and 1 ml syringe	To aspirate air bubbles trapped in the ventricles or along the cortical surface
Refrigerator	To keep the brain in phosphate-buffered saline at 35°F
Polycarbonate desiccator (330 mm × 330 mm × 245 mm)	Vacuum chamber to remove air bubbles from the brain and the container

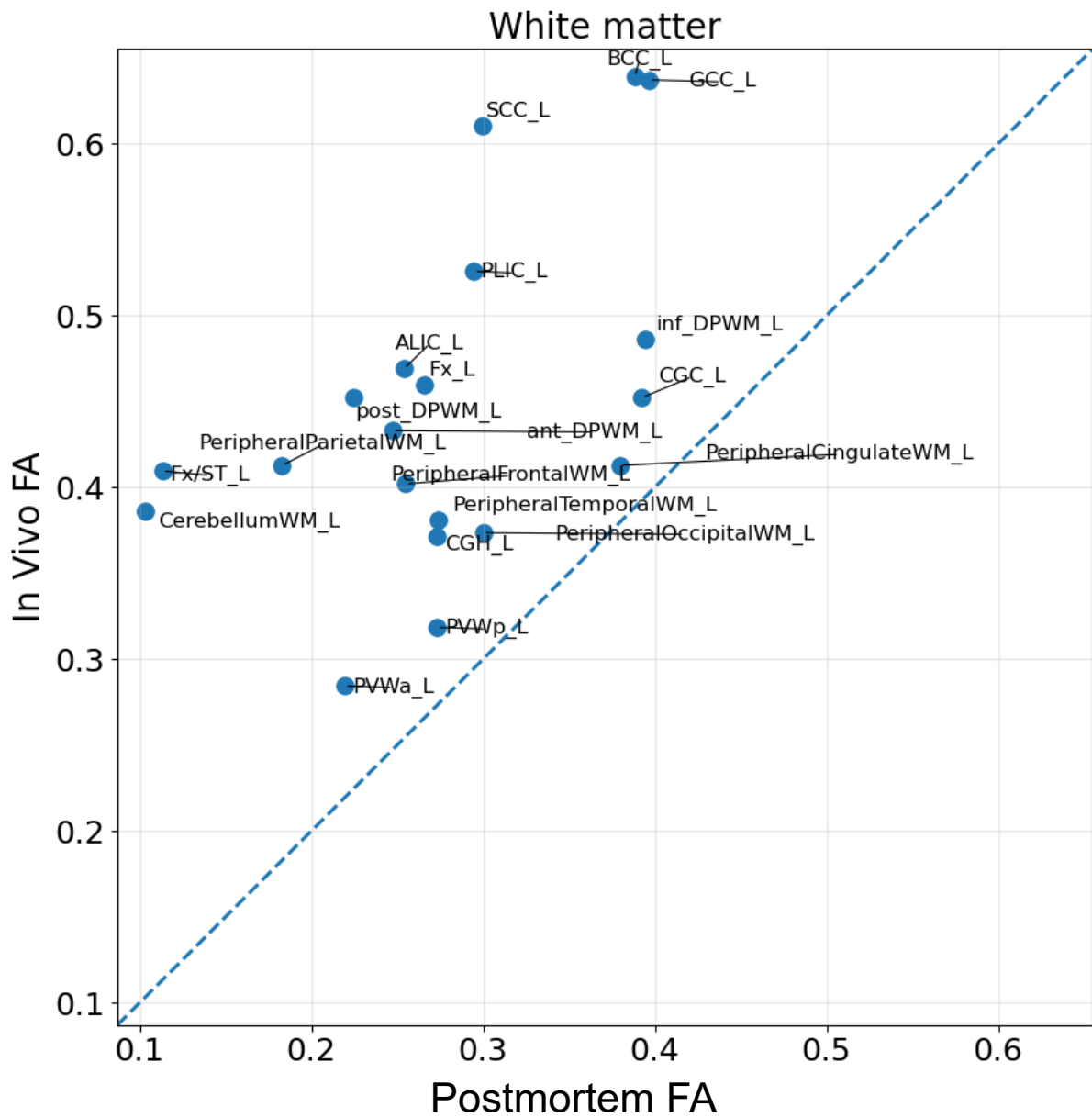
Supplementary Table 4: Material explanation

Materials	Explanations
10% phosphate-buffered formalin solution	pH-neutral solution for histological brain tissue fixation
Phosphate-buffered saline	Buffer solution for maintaining the pH and osmolarity to prevent changes in tissues
Gadopentetate dimeglumine	MRI contrast agents to shorten repetition time without compromising diffusion measures
Liquid perfluoropolyether (Fomblin TM)	Proton-free liquid to reduce magnetic susceptibility artifacts
Polylactic acid filaments	Biodegradable and eco-friendly filaments as the printing materials
Small plugs of plastic epoxy	To seal the spout and any other openings on the lid of the ellipsoid-shaped container
Plastic pipes and pins	To support and pad the brain sample in the container and keep it stable
Polyurethane adhesive (Gorilla TM)	To attach the outer lid to the bottom piece of the container
Spray sealant adhesive (Permatex TM)	To seal potential gaps between the outer lid and the bottom piece of the container

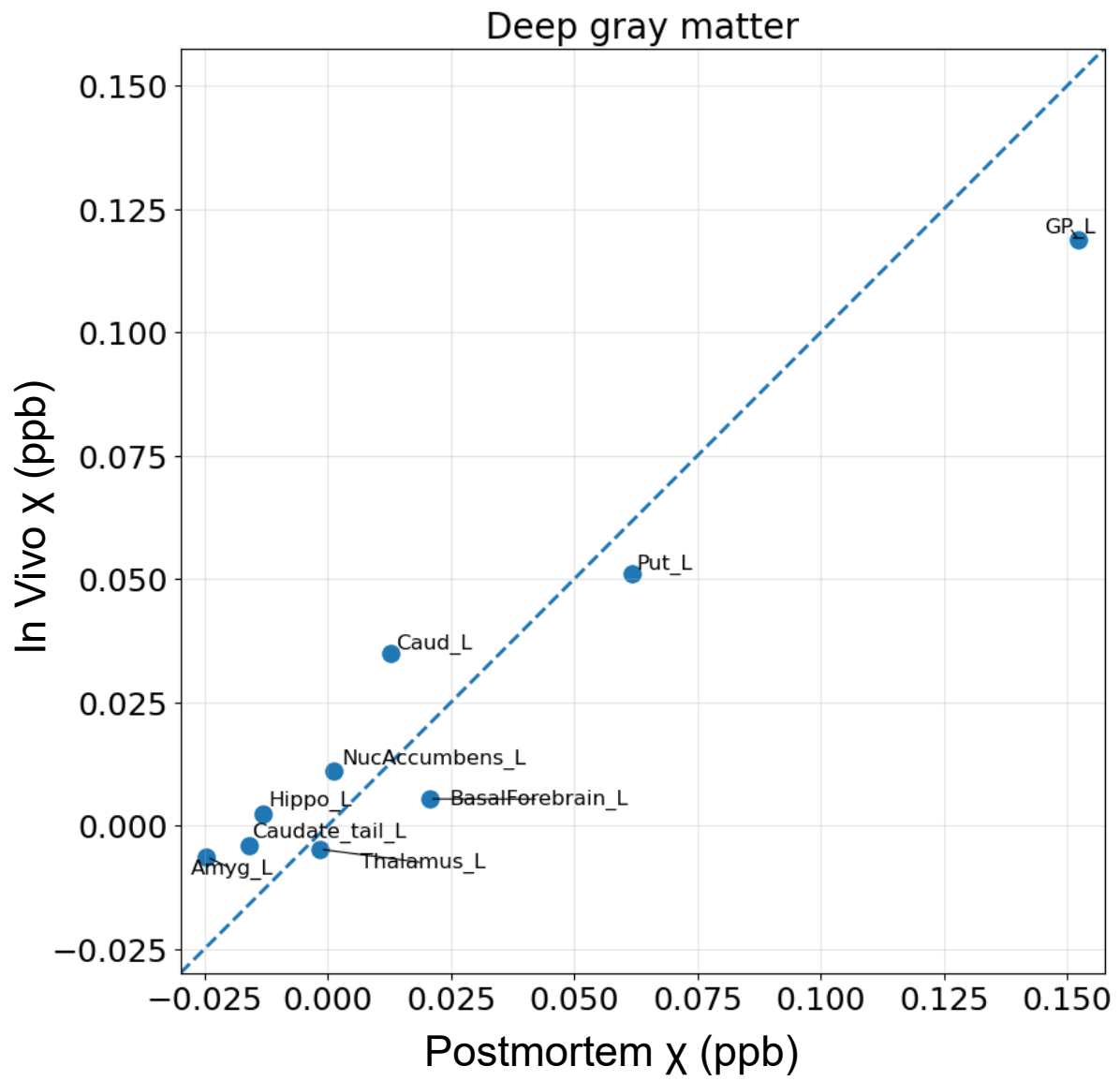
Supplementary Fig. 1: Region-wise comparisons of postmortem vs. in vivo FA and χ values with anatomical labels, shown separately for deep gray matter and white matter regions



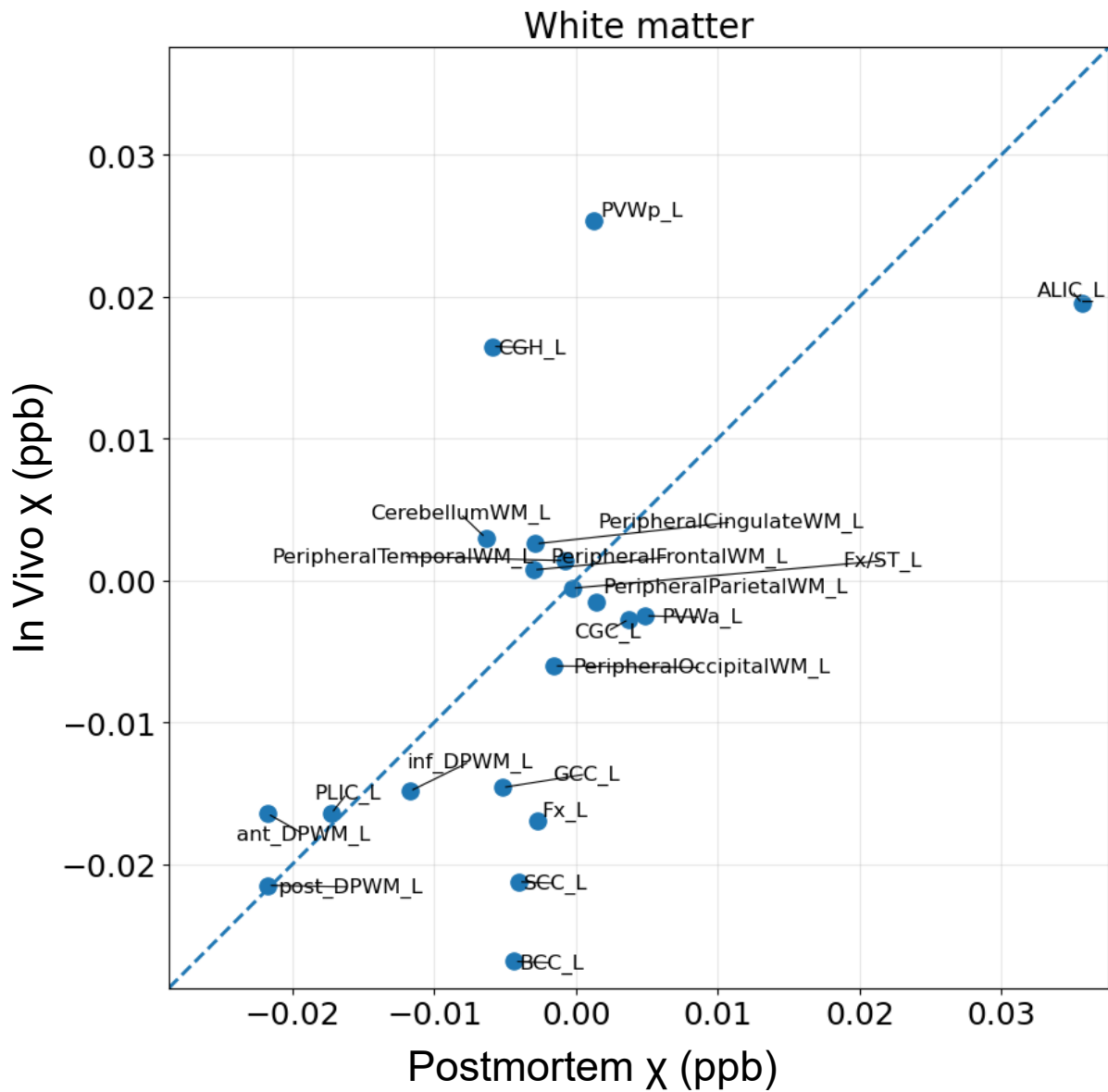
(Pearson's $r = 0.63$, $p = 0.067$)



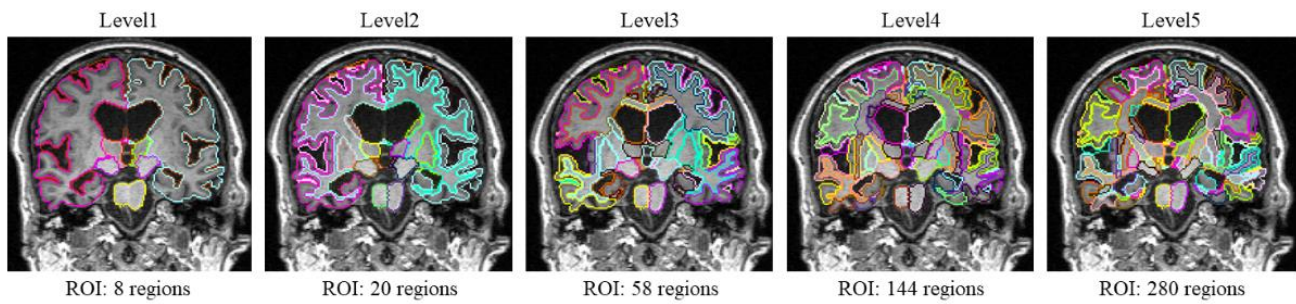
(Pearson's $r = 0.51$, $p = 0.022$)



(Pearson's $r = 0.97$, $p = 1.525 \times 10^{-5}$)



(Pearson's $r = 0.60$, $p = 0.005$)

Supplementary Fig. 2: Multiple hierarchical structural levels

(<https://github.com/OishiLab/OpenMAP-T1>)

OpenMAP-T1 parcellates a whole brain into five hierarchical structural levels (Level 1: Hemispheric level; Level 2: Gray and white matter segmentation level; Level 3: Lobar level; Level 4: Coarse parcellation level; Level 5: Fine parcellation level).