Supplementary

Table S1 The detail of MRS parameters, reported as the Minimum Reporting Standards for *in vivo* MRS checklist.

Site (name or number)	Parameters	Parameters
1. Hardware		
a. Field strength [T]	3T	3T
b. Manufacturer	Philips	Philips
c. Model (software version if available)	Elition X	Elition X
d. RF coils: nuclei (transmit/receive), number of channels, type, body part	32 channel ^{1}H head coil	Dual-tuned (^{1}H/^{31}P) birdcage coil (Rapid Biomed, Germany)
e. Additional hardware	N/A	N/A
2. Acquisition		
a. Pulse sequence	PRESS (GABA/GSH)	2D-CSI
b. Volume of interest (VOI) locations	Anterior cingulate cortex	N/A
c. Nominal VOI size [cm^3, mm^3]	30 × 30 × 25 mm^3	Slice thickness = 20 mm, field of view = 240×240 mm^2, acquired voxel sizes = 40×40×20 mm^3
d. Repetition time (T_R), echo time (T_E) [ms. s]	T_R/T_E = 2000/68 ms for GABA-edited; T_R/T_E = 2000/130 ms for GSH-edited	T_R/T_E = 3500/0.22 ms
e. Total number of excitations or acquisitions per spectrum	128 averages	6 averages
In time series for kinetic studies		
i. Number if averaged spectra (NA) per time point		
ii. Averaging method (eg block-wise or moving average)		
iii. Total number of spectra (acquird/ in time series)		
f. Additional sequence parameters (spectral width in Hz, number id spectral points, frequency offsets). If STEAM: mixing time (TM). If MRSI：2D or 3D，FOV in all directions, matrix size, acceleration factors, sampling method	2000 Hz, 1024 data points	3000 Hz, 2048 data points
g. Water suppression method	VAPOR	N/A
h. Shimming method, reference peak, and thresholds for “acceptance of shim” chosen	Automated second-order pencil beam shim	Automated first-order pencil beam shim and WALTZ-4 broadband heteronuclear decoupling with nuclear Overhauser effect
i. Triggering or motion correction method (respiratory, peripheral, cardiac triggering, incl. device used and delays)	None	None
3. Data analysis methods and outputs		
a. Analysis software	Gannet (version 3.0)	JMRUI (version 7.0.3)
b. Processing steps deviating from quoted reference or product	None	None
c. Output measure (e.g., absolute concentration, institutional units, ratio), processing steps deviating from quoted reference or product	Ratios to creatine/the relaxation correction water	total phosphorus signal
d. Quantification references and assumptions, fitting model assumptions	Default basis set	AMARES Gaussian lineshapes
4. Data quality		
a. Reported variables (SNR, linewidth (with reference peaks))	SNR: 18.856±3.680 (GABA+); 24.910±5.763 (Glx); 8.688±2.053 (GSH)	Frontal lobe: SNR=48.74; Temporal lobe: SNR=50.01; Thalamus: SNR=95.31; Occipital lobe: SNR= 64.06
b. Data exclusion criteria	Fit error < 15%	Manual visual to exclude spurious signals
c. Quality measures of postprocessing model fitting (e.g., CRLB, goodness of fit, SD of residual)	Fit error =4.643±1.194 (GABA+); Fit error =3.521±1.361 (Glx); Fit error =8.288±2.206 (GSH)	Two Occipital lobe raw data were excluded
d. Sample spectrum	*Figure 1*	*Figure 2*

https://dx.doi.org/10.21037/qims-24-1853

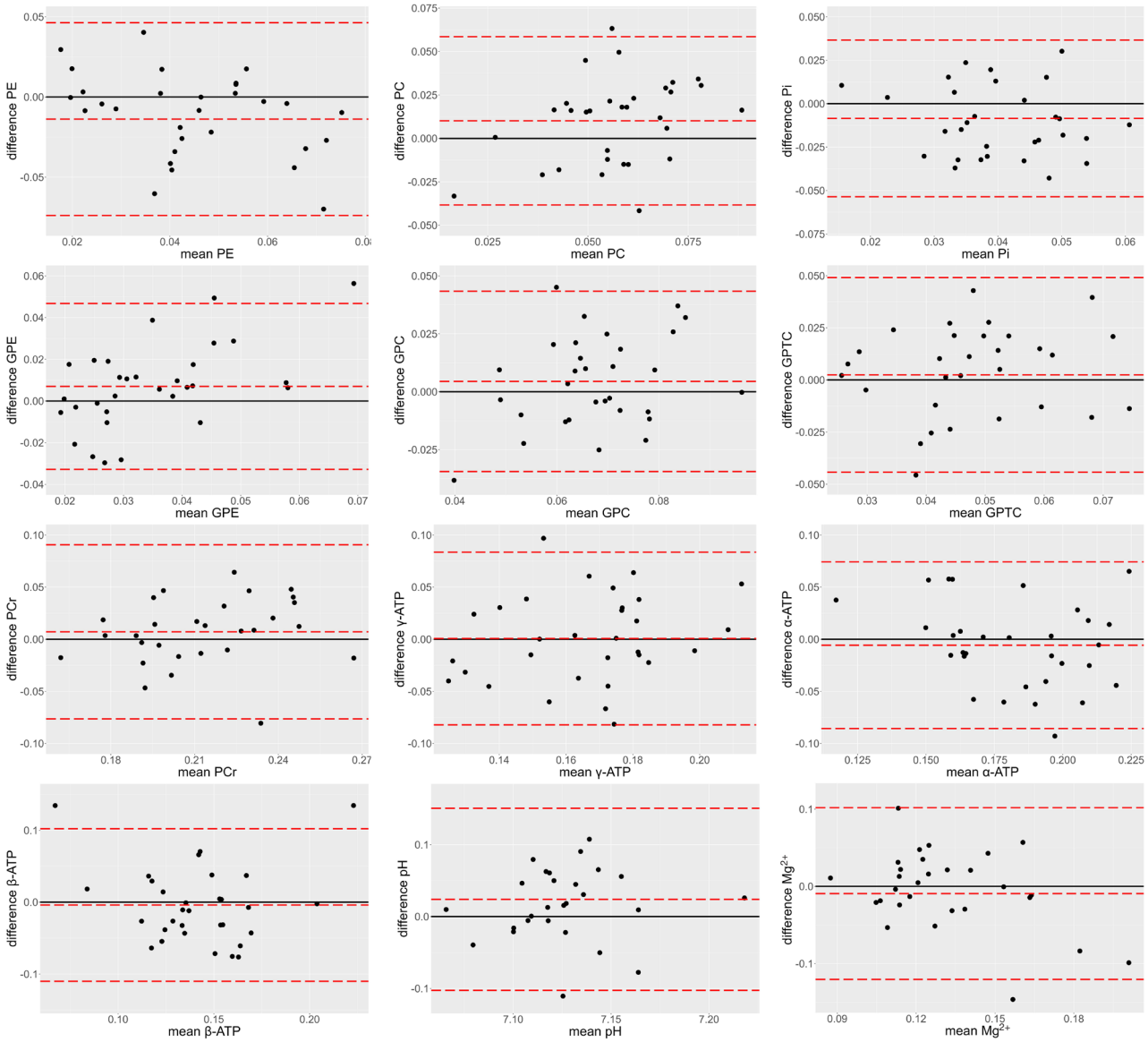

Figure S1 Bland-Altman plots of the two scanned time points of ^{31}P-MRS metabolites in frontal lobe region. All amplitudes were normalized to the total phosphorus signal detected within the respective voxel prior to statistical analyses. From top to bottom, left to right: PE: phosphoethanolamine; PC: phosphocholine; Pi: inorganic phosphate; GPE: glycerophosphoethanolamine; GPC: glycerophosphocholine; GPTC: glycerophosphatidylcholine; PCr: phosphocreatine; γ-, α-, β-ATP: α-, β-, γ-adenosine triphosphate; pH; Mg^{2+}, Magnesium ion.

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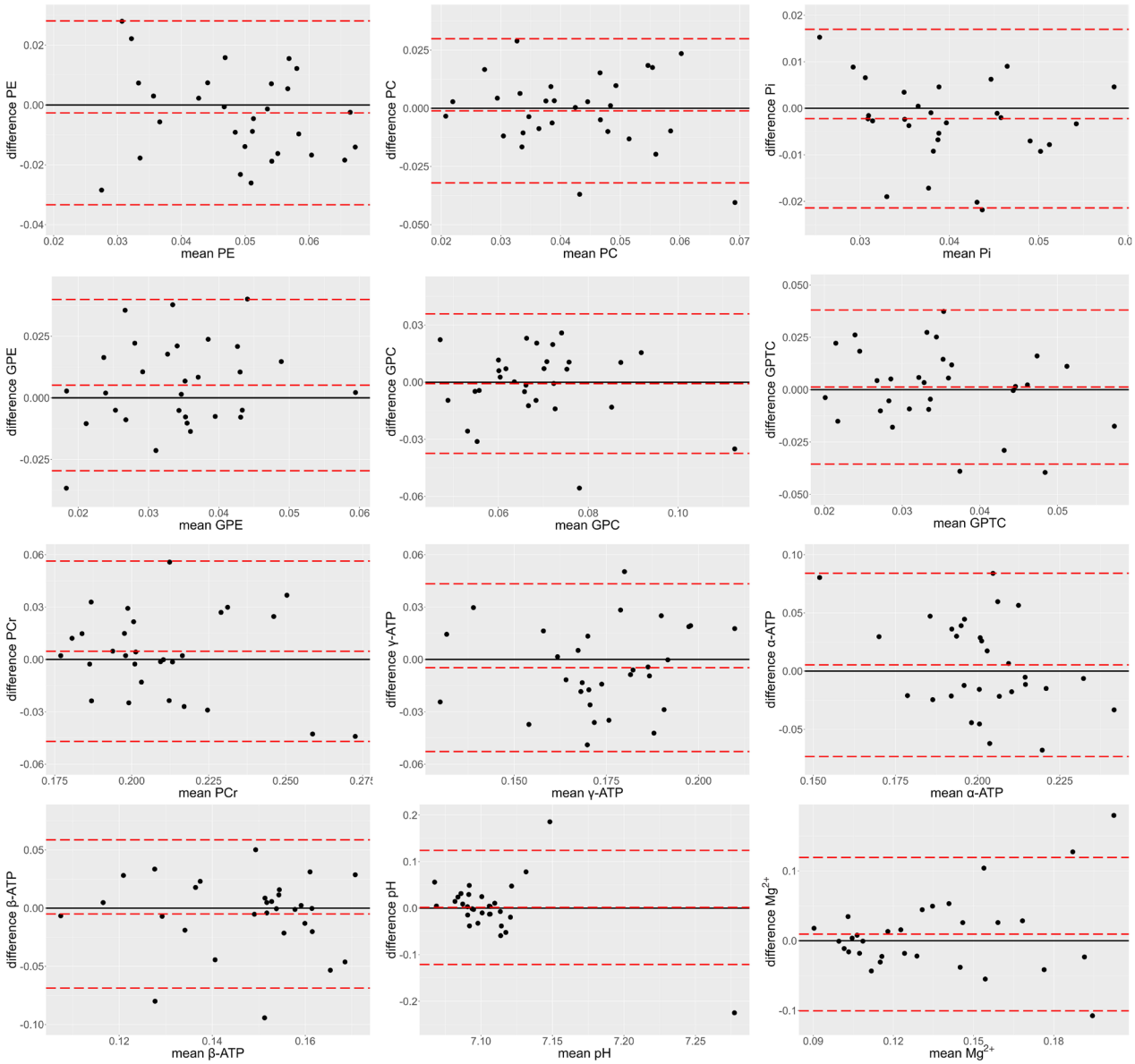

Figure S2 Bland-Altman plots of the two scanned time points of ^{31}P-MRS metabolites in temporal lobe region. All amplitudes were normalized to the total phosphorus signal detected within the respective voxel prior to statistical analyses. From top to bottom, left to right: PE: phosphoethanolamine; PC: phosphocholine; Pi: inorganic phosphate; GPE: glycerophosphoethanolamine; GPC: glycerophosphocholine; GPTC: glycerophosphatidylcholine; PCr: phosphocreatine; γ-, α-, β-ATP: α-, β-, γ-adenosine triphosphate; pH; Mg^{2+}, Magnesium ion.

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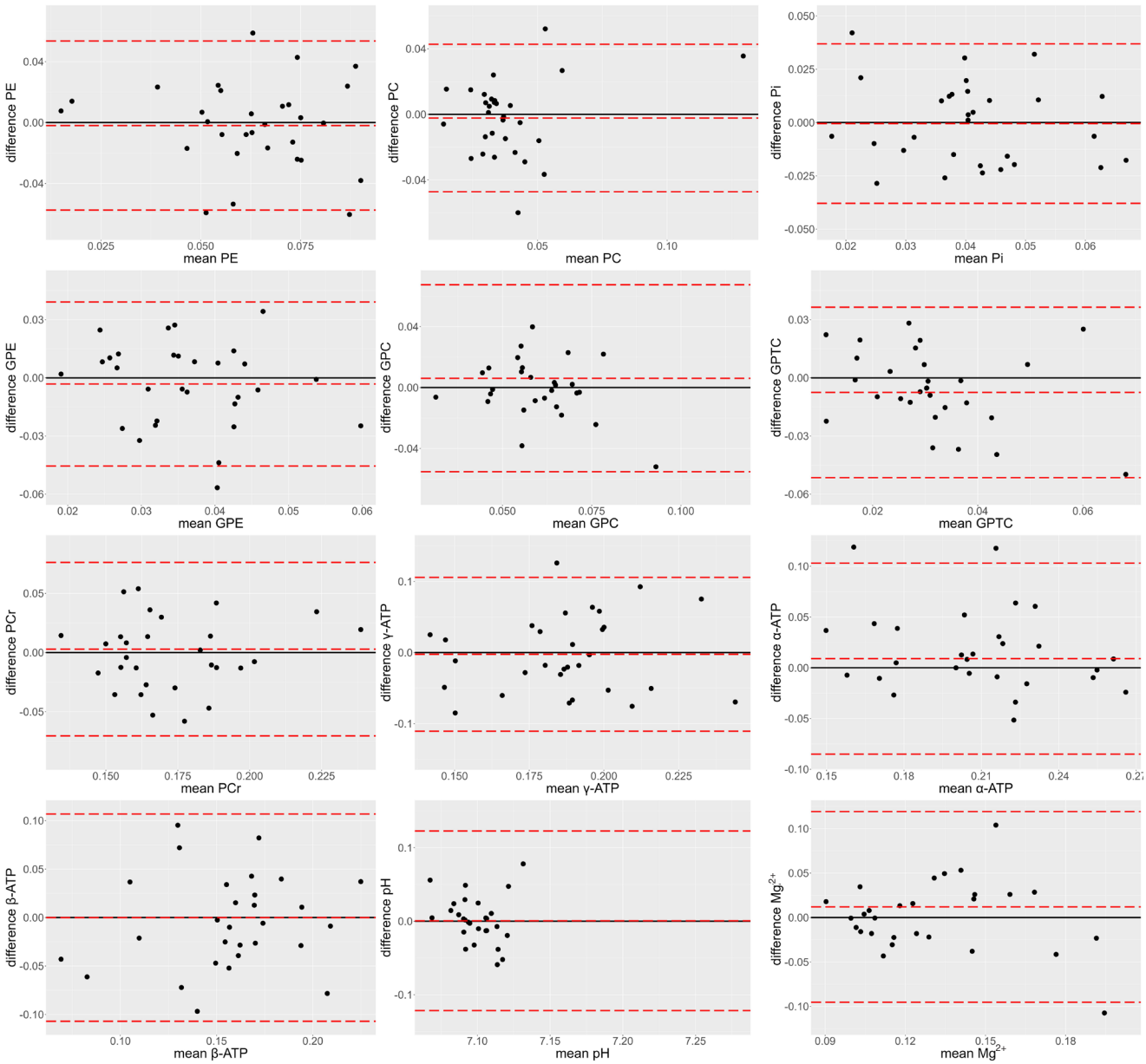

Figure S3 Bland-Altman plots of the two scanned time points of ^{31}P-MRS metabolites in occipital lobe region. All amplitudes were normalized to the total phosphorus signal detected within the respective voxel prior to statistical analyses. From top to bottom, left to right: PE: phosphoethanolamine; PC: phosphocholine; Pi: inorganic phosphate; GPE: glycerophosphoethanolamine; GPC: glycerophosphocholine; GPTC: glycerophosphatidylcholine; PCr: phosphocreatine; γ-, α-, β-ATP: α-, β-, γ-adenosine triphosphate; pH; Mg^{2+}, Magnesium ion.

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