Sample figure and tables
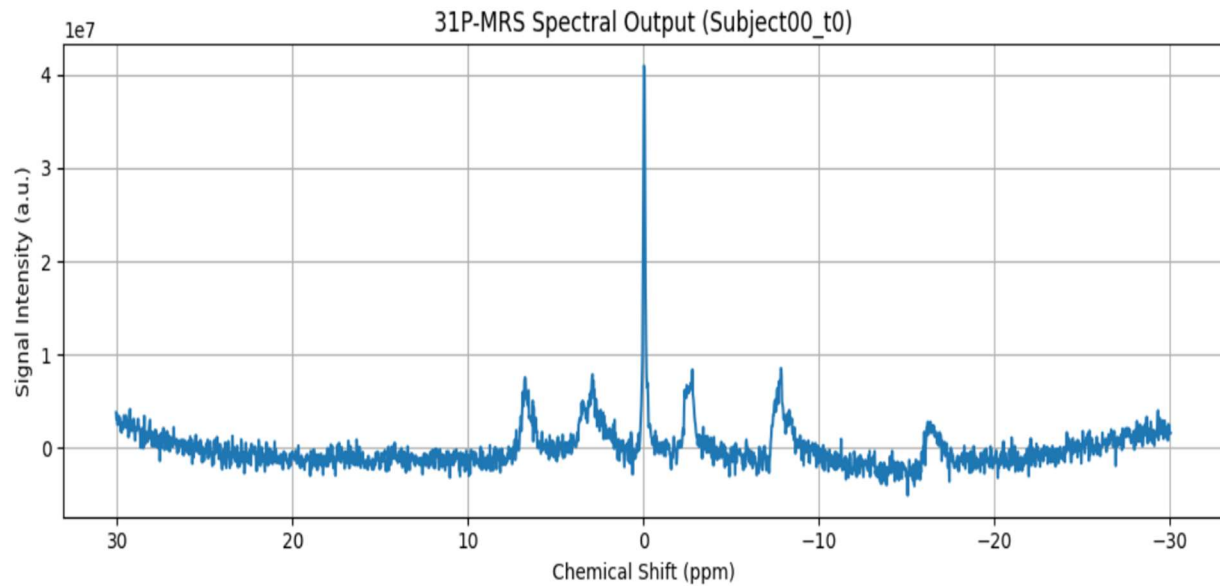

Figure 1: Original visualization by Deelchand et al [1].

Thanks to the authors, Fear et al [2] for providing access to the 31p-mrs-redesign dataset
https://git.app.uib.no/biomedvis2025/31p-mrs-redesign/-/tree/main

This folder has a data subfolder containing the .csv files (chemical shifts, spectra and single spectrum). It also contains two .png images of existing visualization (including figure 1

above). It also has the .py file containing the code used produce the existing visualization above and the dictionary table containing the chemical shifts dictionary.
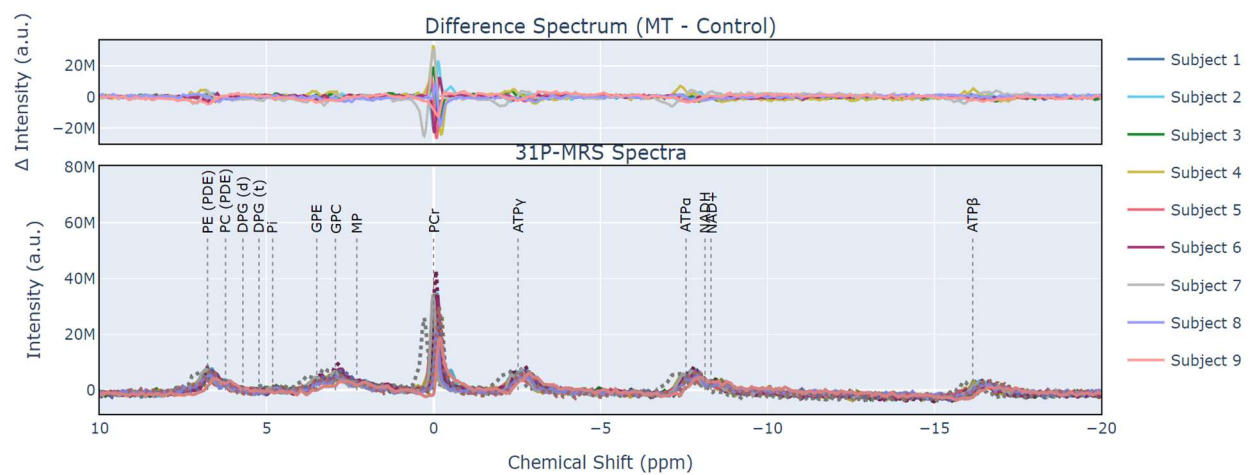

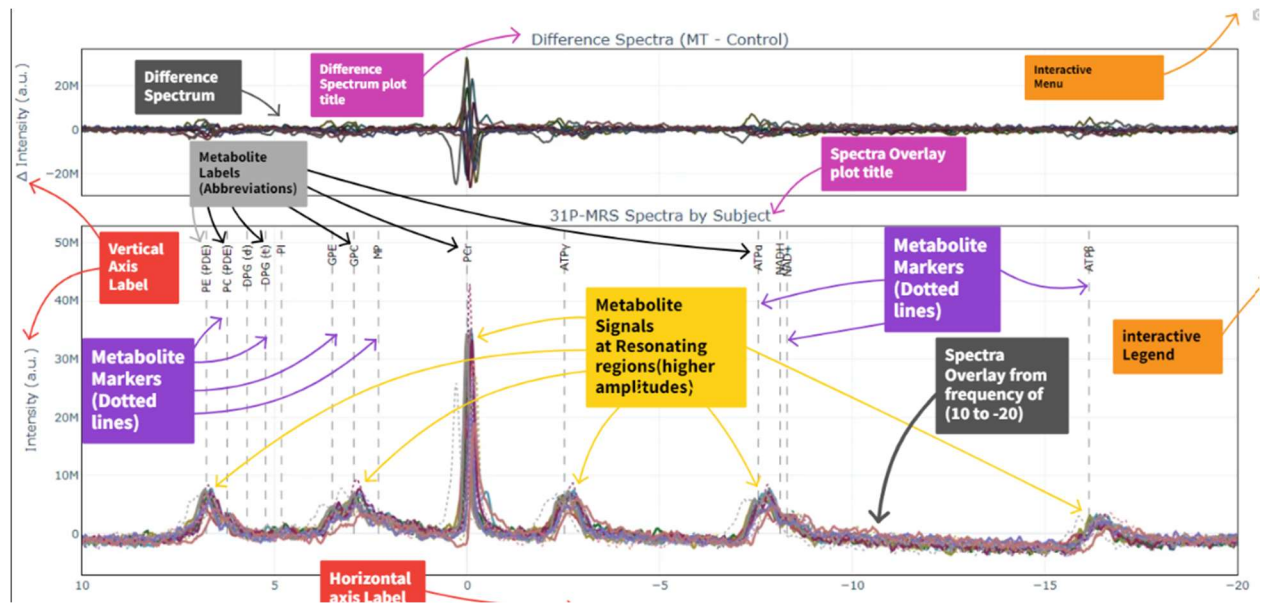Figure 2: Spectra overlay (Proposed visualization)

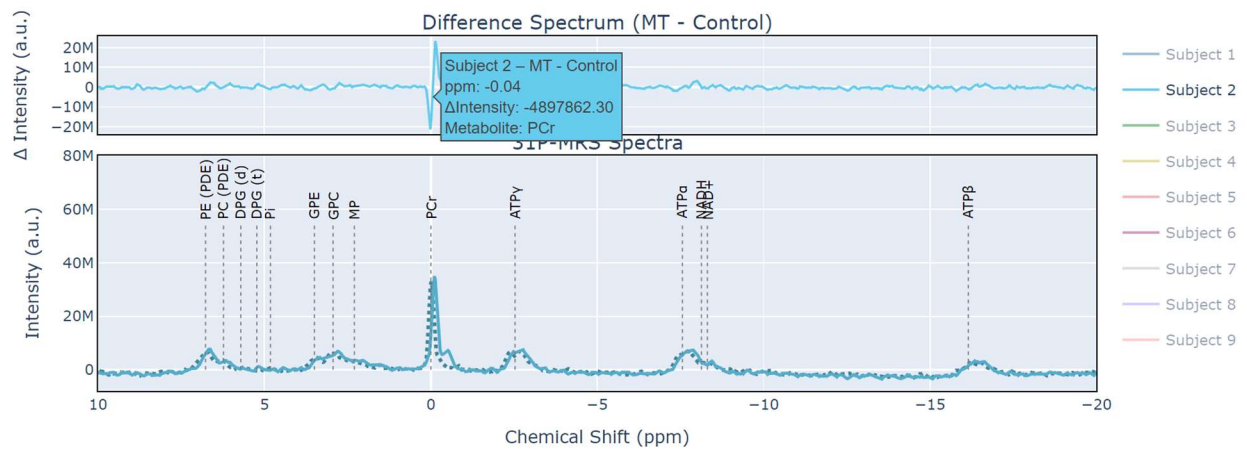Figure 3: Spectra overlay with descriptive labels

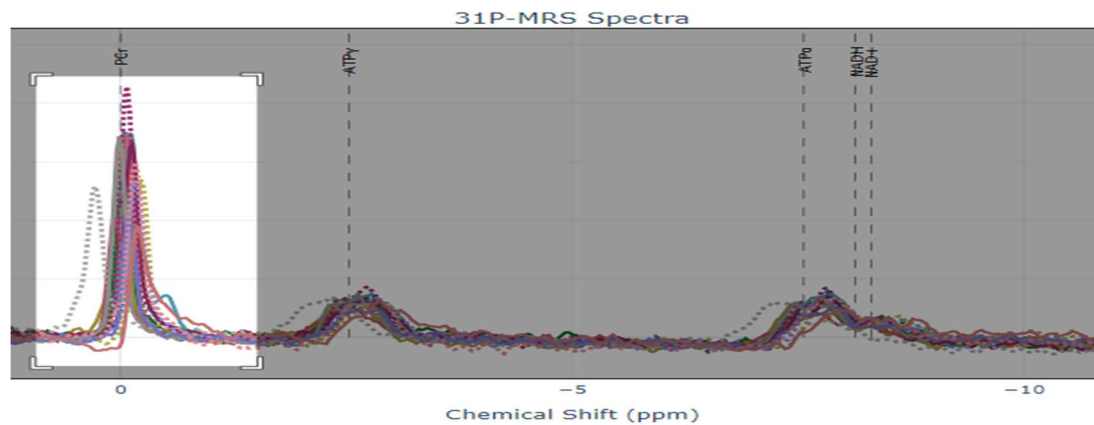Figure 4: Subject-wise Spectra pair and difference spectrum

Figure 5: Click & hold, then drag to highlight the intended zooming space
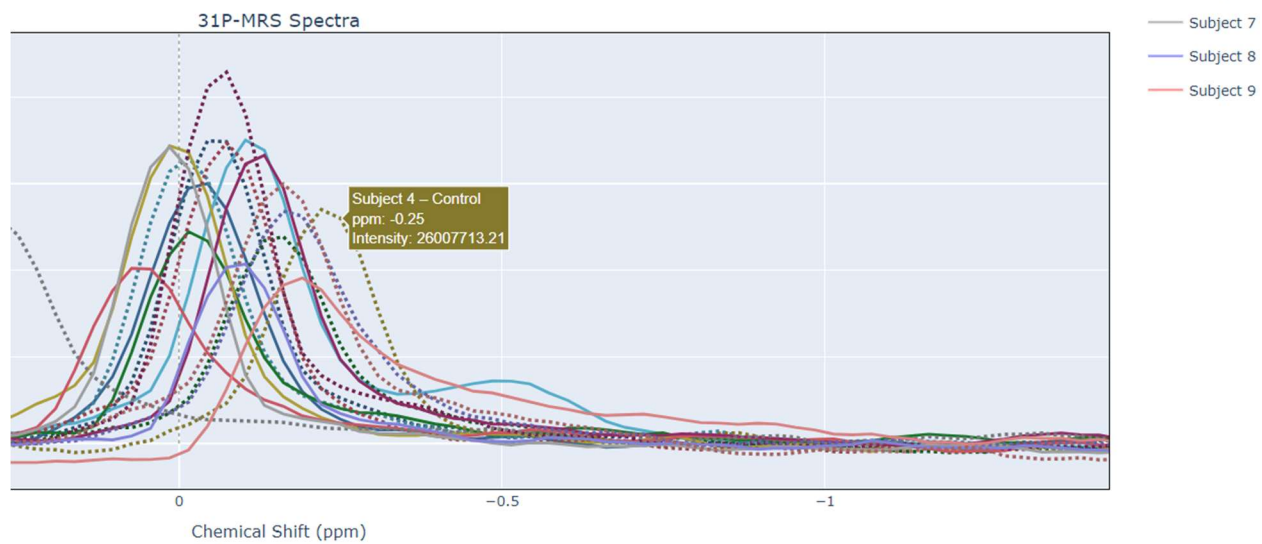
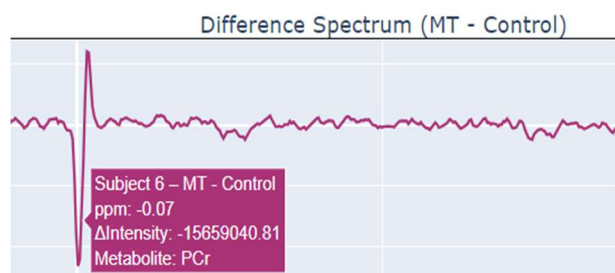Figure 6: Release the mouse button to visualize the zooming effect

Figure 7: Difference spectrum for subject 6 with visual tooltip
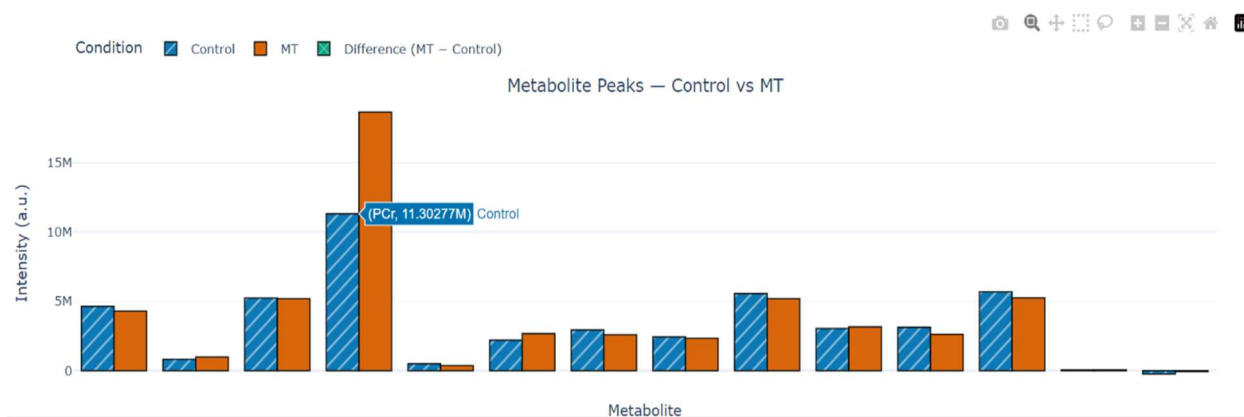

Figure 8: Legend section
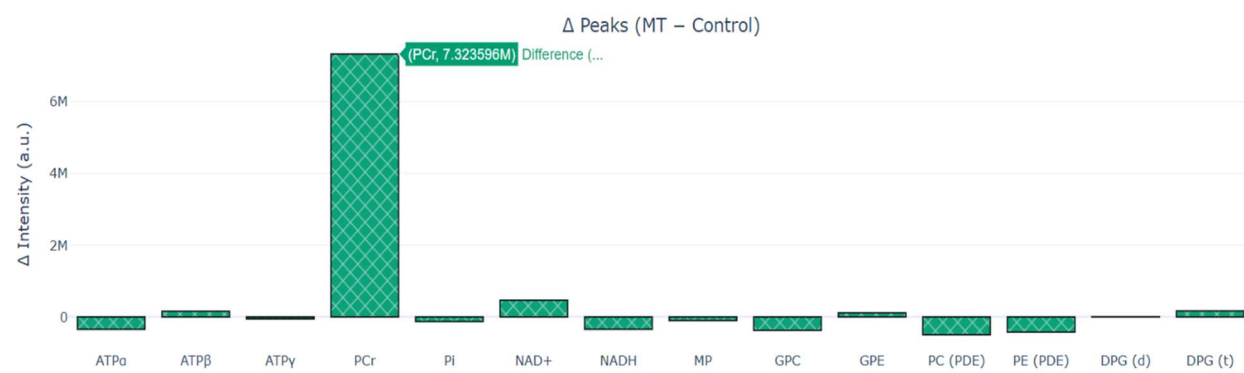
Figure 9: Peaks comparison

Figure 10: Peak difference

Table 1: Average peak comparison (control vs MT)

Metabolite	n_pairs	Mean_Control	Mean_MT	Mean_Diff	Pct_Change_%
ATPα	9	4633318.009	4288490.926	-344827.083	-7.44
ATPβ	9	823846.898	980989.821	157142.923	19.07
ATPγ	9	5238246.485	5182576.495	-55669.991	-1.06
PCr	9	11302765.686	18626362.11	7323596.425	64.79
Pi	9	498245.74	369474.007	-128771.733	-25.85
NAD+	9	2202049.66	2668784.696	466735.036	21.2
NADH	9	2935307.251	2591285.861	-344021.39	-11.72
MP	9	2432963.9	2332129.322	-100834.578	-4.14
GPC	9	5557329.34	5183769.763	-373559.577	-6.72
GPE	9	3041620.59	3156318.571	114697.981	3.77
PC (PDE)	9	3125640.732	2627704.15	-497936.582	-15.93
PE (PDE)	9	5682217.436	5259998.412	-422219.024	-7.43
DPG (d)	9	50484.989	54748.517	4263.528	8.45
DPG (t)	9	-235694.006	-68526.261	167167.745	-70.93

Table 2: peak Paired t-test (MT vs control)

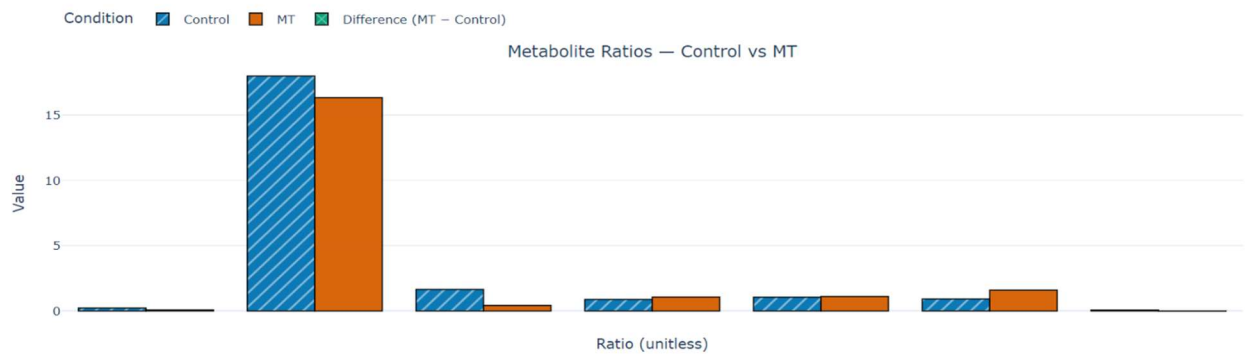| Metabolite	t_stat	p_value	Significance
ATPα	-0.578	0.579	
ATPβ	0.214	0.836	
ATPγ	-0.138	0.893	
PCr	0.99	0.351	
Pi	-0.326	0.753	
NAD+	0.763	0.467	
NADH	-0.828	0.432	
MP	-0.341	0.742	
GPC	-0.431	0.678	
GPE	0.152	0.883	
PC (PDE)	-1.374	0.207	
PE (PDE)	-0.413	0.69	
DPG (d)	0.011	0.991	
DPG (t)	0.344	0.74	

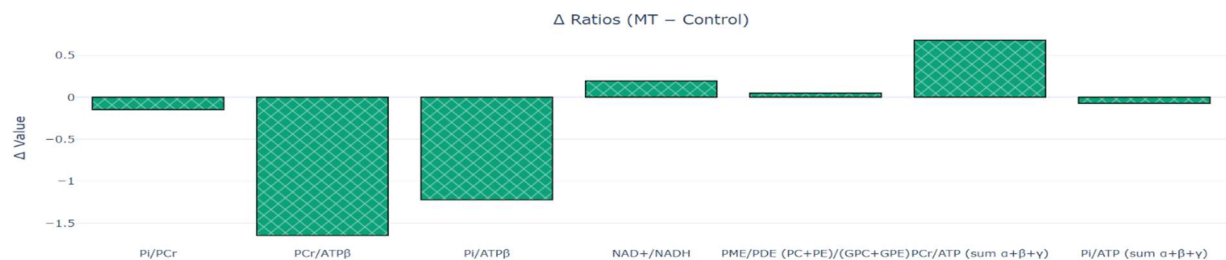Figure 11: Metabolite ratio comparison

Figure 12: Ratio difference

Table 3: Ratios - Average Comparison (Control vs MT)

Metric	n_pairs	Mean_Control	Mean_MT	Mean_Diff	Pct_Change_%
Pi/PCr	9	0.221	0.072	-0.148	-67.21
PCr/ATPβ	9	17.991	16.343	-1.648	-9.16
Pi/ATPβ	9	1.644	0.422	-1.223	-74.35
NAD+/NADH	9	0.874	1.068	0.194	22.23
PME/PDE	9	1.056	1.105	0.049	4.6
PCr/ATP_total	9	0.912	1.59	0.678	74.42
Pi/ATP_total	9	0.065	-0.008	-0.073	-113.04

Table 4: Ratio Paired t-test (MT - control)

Metric	Mean_Control	Mean_MT	Mean_Diff	t_stat	p_value	Significance
Pi/PCr	0.221	0.072	-0.148	-0.931	0.379	
PCr/ATPβ	17.991	16.343	-1.648	-0.133	0.897	
Pi/ATPβ	1.644	0.422	-1.223	-0.53	0.61	
NAD+/NADH	0.874	1.068	0.194	0.873	0.408	
PME/PDE	1.056	1.105	0.049	0.304	0.769	
PCr/ATP_total	0.912	1.59	0.678	1.065	0.318	
Pi/ATP_total	0.065	-0.008	-0.073	-1.019	0.338	

[1]   D. K. Deelchand, T. M. Nguyen, X. H. Zhu, F. Mochel, and P. G. Henry, "Quantification of in vivo 31P NMR brain spectra using LCModel," *Wiley Online LibraryDK Deelchand, TM Nguyen, XH Zhu, F Mochel, PG HenryNMR in Biomedicine, 2015•Wiley Online Library*, vol. 28, no. 6, pp. 633–641, Jun. 2015, doi: 10.1002/NBM.3291.

[2]   E. J. Fear *et al.*, "Use of 31P magnetisation transfer magnetic resonance spectroscopy to measure ATP changes after 670 nm transcranial photobiomodulation in older adults," *Aging Cell*, vol. 22, no. 11, 2023, doi: 10.1111/acel.14005.