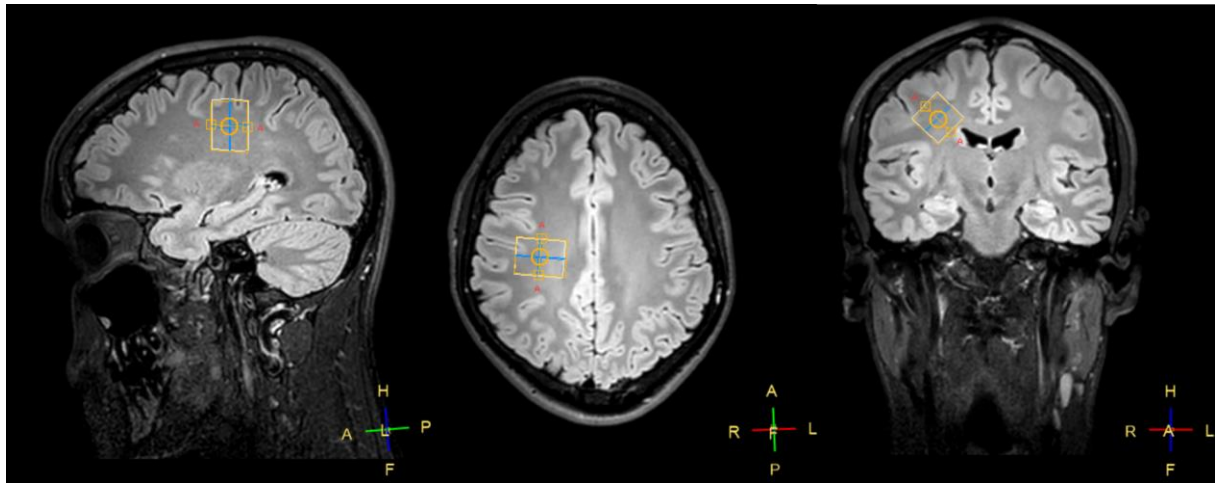


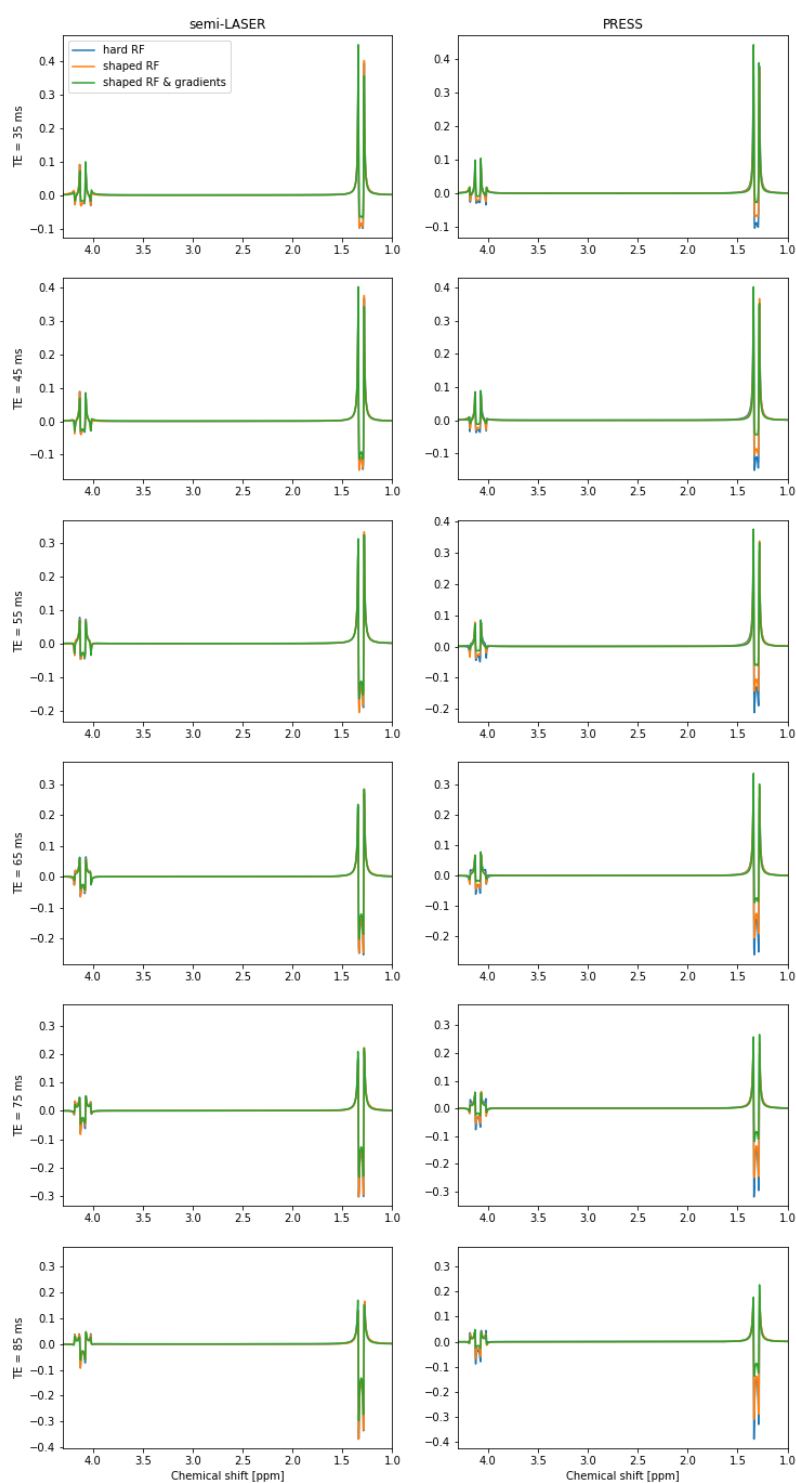
Supplementary material

Figure S1. VOI position used for in vivo measurements shown on a FLAIR image acquired for VOI planning

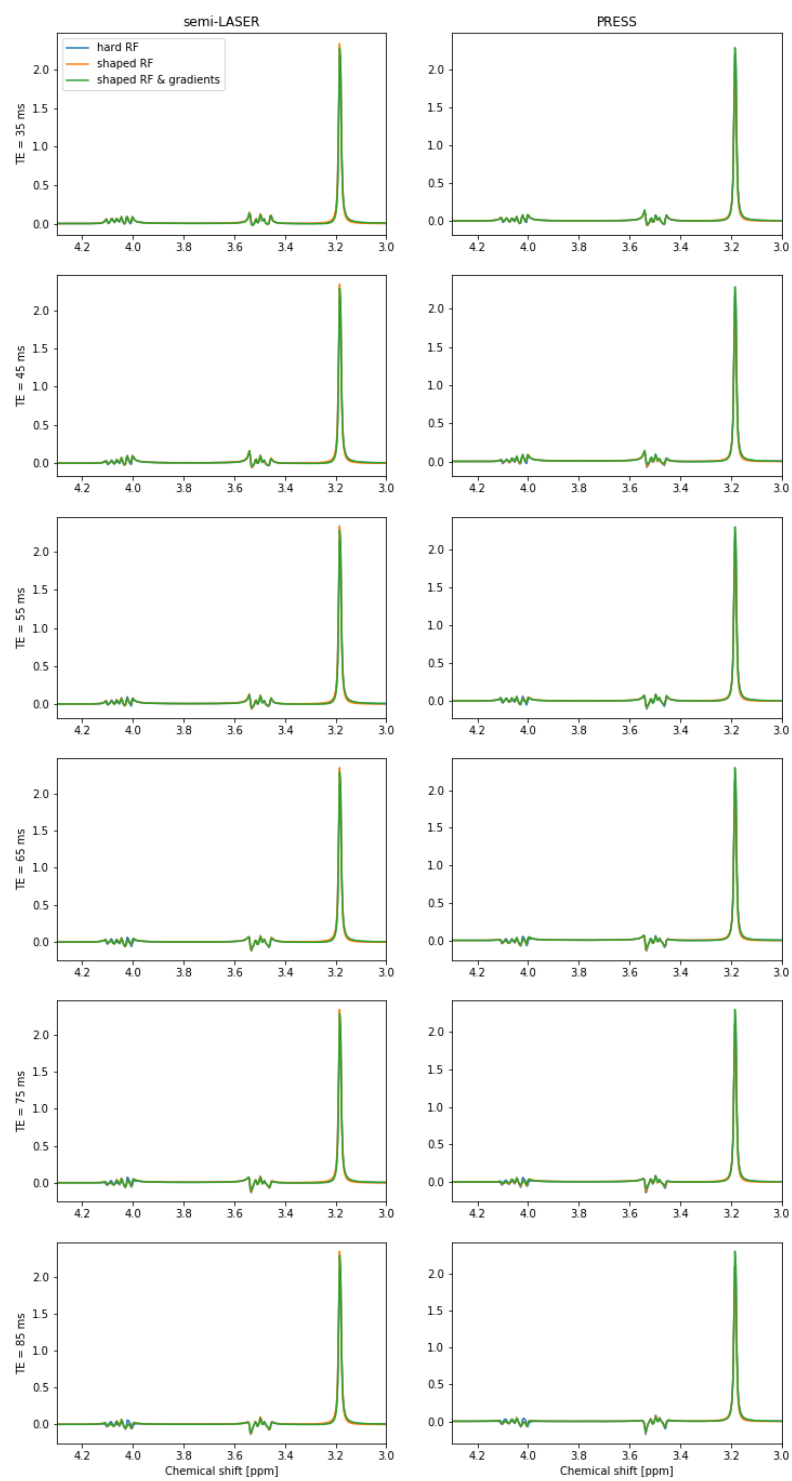


Supplementary figures S2-S7. Simulated spectra for different simulation methods and pulse sequences.

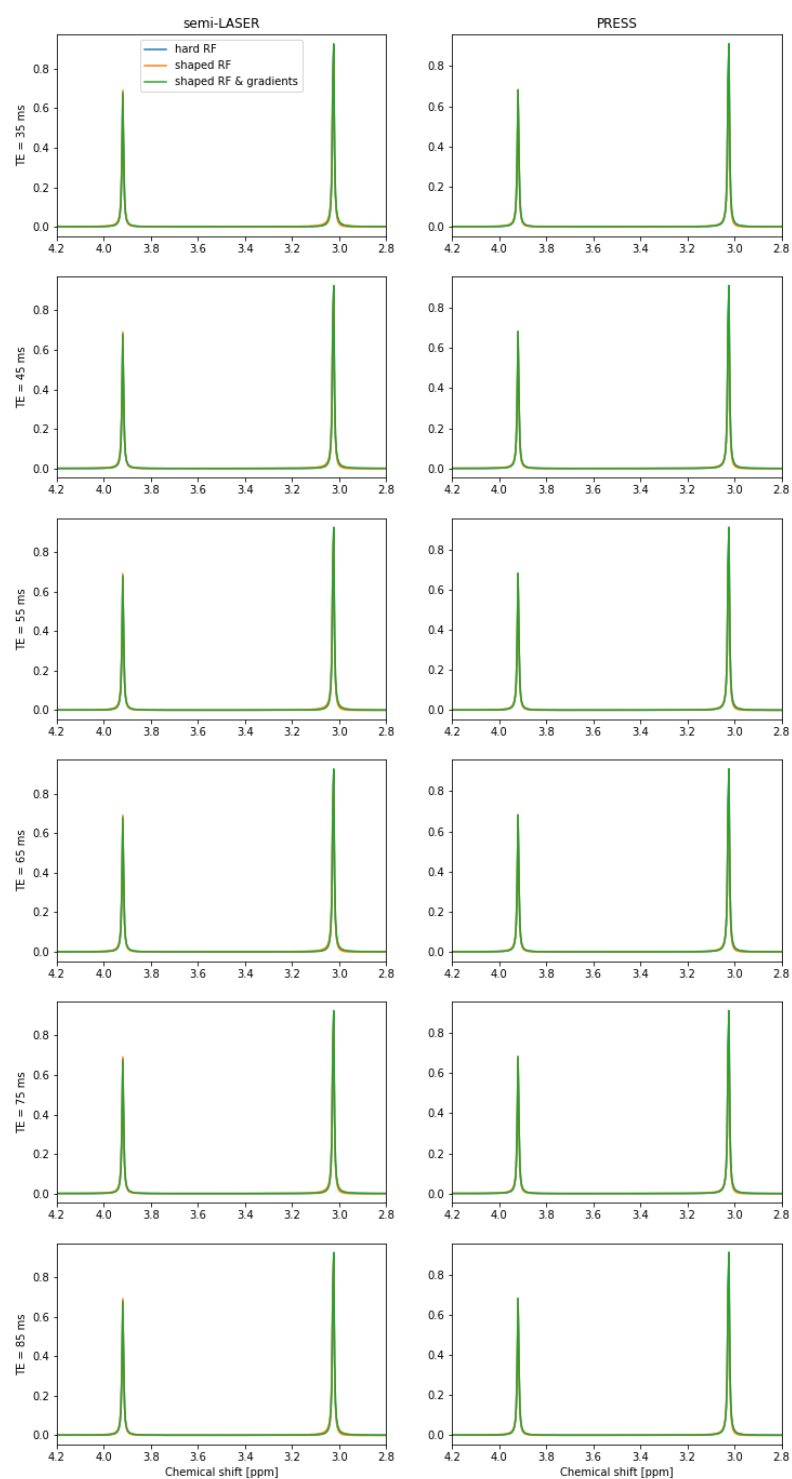
S2. Lactate



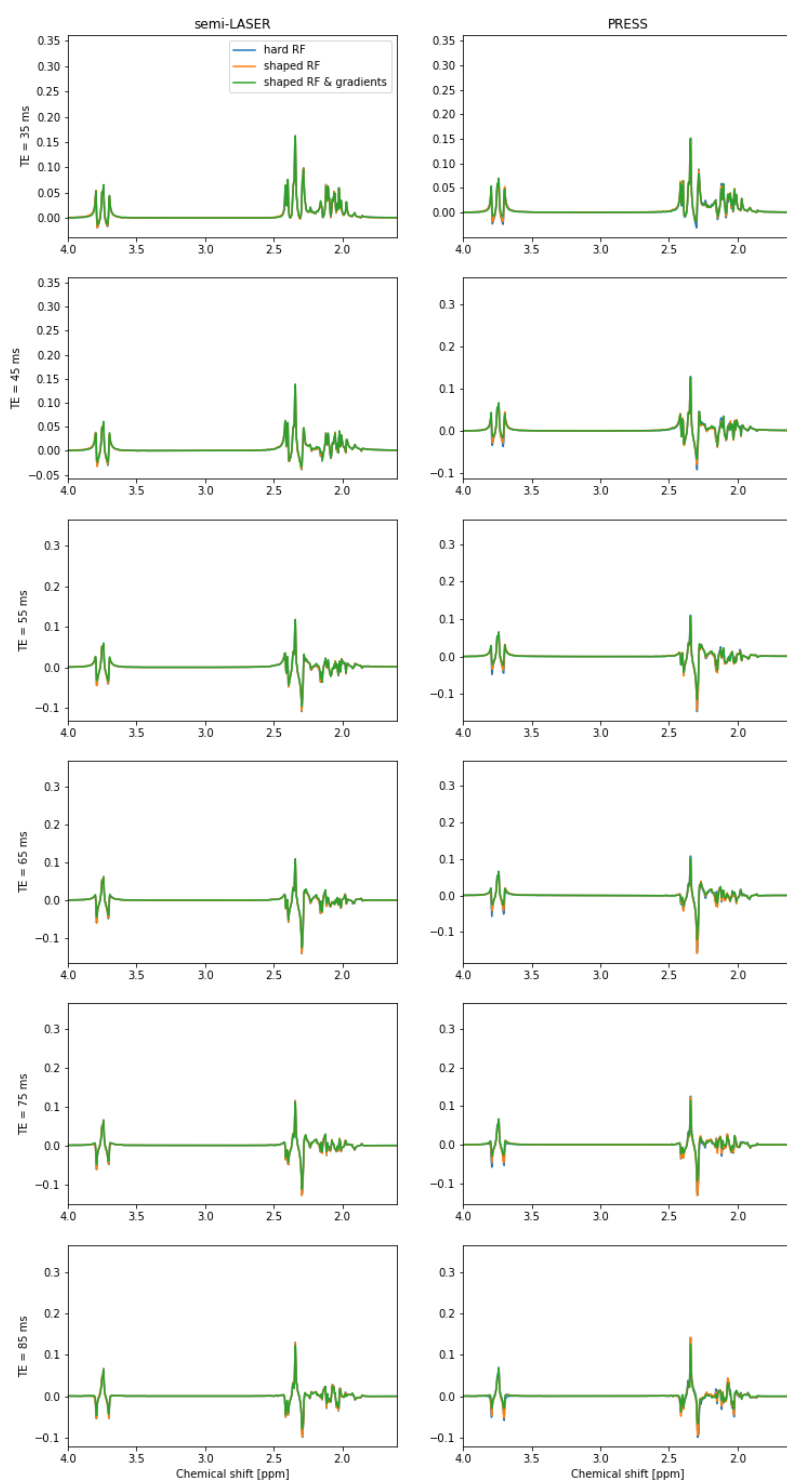
S3. Choline



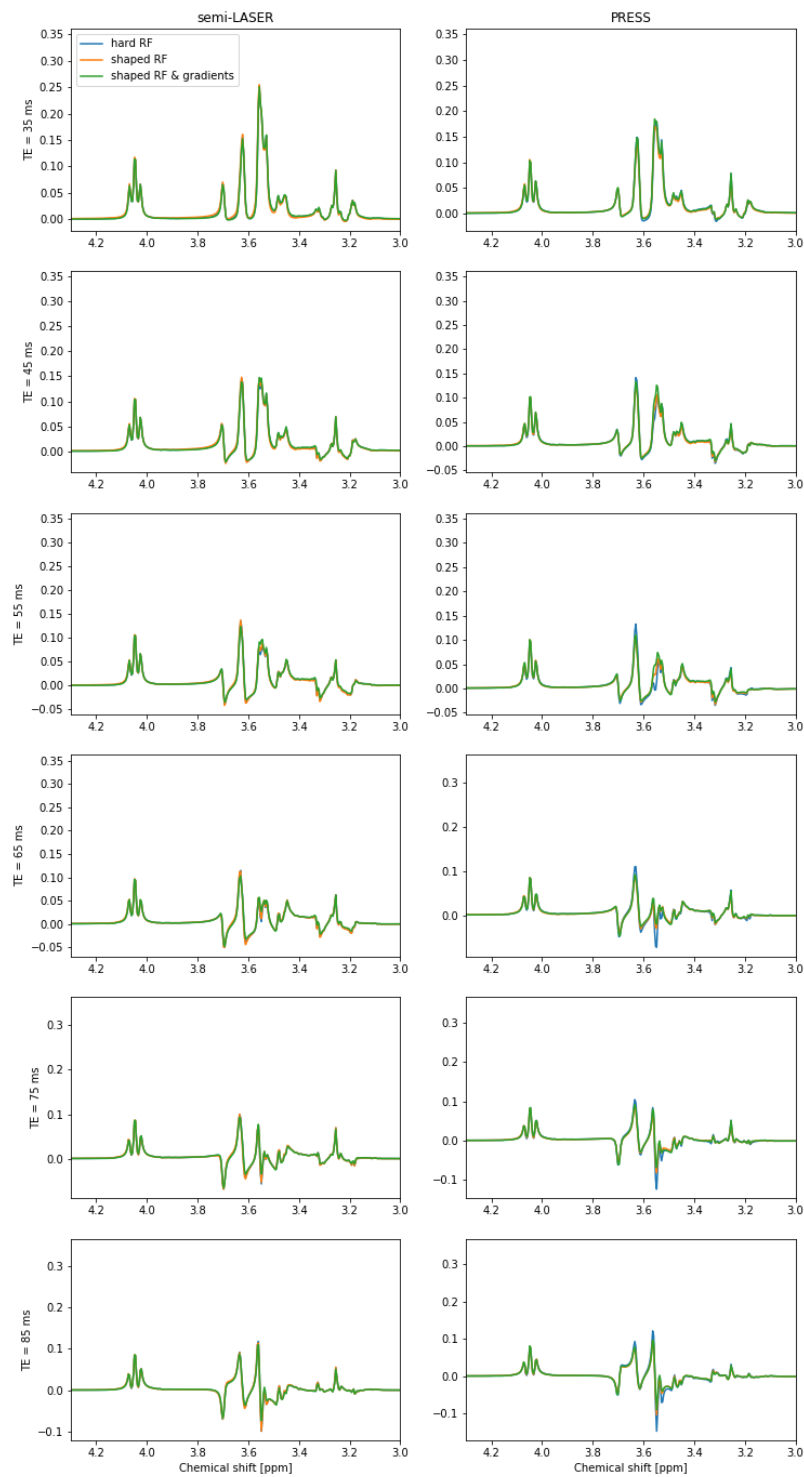
S4. Creatine



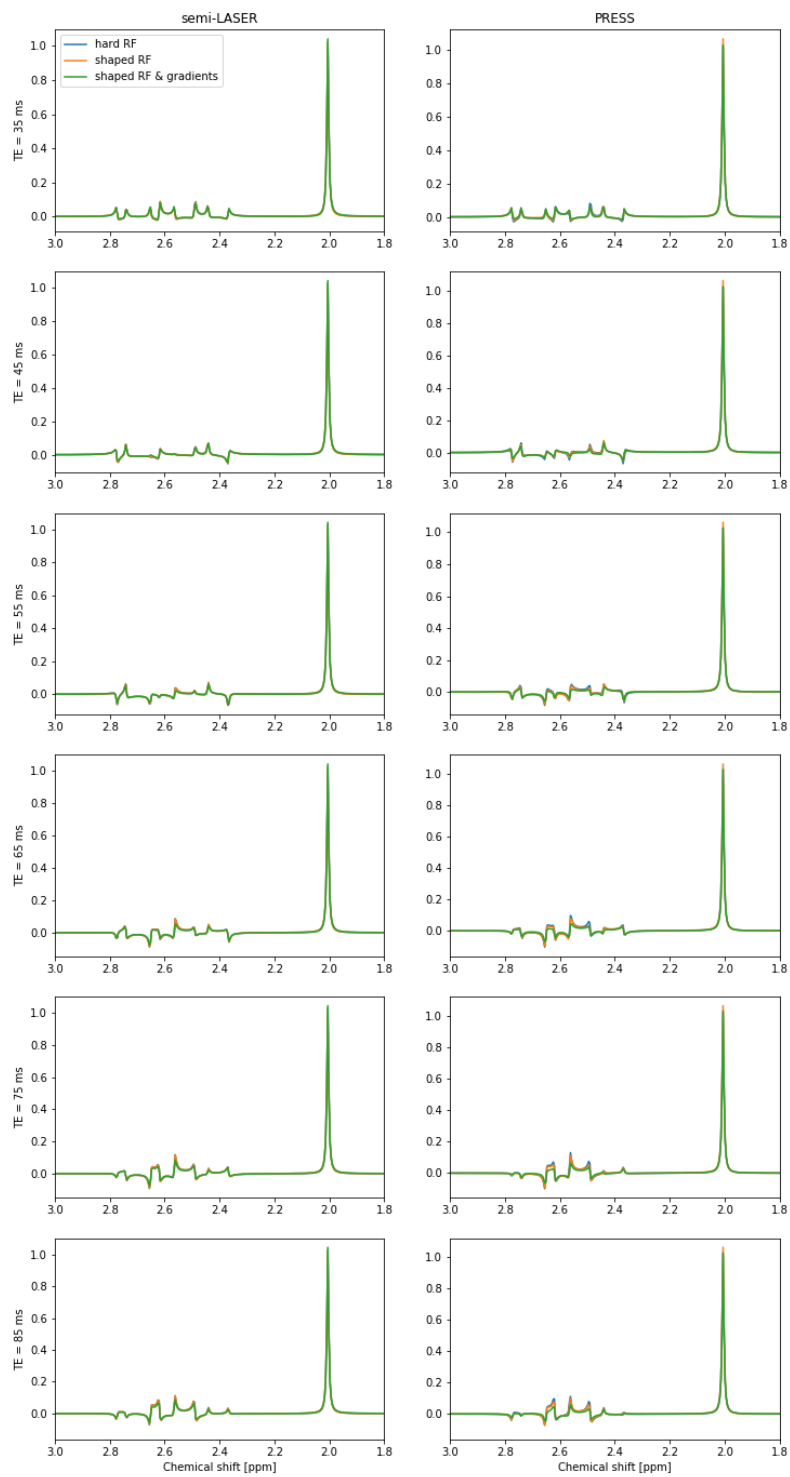
S5. Glutamate



S6. Myo-Inositol

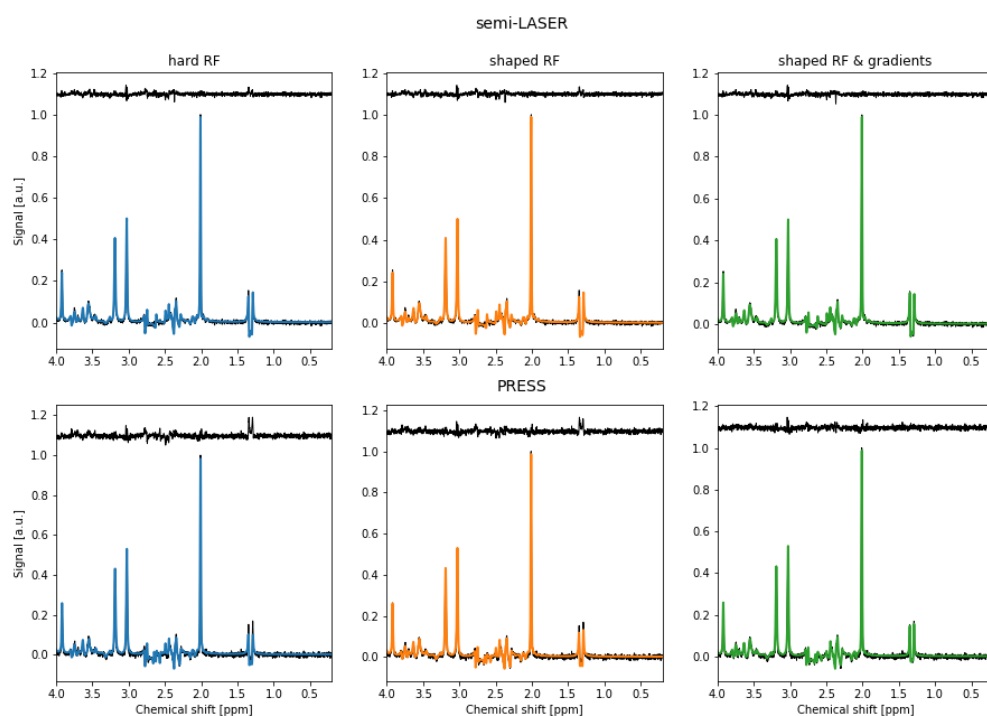


S7. NAA

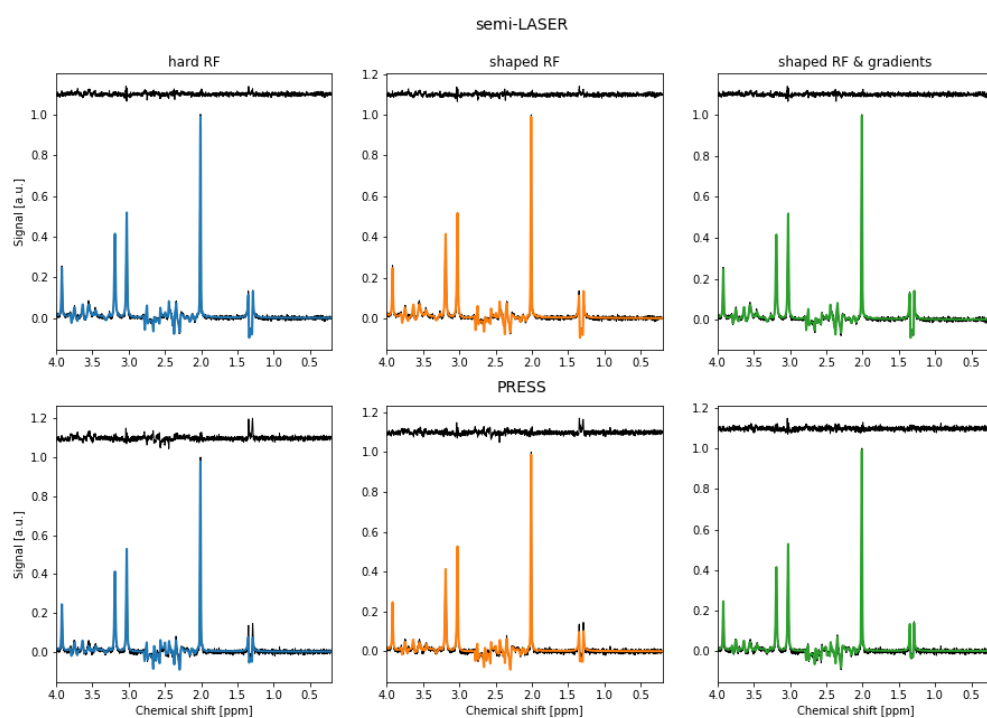


Supplementary figures S8-S12. Measured phantom spectra (black), LCModel fit (colored) and residual (black elevated) for each simulation method and pulse sequence.

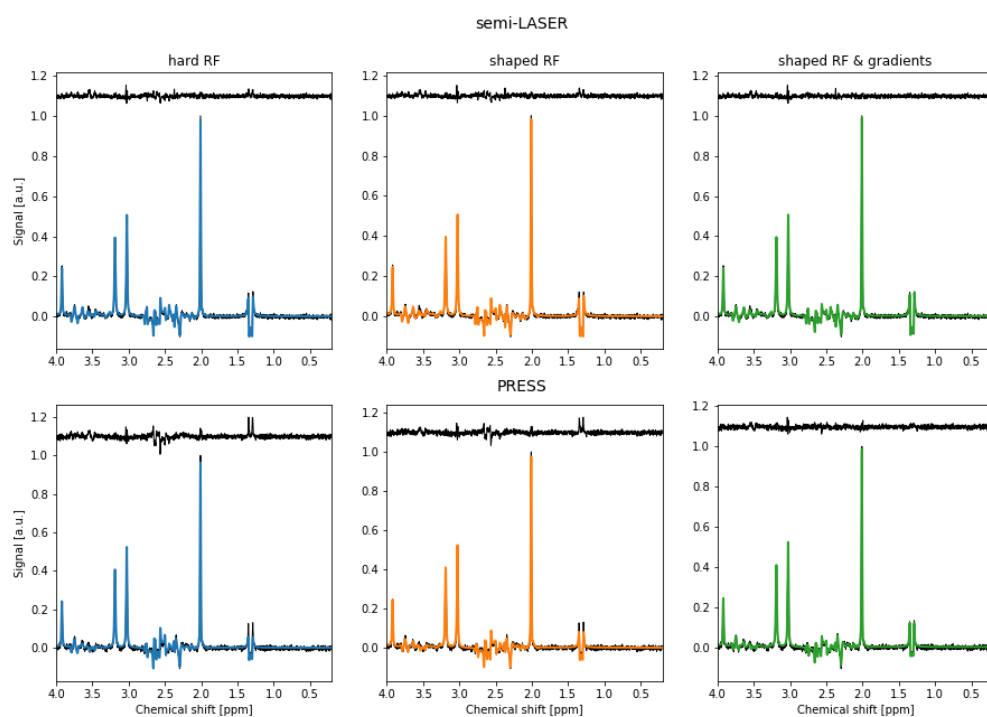
S8. TE = 45 ms



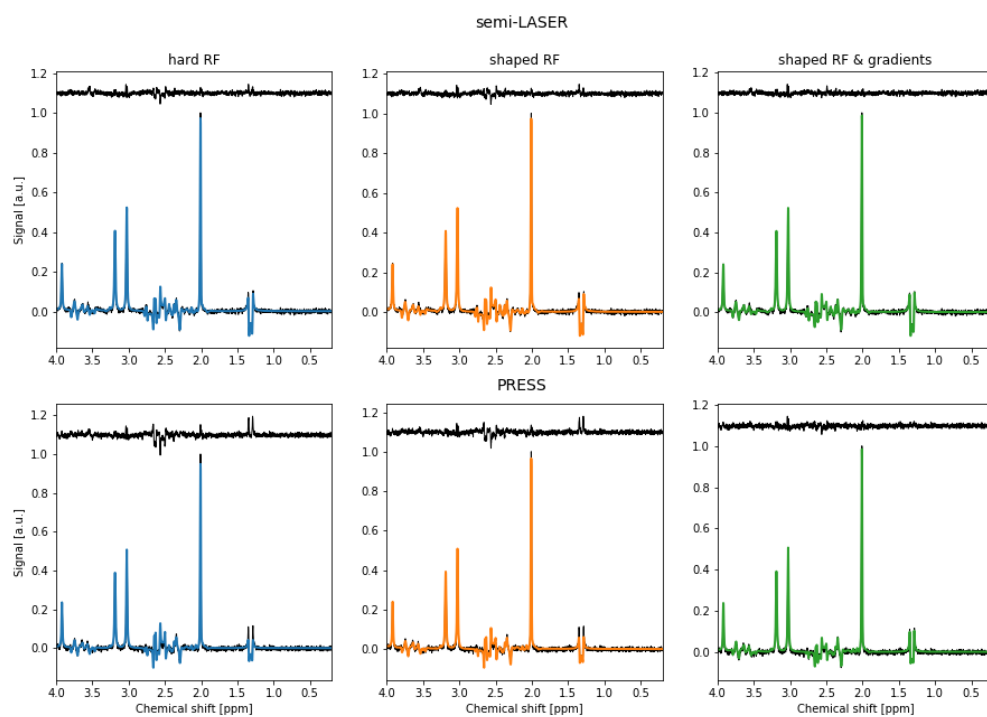
S9. TE = 55 ms



S10. TE = 65 ms



S11. TE = 75 ms



S12. TE = 85 ms

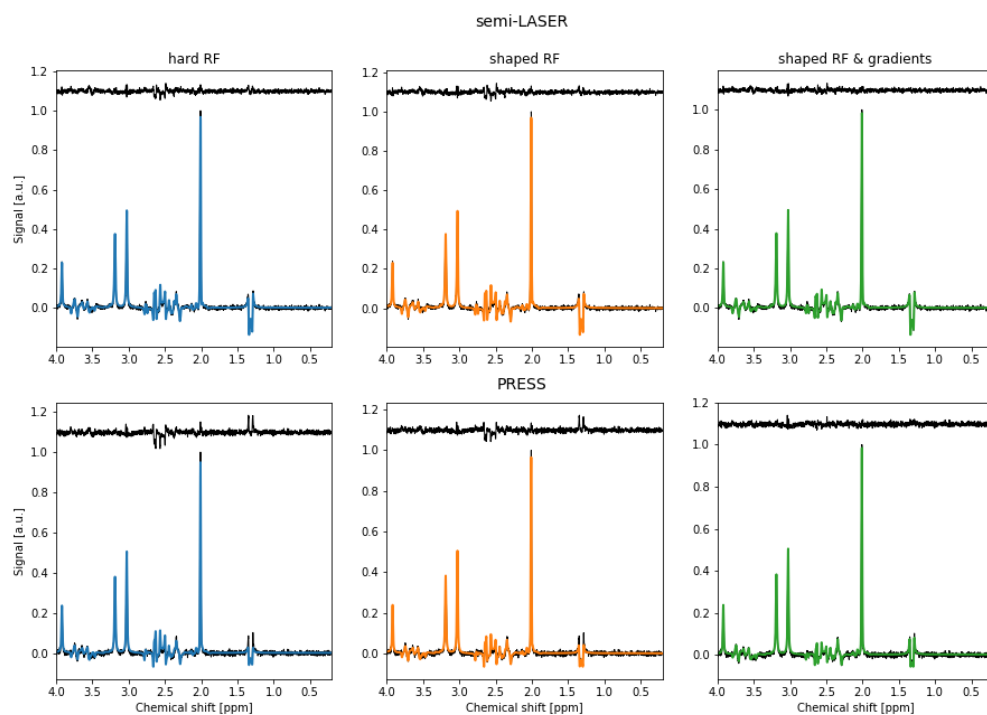


Figure 3 displays four bar charts quantifying metabolite concentrations and relative bias for the semi-LASER and PRESS methods. The charts are arranged in a 2x2 grid. The top row shows results for the semi-LASER method, and the bottom row shows results for the PRESS method. The left column displays metabolite concentrations in mM, and the right column displays relative bias in %.

Top Left: semi-LASER Concentration [mM]

Metabolite	hard RF	shaped RF	shaped RF & gradients	specified
Lac	4.5	4.8	4.5	5.0
Cho	3.2	3.2	3.2	2.8
Cr	10.0	10.0	10.0	10.0
Glu	11.5	11.5	9.5	12.5
Ins	10.5	10.5	9.0	7.5
NAA	12.0	12.0	11.5	12.5

Top Right: semi-LASER Relative bias [%]

Metabolite	hard RF	shaped RF	shaped RF & gradients
Lac	-2	-2	-10
Cho	10	10	10
Cr	-1	-1	-2
Glu	-10	-10	-20
Ins	38	38	22
NAA	-2	-2	-5

Bottom Left: PRESS Concentration [mM]

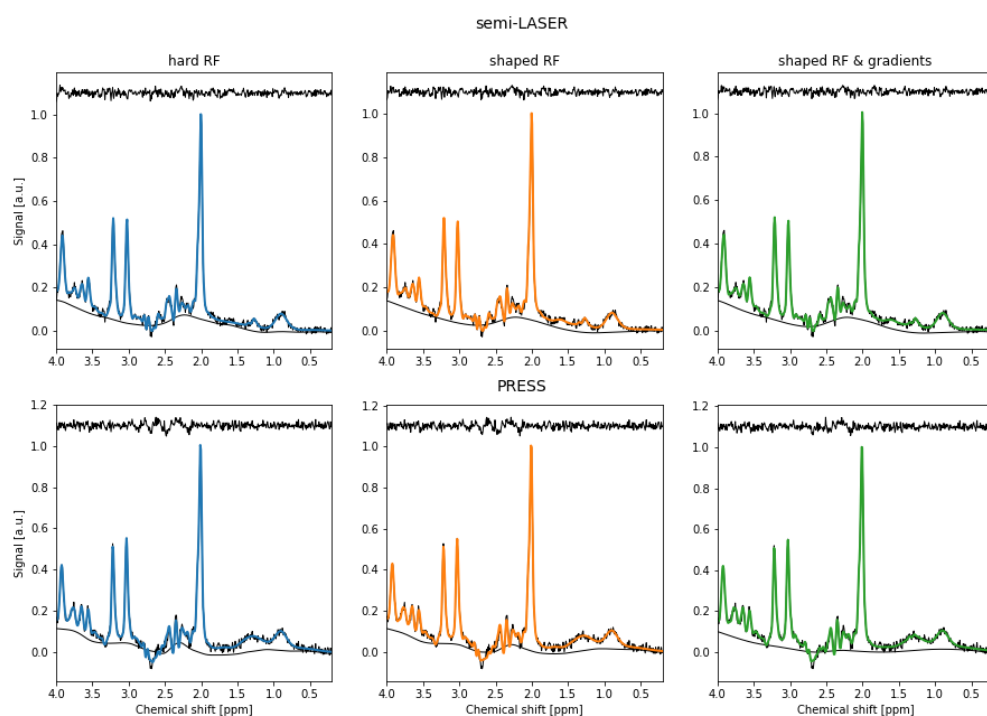
Metabolite	hard RF	shaped RF	shaped RF & gradients	specified
Lac	7.0	7.0	4.5	4.8
Cho	3.5	3.5	3.5	2.8
Cr	10.5	10.5	10.0	10.0
Glu	11.5	10.5	9.5	12.5
Ins	13.0	10.0	8.0	7.5
NAA	13.0	11.5	11.5	12.5

Bottom Right: PRESS Relative bias [%]

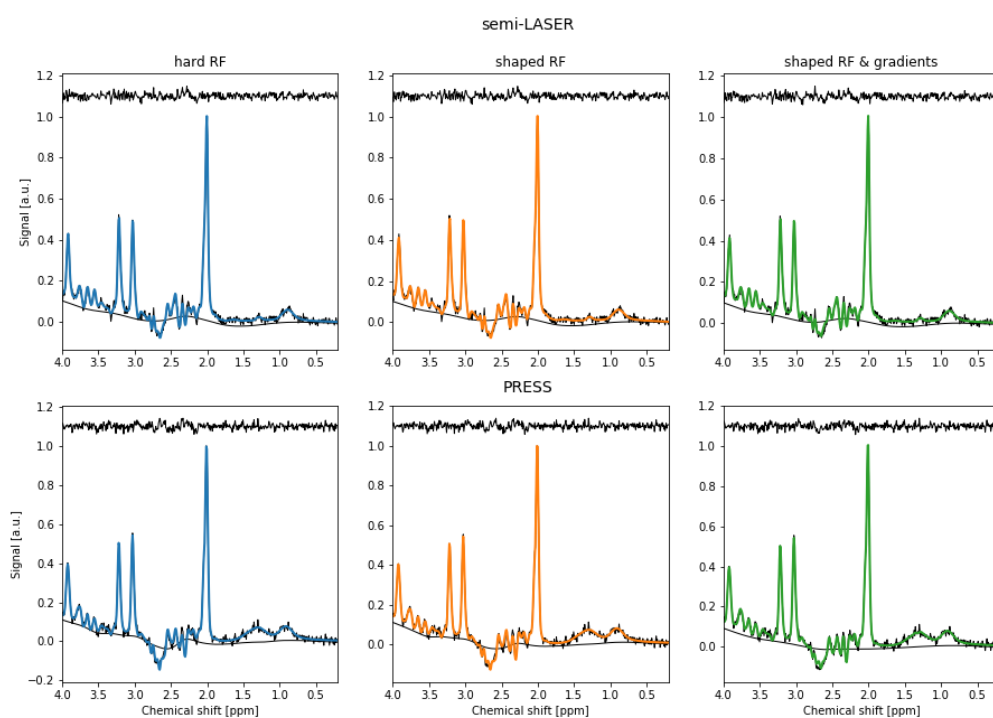
Metabolite	hard RF	shaped RF	shaped RF & gradients
Lac	45	45	-5
Cho	20	20	18
Cr	4	4	2
Glu	-5	-15	-25
Ins	72	32	10
NAA	3	-10	2

Supplementary figures S15-S19. Measured *in vivo* spectra (black), LCModel fit (colored) and residual (black elevated) for each simulation method and pulse sequence.

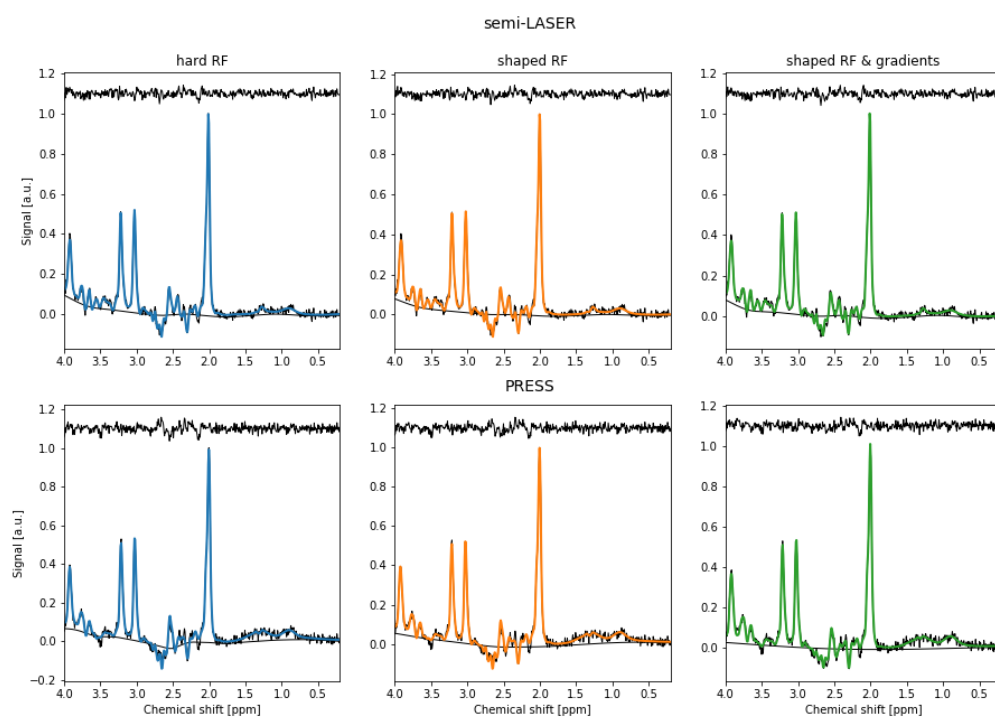
S15. TE = 45 ms



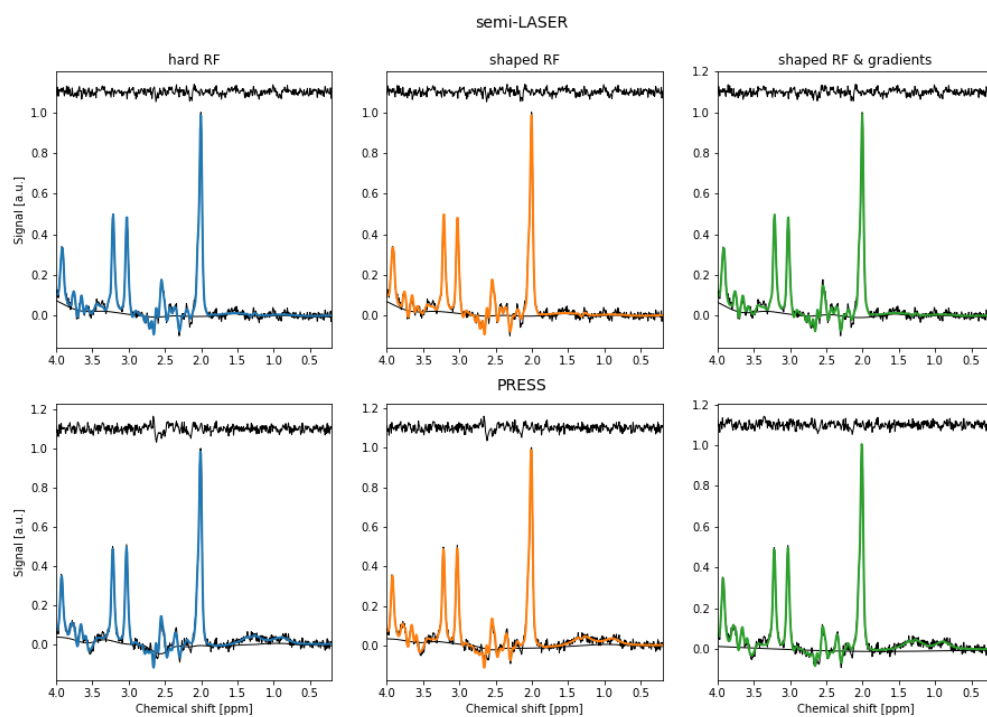
S16. TE = 55 ms



S17. TE = 65 ms



S18. TE = 75 ms



S19. TE = 85 ms

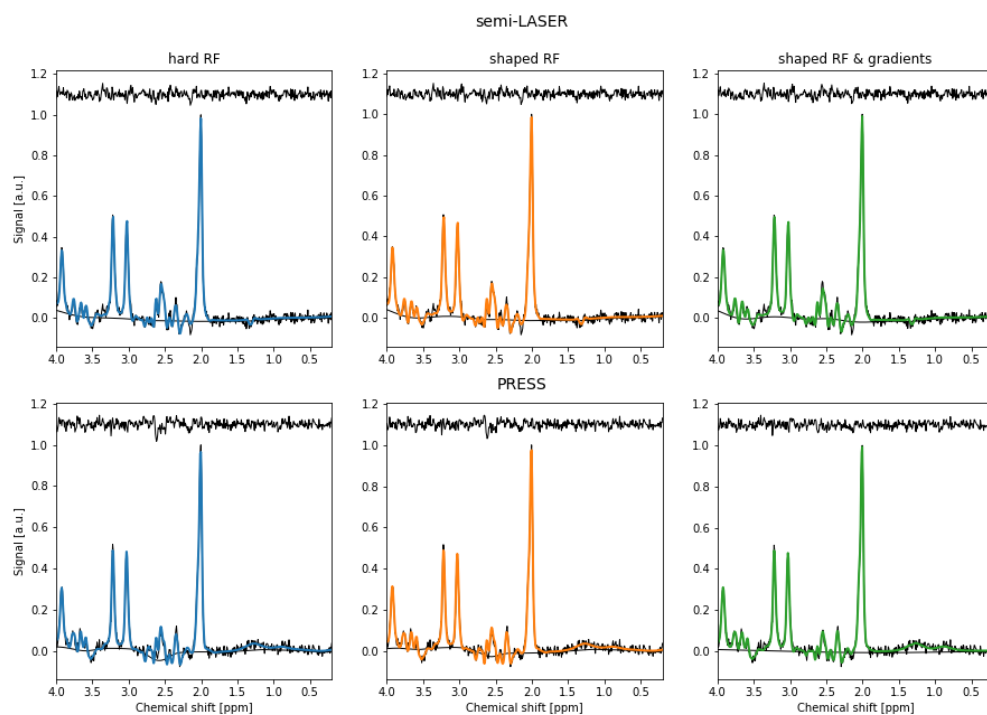
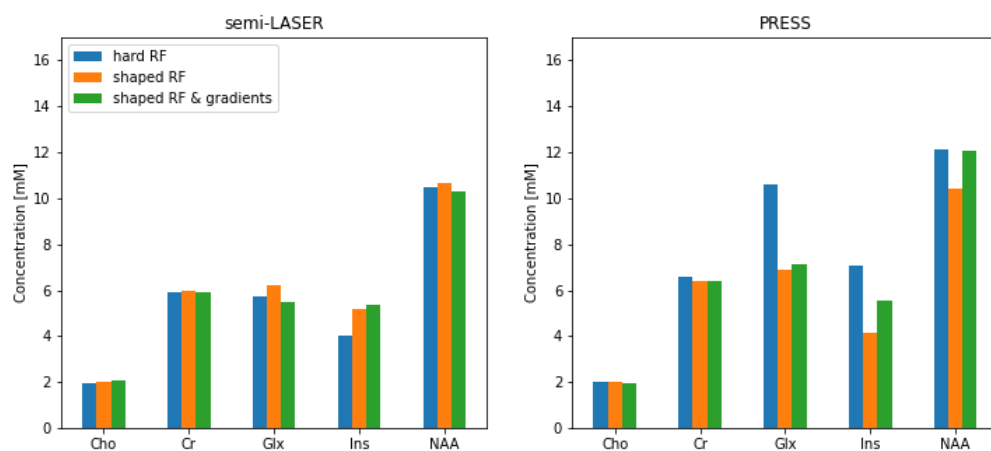


Fig S20 Estimated *in vivo* metabolite concentrations corrected for T2 relaxation (extrapolated to TE = 0 ms based on monoexponential fit of multi-TE data)



Supplementary figures S21. Estimated *in vivo* metabolite concentrations vs TE and exponential model fit (related to Fig. S20)

