

Parameter Values For Metabolite Quantification at 9.4T

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1 T₁ Values

The T₁ values of metabolites and water in tissue were taken from the following reference:

Reference	ROI	Animal	Sequence
de Graaf, R. A., Brown, P. B., McIntyre, S., Nixon, T. W., Behar, K. L., & Rothman, D. L. (2006). High magnetic field water and metabolite proton T ₁ and T ₂ relaxation in rat brain in vivo. <i>Magnetic Resonance in Medicine</i> , 56(2), 386–394. https://doi.org/10.1002/mrm.20946	<ul style="list-style-type: none">Cerebral cortex (60-70%) + corpus callosum and hippocampus (30-40%)5 x 3 x 5 mm³ voxel	Sprague-Dawley rats	<ul style="list-style-type: none">Nonselective AHP excitation and 3 pairs of AFP for selective refocussing
This reference was chosen because they used a sequence that was similar to ours for their parameter measurement.			

The T₁ value of water in CSF was taken from the following reference:

Reference	ROI	Animal	Sequence
Kuo, Y. T., Herlihy, A. H., So, P. W., Bhakoo, K. K., & Bell, J. D. (2005). In vivo measurements of T ₁ relaxation times in mouse brain associated with different modes of systemic administration of manganese chloride. <i>Journal of Magnetic Resonance Imaging</i> , 21(4), 334–339. https://doi.org/10.1002/jmri.20285	Left Ventricle	C57/BL6 Mice	<ul style="list-style-type: none">Spin-echo sequenceTE=18 ms5 TRs (800 – 6000 ms)
Though CSF in tissue and CSF in a ventricle have different relaxations, there has not been reports in literature of the relaxation rates of CSF within the rat or mouse brain tissue. Thus, a CSF measurement was used.			

1.1 Summary of T₁ Values for Metabolites

The T₁ values of metabolites used for metabolite quantification at 9.4T are summarized below:

Metabolite	T ₁ in Tissue [sec]	Notes
NAA	1.6740	
NAAG	1.6740	Assumed to be the same as NAA
Ala	1.3701	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
GABA	1.3701	
Asp	1.3701	
Cho	1.3484	Total choline
Cre	1.6792	Total creatine, 3.03 ppm singlet only
Glc	1.3701	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Glu	1.4975	de Graaf measured the Glx complex (glutamate + glutamine)
Gln	1.4975	
GSH	1.3701	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Gly	1.3701	
Myo	1.3701	
Scy	1.3701	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Lac	1.3701	
Eth	1.3701	
Tau	2.3289	

1.2 Summary of T₁ Values for Water

The T₁ values of water used for metabolite quantification at 9.4T are summarized below:

	T ₁ in Tissue [sec]	T ₁ in CSF [sec]
Water	<ul style="list-style-type: none">• 2.0597 (hippocampus)• From de Graaf et al, 2006	<ul style="list-style-type: none">• 4.2867 (left ventricle)• From Kuo et al, 2005

2 T₂ Values

The T₂ values of metabolites and water in tissue were taken from the following reference:

Reference	ROI	Animal	Sequence
Deelchand, D. K., Henry, P. G., & Marjańska, M. (2015). Effect of Carr-Purcell refocusing pulse trains on transverse relaxation times of metabolites in rat brain at 9.4 Tesla. <i>Magnetic Resonance in Medicine</i> , 73(1), 13–20. https://doi.org/10.1002/mrm.25088	<ul style="list-style-type: none">• On the midline, 2mm posterior to bregma and 3 mm ventral• 5 x 2.5 x 5 mm³	Sprague-Dawley Rats	<ul style="list-style-type: none">• LASER• 8 TEs between 18 ms and 400 ms

¹ Marjańska, M., Auerbach, E. J., Valabrègue, R., Van de Moortele, P.-F., Adriany, G., & Garwood, M. (2012). Localized 1H NMR spectroscopy in different regions of human brain in vivo at 7 T: T2 relaxation times and concentrations of cerebral metabolites. *NMR in Biomedicine*, 25(2), 332–339. <https://doi.org/10.1002/nbm.1754>

² Kreis, R., Slotboom, J., Hofmann, L., & Boesch, C. (2005). Integrated data acquisition and processing to determine metabolite contents, relaxation times, and macromolecule baseline in single examinations of individual subjects. *Magnetic Resonance in Medicine*, 54(4), 761–768. <https://doi.org/10.1002/mrm.20673>

This reference was used because it employed a LASER sequence, the same as what was used on our 9.4T Varian scanner. The authors were also able to measure T₂ values for glutamate and glutamine separately. There were also able to measure separate T₂ values for

The T₂ value of water in CSF was taken from the following reference:

Reference	ROI	Animal	Sequence
Kuo, Y. T., Herlihy, A. H., So, P. W., Bhakoo, K. K., & Bell, J. D. (2005). In vivo measurements of T1 relaxation times in mouse brain associated with different modes of systemic administration of manganese chloride. Journal of Magnetic Resonance Imaging, 21(4), 334–339. https://doi.org/10.1002/jmri.20285	Left Ventricle	C57/BL6 Mice	<ul style="list-style-type: none"> Spin-echo sequence TE=18 ms 5 TRs (800 – 6000 ms)
Though CSF in tissue and CSF in a ventricle have different relaxations, there has not been reports in literature of the relaxation rates of CSF within the rat or mouse brain tissue. Thus, a CSF measurement was used.			

2.1 Summary of T₂ Values for Metabolites

The T₂ values use of metabolites used for metabolite quantification at 9.4T are summarized below:

Metabolite	T ₂ in Tissue [ms]	Notes
NAA	321	CH ₃ singlet only
NAAG	321	Assumed to be the same as NAA
Ala	161	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
GABA	161	
Asp	161	
Cho	445	
Cho	445	Total choline
Cre	104	Creatine + phosphocreatine, 3.03 ppm singlet only
Glc	161	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Glu	70	
Gln	56	
GSH	161	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Gly	161	
Myo	161	
Scy	161	Assumed to be the same as Myo, per Marjanska ¹ and Kreis ²
Lac	161	
Eth	161	
Tau	162	

2.2 Summary of T₂ Values for Water

The T₂ values of water used for metabolite quantification at 9.4T are summarized below:

	T ₂ in Tissue [ms]	T ₂ in CSF [ms]
Water	<ul style="list-style-type: none">• 44• From Deelchand et al, 2015	<ul style="list-style-type: none">• 111.3• From Kuo et al, 2005