

3.1. From Tables 2.01 and 2. it follows that $\delta([2-^1\text{H}]\text{-acetate}) = 1.904$ ppm, $\delta([4-^1\text{H}]\text{-glutamate}) = 2.344$ ppm (average), $\delta([2-^{13}\text{C}]\text{-acetate}) = 24.5$ ppm and $\delta([4-^{13}\text{C}]\text{-glutamate}) = 34.2$ ppm.

One of several different routes is to calculate the glutamate frequencies at 7.05 T, after which the frequency at 4.0 T can be obtained by simple scaling, i.e.

$$\nu([4-^{13}\text{C}]\text{-glutamate})_{7\text{T}} = \nu([2-^{13}\text{C}]\text{-acetate})_{7\text{T}} + (\delta([4-^{13}\text{C}]\text{-glutamate}) - \delta([2-^{13}\text{C}]\text{-acetate}))$$

resonance frequency

$$\nu([4-^{13}\text{C}]\text{-glutamate})_{7\text{T}} = 75.230404 \text{ MHz}$$

and

$$\nu([4-^1\text{H}]\text{-glutamate})_{7\text{T}} = \nu([2-^1\text{H}]\text{-acetate})_{7\text{T}} + (\delta([4-^1\text{H}]\text{-glutamate}) - \delta([2-^1\text{H}]\text{-acetate})) \times$$

resonance frequency

$$\nu([4-^1\text{H}]\text{-glutamate})_{7\text{T}} = 300.015755 \text{ MHz}$$

and finally:

$$\nu([4-^{13}\text{C}]\text{-glutamate})_{4\text{T}} = [\nu([4-^1\text{H}]\text{-glutamate})_{4\text{T}} / \nu([4-^1\text{H}]\text{-glutamate})_{7\text{T}}] \times \nu([4-^{13}\text{C}]\text{-glutamate})_{7\text{T}}$$

$$\nu([4-^{13}\text{C}]\text{-glutamate})_{4\text{T}} = 42.742498 \text{ MHz}$$

3.2. If 2-oxoglutarate is continuously saturated, the magnetization of glutamate is given by:

$$\frac{M_{z,\text{Glu}}(\infty)}{M_{z,\text{Glu}}^0} = \frac{1}{1 + k_{2\text{OG-Glu}} T_{1,\text{Glu}}} \quad [\text{s.1}]$$

$T_{1,\text{Glu}}$ can be obtained from Eq. [3.36] and is equal to 5.313 s. Substitution of the parameters in Eq. [s.1] given a signal decrease of 68% in the glutamate resonance.

3.3.A. Eq. [3.12] can be rewritten as:

$$\frac{1}{T_1} = C \left(\frac{\tau_c}{1 + 4\pi^2 \nu^2 \tau_c^2} + \frac{4\tau_c}{1 + 16\pi^2 \nu^2 \tau_c^2} \right)$$

Substituting $\{T_1, \tau_c, \nu\} = \{4.0 \text{ s}, 10^{-11} \text{ s}, 300 \text{ MHz}\}$ allows the determination of the constant C as $5.006 \times 10^{+9} \text{ s}^{-2}$. Using C, the bone T_1 under conditions of pure dipolar relation then becomes 354.9 s.

B.

Solving for the real root of $(d(1/T_1)/d\tau_c) = 0$ gives $T_{1\text{minimum}} = 0.264 \text{ s}$ for $\tau_c = 3.27 \times 10^{-10} \text{ s}$. Note that the calculation involves a cubic equation of which the solutions can be found in any standard textbook.

C.

After noting that the constant in Eq. [3.14] is half that of Eq. [3.13], the T_2 s can be directly calculated and are given by : $T_{2\text{water}} = 3.997 \text{ s}$ and $T_{2\text{lipids}} = 0.133 \text{ ms}$. Note that $T_{1\text{water}} \approx T_{2\text{water}}$ as predicted by Eq. [3.16] for the ‘extreme narrowing condition’.

D.

$T_{1\text{water}} = 4.025 \text{ s}$, $T_{2\text{water}} = 4.007 \text{ s}$, $T_{1\text{lipids}} = 2218 \text{ s}$ and $T_{2\text{lipids}} = 0.133 \text{ ms}$. The relaxation times for free water are fairly independent of the magnetic field, in accordance with Figs. 3.4 and 3.5.

3.4.A. The ^{33}S NMR spectrum will only consist of a single resonance originating from the SO_4^{2-} ion. This is because the quadrupolar relaxation pathway is not dominant due to molecular symmetry of the SO_4^{2-} ion. The sulfur group in glutathione on the other hand is highly asymmetric, such that quadrupolar relaxation according to Eq. [3.21] is dominant, resulting in very short T_2 relaxation times and hence very broad resonance lines.

B. The ^1H NMR spectrum will consist of all resonances from glutathione and water. The H_2SO_4 molecule is not visible as the protons are in rapid exchange with the water.

3.5.A.

Using Eq. [1.72] and the fact that $M_{xy}(\alpha) = M_z(\alpha)\sin\alpha$, the expression for T_1 is readily derived as:

$$T_1 = \frac{-TR}{\ln\left(\frac{M_1 \sin \alpha_2 - M_2 \sin \alpha_1}{M_1 \sin \alpha_2 \cos \alpha_1 - M_2 \sin \alpha_1 \cos \alpha_2}\right)}$$

B.

$$T_1 = 426.2 \text{ ms.}$$

C.

The main advantage of a two-angle-method is speed. The disadvantage is that the range of T_1 relaxation times that can be determined accurately is dependent on α_1 and α_2 . Since an inversion recovery method samples multiple delays, it can accurately determine a wide range of T_1 relaxation times.

3.6.A.

Direct substitution of Eqs. [3.29] and [3.30] into Eqs. [3.27] and [3.28] demonstrate that Eqs. [3.29] and [3.30] are valid solutions of the Bloch equations extended to incorporate the effects of chemical exchange. Note that Eqs. [3.36] and [3.37] need to be used to replace R_A and R_B .

B.

For $M_{zB}(t) = 0$, Eq. [3.27] reduces to:

$$\frac{dM_{zA}(t)}{dt} = \frac{M_{zA}^0}{T_{1A}} - M_{zA}(t)R_A$$

The general solution to this first order, non-homogeneous differential equation equals

$$M_{zA}(t) = \frac{M_{zA}^0}{R_A T_{1A}} + C e^{-R_A t}$$

which reduces to Eq. [3.39] when substituting $M_{zA}(0)=M_{zA}^0$.

C.

Eq. [3.40] follows directly from Eq. [3.39] when $t \rightarrow \infty$.

3.7.

Consider flow of particles through a 2D plane of area A and thickness Dx . The number of particles entering the plane, N_{in} , minus the number of particles leaving the plane, N_{out} , per unit time must equal the change in concentration of particles Δc within the volume $A\Delta x$ per unit of time. In other words:

$$(N_{in} - N_{out})/\Delta t = \Delta c A \Delta x / \Delta t$$

Since the flux is defined as the number of particles flowing through an area per unit of time, i.e. $J = (N_{out} - N_{in})/(A\Delta t)$, this equation reduces to Eq. [3.45] for $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$.

3.8.A. Consider a spin-echo sequence with a constant background gradient G during the entire echo-time. The function $F(t)$ over the interval $0 \leq t < TE/2$ then becomes γGt . The 180° pulse resets the acquired phase, such that the function $F(t)$ over the interval $TE/2 \leq t \leq TE$ becomes $-\gamma GTE/2 + \gamma G(t - TE/2)$. Substituting $F(t)$ into Eq. [3.61] gives

$$b = \gamma^2 \int_0^{TE/2} G^2 t^2 dt + \gamma^2 \int_{TE/2}^{TE} \left(G \left(t - \frac{TE}{2} \right) - G \frac{TE}{2} \right)^2 dt \quad [s.3]$$

After expanding and grouping terms and using the fact that $f(TE/2) = GTE/2$, it follows that Eq [s.3] is identical to Eq. [3.62].

B.

Without loss of generality, let the diffusion gradients in Fig. 3.19B start immediately following the RF pulses, such that the function $F(t)$ (for use with Eq. [3.61]) becomes γGt for $0 \leq t \leq \delta$, $\gamma G\delta$ for $\delta \leq t \leq \Delta$ and $-\gamma G\delta + \gamma G(t - \Delta)$ for $\Delta \leq t \leq \Delta + \delta$. Substituting $F(t)$ into Eq. [3.61] yields the b-value expression given by Eq. [3.63].

C.

Maximum diffusion-weighting ('b-value') will be achieved when maximum gradients are present in all three directions simultaneously during the entire echo-time, such that $\delta = 10$ ms and $\Delta = 10$ ms. The maximum gradient strength G then becomes $\sqrt{3} \cdot 40$ mT/m = 69.28 mT/m = 2949.3 Hz/mm, which will lead to a b-value of 5.80 s/mm².

D.

$\delta = 9.5$ ms, $\varepsilon = 0.5$ ms and $\Delta = 10$ ms, such that $b = 5.36$ s/mm².

3.9A.

Eq. [3.58] can be derived directly from Eqs. [3.54] – [3.57]. However a much simpler derivation is provided when the background field is considered as two pulse gradients of amplitude G_0 , duration δ of $TE/2$ and separation Δ of $TE/2$. Substitution of these parameters into Eq. [3.63] gives, in combination with Eq. [3.60], the result of Eq. [3.58].

B.

$TE = 9.58$ s.

C.

The extremely long echo-time required to produce a 5% diffusion-related signal reduction will lead to 100% signal loss due to T_2 relaxation.

D.

In order to retain a reasonable echo-time (< 100 ms), G_0 must be increased to circa 1000 Hz/cm. Unfortunately, this background magnetic field inhomogeneity will persist during

the acquisition time, thereby causing severe line broadening and loss in spectral resolution. During the Stejskal-Tanner experiment, the magnetic field gradients are not present during acquisition, such that diffusion-weighting can be achieved *without* an associated loss in spectral resolution.

E.

Standard Hahn sequence : $M_{xy} = 0.1664M_0$

CMPG sequence : $M_{xy} = 0.2396M_0$

3.10.

A. $b = 5,403 \text{ s.mm}^{-2}$.

B. $D = 1.88 \times 10^{-4} \text{ mm}^2.\text{s}^{-1}$.

C. On an unrestricted phantom the ADC should be largely independent of the diffusion time (or TM), while in the presence of restrictions as found *in vivo*, the ADC should decrease with increasing diffusion times. However, additional signal loss may be observed in the presence of macroscopic motion and signal averaging. Since motion related artifacts increase at longer TM times, the observed ADC also increases at longer diffusion times.

D. $b_{xyz} = 3b_x = 16,209 \text{ s.mm}^{-2}$.

E. Since the magnetization is along the z axis during the TM period, the TM gradient does not affect the diffusion weighting.

3.11A.

Eq. [3.81] is a standard first-order linear non-homogeneous differential equation of which Eq. [3.82] is the direct solution (using $P^*(0) = 0$).

B.

Fractional enrichment (FE) of compound P = $[P^*]/[P] = 0.7$.

C.

$V_{in} = 0.466 \text{ mM/min}$.

D.

$$V_{in} = 0.933 \text{ mM/min.}$$

3.12.

The 2D diffusion tensor in the cell frame of reference is given by:

$$D' = \begin{pmatrix} D'_{xx} & 0 \\ 0 & D'_{yy} \end{pmatrix}$$

Following a 2D rotation over an arbitrary angle α , the diffusion tensor is equal to:

$$D = \begin{pmatrix} D'_{xx} \cos^2 \alpha + D'_{yy} \sin^2 \alpha & D'_{xx} \sin \alpha \cos \alpha - D'_{yy} \sin \alpha \cos \alpha \\ D'_{xx} \sin \alpha \cos \alpha - D'_{yy} \sin \alpha \cos \alpha & D'_{xx} \sin^2 \alpha + D'_{yy} \cos^2 \alpha \end{pmatrix}$$

Even though the two matrices are very different, the traces are identical, i.e.

$$\text{Tr}(D') = \text{Tr}(D) = D'_{xx} + D'_{yy}$$