

Appendix 4

Biochemical Reactions and Molecular Structures of Common MRS-Detectable Metabolites

Most of the metabolites routinely detected in vivo by MRS are involved in a limited number of metabolic interconversions. This appendix is therefore presented in the form of simplified metabolic pathway diagrams. MRS-detectable metabolites are depicted in boldface in boxes; intermediates that are usually undetectable by MRS are shown in faint text. Cofactor

substrates (e.g., methyl donors) are omitted for clarity. Broken lines indicate multiple steps in a pathway (Figures 1–5).

The structural formulae of the MRS-detectable metabolites in these diagrams are also shown in Appendix 6, along with their spectra and peak assignments.

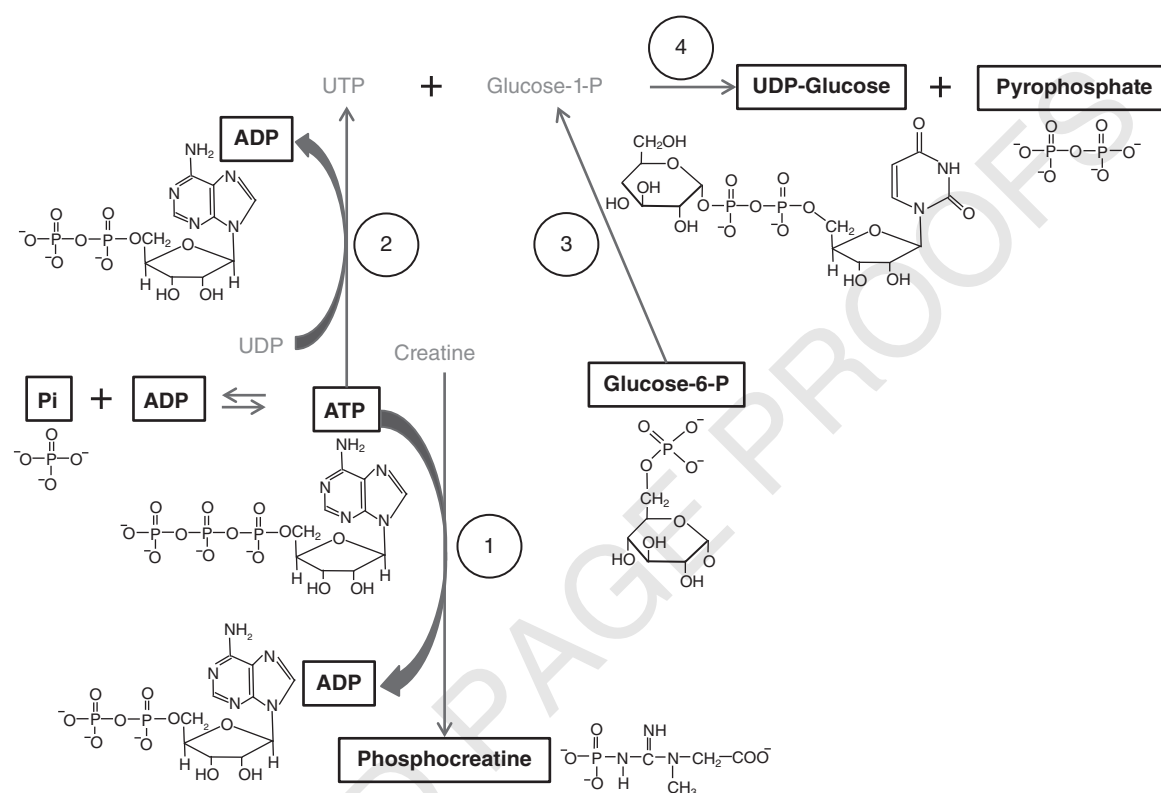


Figure 1. Interconversions of metabolites detectable in vivo by ^{31}P MRS: adenosine triphosphate (ATP)-based reactions. 1, Creatine kinase; 2, nucleoside diphosphate kinase; 3, phosphoglucomutase; and 4, uridine diphosphate (UDP)-glucose pyrophosphorylase (UTP = uridine triphosphate; Pi = inorganic phosphate). Note that the total creatine pool (creatine and phosphocreatine) is also detectable by ^1H MRS

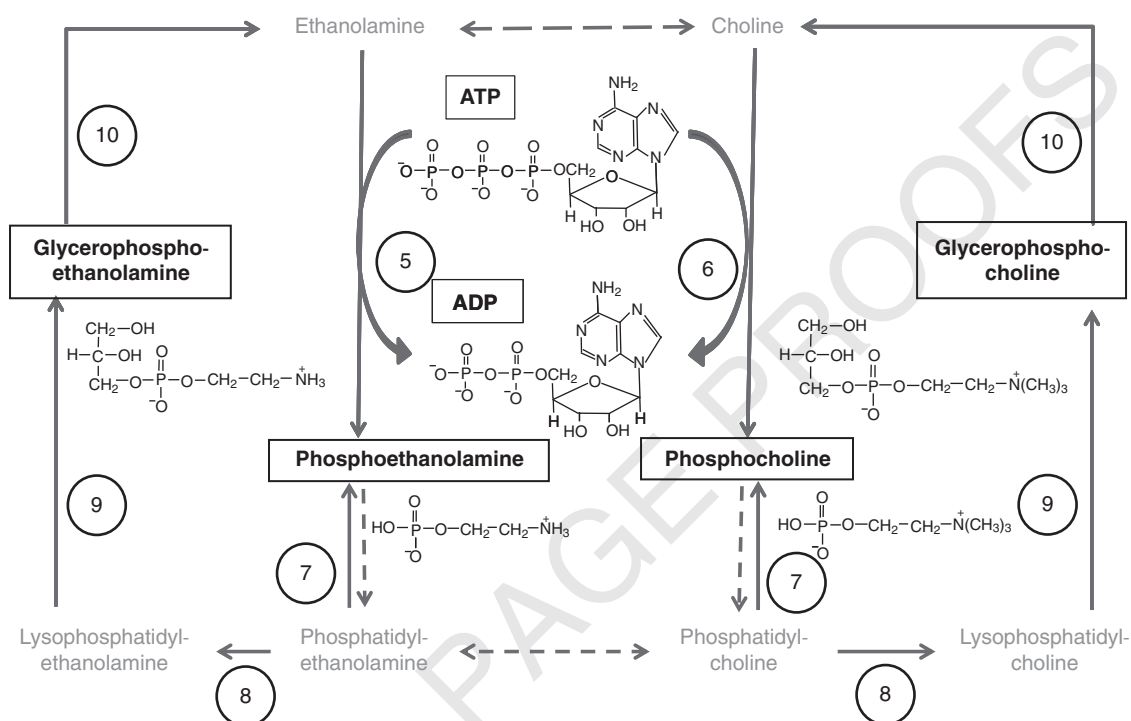


Figure 2. Interconversions of metabolites detectable in vivo by ^{31}P MRS: choline and ethanolamine metabolism. 5, Ethanamine kinase; 6, choline kinase; 7, phospholipase C; 8, phospholipase A2; 9, lysophospholipase; and 10, glycerophosphocholine phosphodiesterase. Note that the total choline pool (choline, phosphocholine, and glycerophosphocholine) and total ethanolamine pool (ethanolamine, phosphoethanolamine, and glycerophosphoethanolamine) are also detectable by ^1H MRS

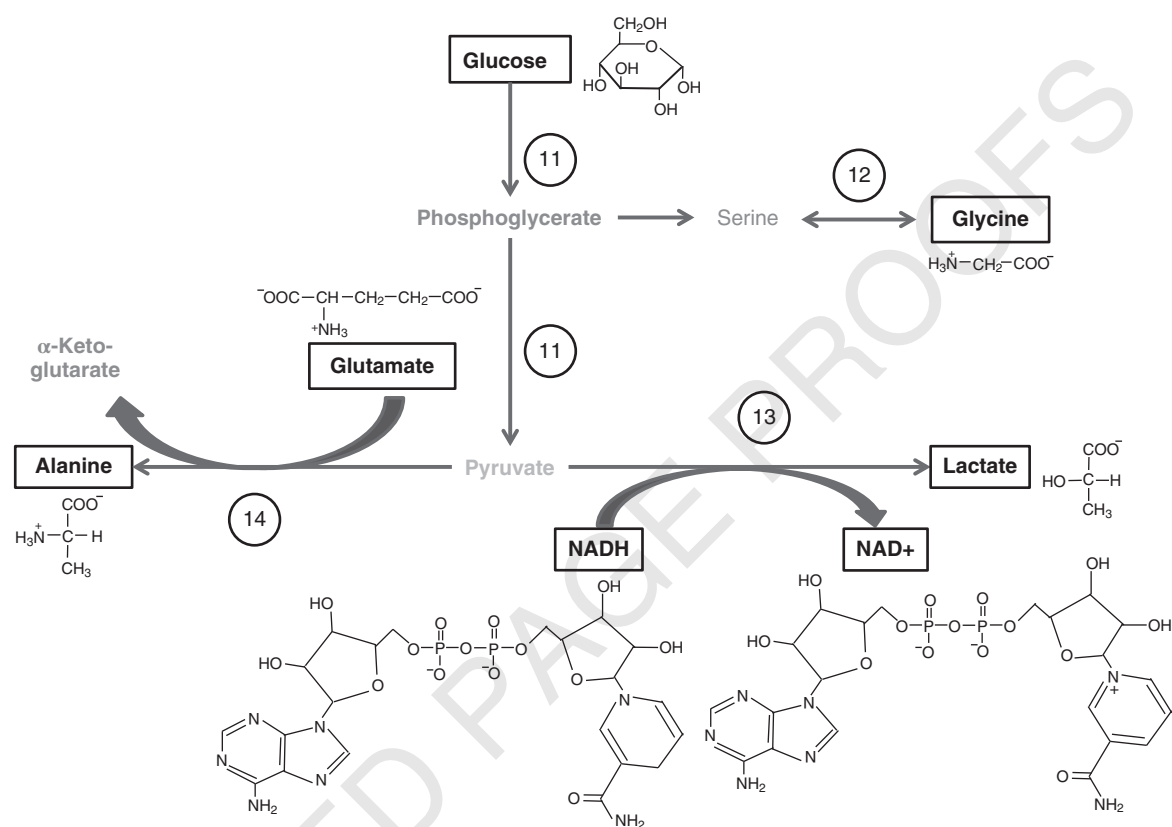


Figure 3. Interconversions of metabolites detectable in vivo by ^1H MRS: Products of glycolysis. 11, Glycolytic pathway; 12, serine hydroxymethyl transferase; 13, lactate dehydrogenase; and 14, alanine aminotransferase

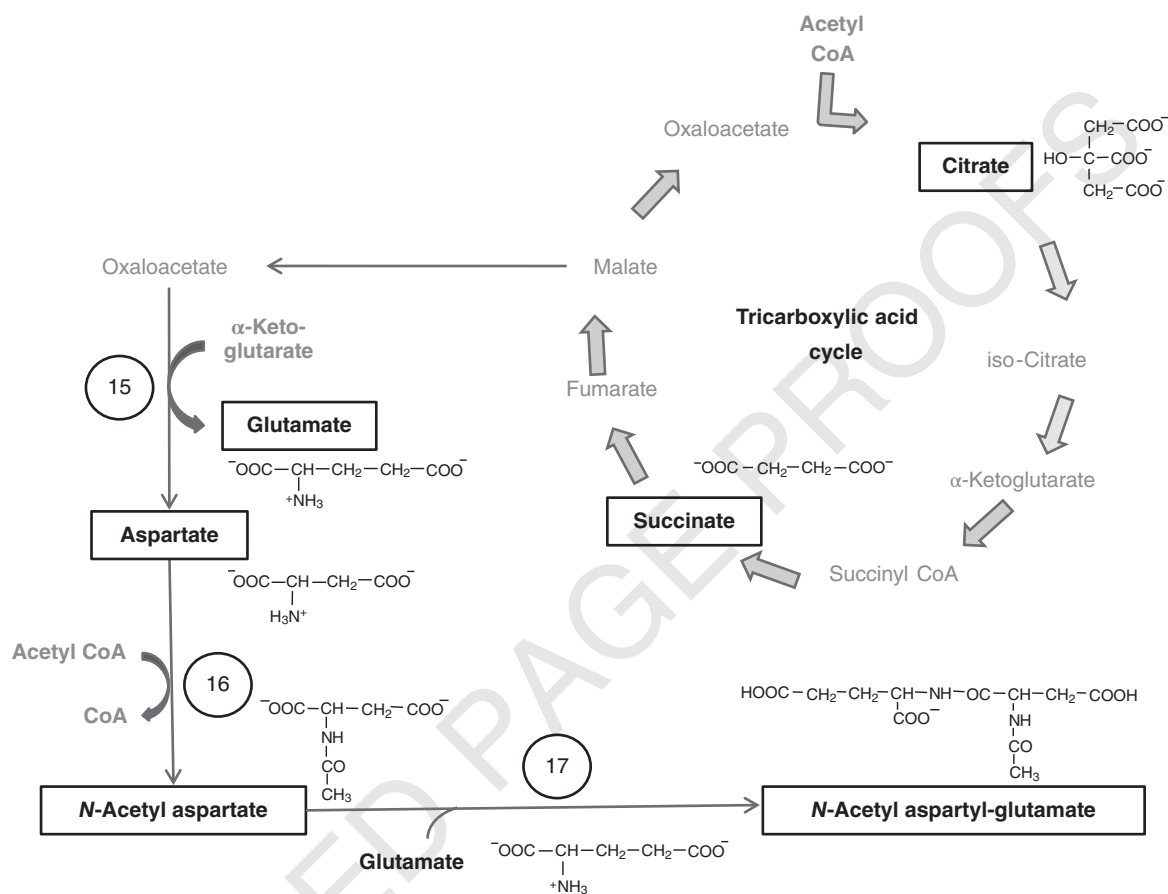


Figure 4. Interconversions of metabolites detectable in vivo by ^1H MRS: Products of acetyl-CoA and succinate metabolism. 15, Aspartate aminotransferase; 16, L-aspartate *N*-acetyltransferase; and 17, *N*-acetylasparylglutamic acid synthetase

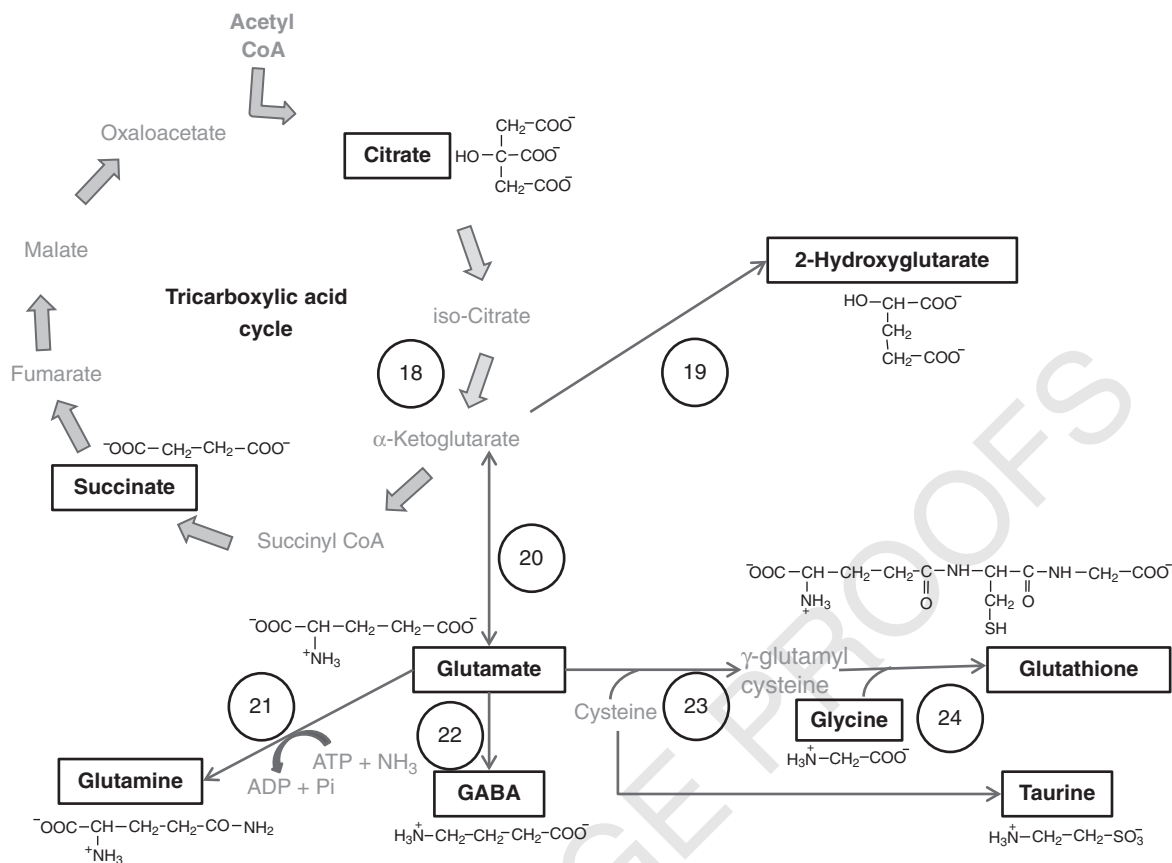


Figure 5. Interconversions of metabolites detectable in vivo by ^1H MRS: Products of citrate and α -ketoglutarate metabolism. 18, Isocitrate dehydrogenase, wild-type enzyme; 19, isocitrate dehydrogenase mutant enzyme; 20, glutamate dehydrogenase; 21, glutamine synthetase; 22, glutamic acid decarboxylase; 23, γ -glutamyl cysteine synthetase; and 24, glutathione synthetase; Note that wild-type isocitrate dehydrogenase (numbered 18) is the normal enzyme and that mutant isocitrate dehydrogenase (numbered 19) is the mutant form that synthesizes the oncometabolite 2-hydroxyglutarate (see *Characterizing Brain Tumors by MRS*)

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