**Table 1: Metabolites that can be measured in cancer cells and tumours by 1H- and 31P HR-MRS**

|  |
| --- |
| ***Amino acids and related metabolites:*** |
| Alanine | Asparagine | Aspartate | Glutamate | Glutamine |
| Glycine | Histidine | Iso-leucine | Leucine | Lysine |
| Phenylalanine | Threonine | Taurine | Valine | Glutathione |
| N-acetyl aspartate |  |  |  |  |
| ***Glycolytic metabolites:*** |
| α-Glucose | β-Glucose | Lactate | Pyruvate |  |
| ***TCA cycle and related metabolites:*** |
| β-Hydroxybutyrate | Acetate  | Fumarate | Succinate |  |
| ***Bioenergetics metabolites:*** |
| Inorganic phosphate | ADP+ADP | NTP | NDP | Phosphocreatine |
| NAD+ and NADH | Inosine | Sugar phosphate | UTP and UDP | Creatine |
| ***Membrane and related metabolites:*** |
| Glycerophosphocholine | Choline | Phosphocholine | Carnitine | Phosphoethanolamine |
| Glycero-phosphoethanolamine | Phosphatidyl-ethanolamine | Cholesterol and esters | Sphingomyelin | Phosphatidylcholine |
| Triacylglycerol | Plasmalogen | Saturated fatty acids | Unsaturated fatty acids | Phosphatidyl-glycerol |
| ***Other:*** |  |  |  |  |
| Betaine | Myo-inositol | Scyllo-inositol | Formate |  |

**Table 2:** Example MR spectral acquisition parameters for various sample types (see **Note 11**):

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Types of metabolite | Spectral width (Hz) | Time domain points | Repetition time (s) | Number of scans\* |
| 1H-MRS of cell/tumour extract | Water-soluble | 7,500 | 32,768 | 2.7 | 256 |
| 1H-MRS of cell/tumour extract | Lipid | 7,500 | 32,768 | 2.7 | 128 |
| 1H-MRS of culture media | Water-soluble | 7,500 | 32,768 | 2.7 | 64 |
| 31P-MRS of cell/tumour extract | Water-soluble | 12,000 | 32,768 | 5.0 | 4096 |

\*This is only a guide as more or less scans maybe required depending on the sample sizes (i.e., the number of cells or the size of extracted tumour).