| Metabolites                     | Spectrum No. | Class                       |
|--------------------------------|--------------|-----------------------------|
| 1-Methylnicotinamide           | 1            | vitamin/cofactors           |
| 2-Hydroxyisobutyrate           | 2            | organic acids               |
| 2-Hydroxyisovalerate           | 3            | organic acids               |
| 3-Aminoisobutyrate             | 4            | amino acids                 |
| 3-Hydroxybutyrate              | 5            | organic acids               |
| 3-Hydroxyisovalerate           | 6            | organic acids               |
| 3-Indoxylsulfate               | 7            | amino acid derivatives      |
| 4-Hydroxyphenylacetate         | 8            | organic acids               |
| Acetate                        | 9            | organic acids               |
| Acetone                        | 10           | ketones                     |
| Alanine                        | 11           | amino acids                 |
| Arabinose                      | 12           | sugars                      |
| Betaine                        | 13           | amino acids                 |
| Carnitine                      | 14           | amino acids                 |
| Choline                        | 15           | ammoniums compounds         |
| Creatine                       | 16           | amino acid derivatives      |
| Creatinine                     | 17           | amines                      |
| Dimethylamine                  | 18           | amines                      |
| Ethanolamine                   | 19           | amines                      |
| Formate                        | 20           | organic acids               |
| Fumarate                       | 21           | organic acids               |
| Glucose                        | 22           | sugars                      |
| Glutamate                      | 23           | amino acids                 |
| Glutamine                      | 24           | amino acids                 |
| Glycine                        | 25           | amino acids                 |
| Guanidooacetate                | 26           | amino acid derivatives      |
| Hippurate                      | 27           | amino acid derivatives      |
| Hypoxanthine                   | 28           | nucleic acid components     |
| Isoleucine                     | 29           | amino acids                 |
| Lactate                        | 30           | organic acids               |
| Leucine                        | 31           | amino acids                 |
| Lysine                         | 32           | amino acids                 |
| Mannitol                       | 33           | sugars                      |
| Methanol                       | 34           | alcohols                    |
| N-Phenylacetylglcine           | 35           | amides                      |
| Phenylalanine                  | 36           | amino acids                 |
| Propylene glycol               | 37           | alcohols                    |
| Pyroglutamate                  | 38           | amino acid derivatives      |
| Pyruvate                       | 39           | organic acids               |
| Serine                         | 40           | amino acids                 |
| Succinate                      | 41           | organic acids               |
| Taurine                        | 42           | amino acids                 |
| Threonine                      | 43           | amino acids                 |
| Trigonelline                   | 44           | food and drug compounds     |
| Tryptophan                     | 45           | amino acids                 |
| Tyrosine                       | 46           | amino acids                 |
| Uracil                         | 47           | nucleic acid components     |
| Valine                         | 48           | amino acids                 |
| Xylose                         | 49           | sugars                      |
| trans-Aconitate                | 50           | organic acids               |