

# Metabolite Identification with the Q Exactive and LTQ Orbitrap Elite

## Course Programme

| Date  | Time          | Session  |   |
|-------|---------------|--|---|
| Day 1 | 09.00 – 09.15 | Registration   |   |
|       | 09.15 – 09.30 | <b>Lecture : Introduction to the course and Birmingham Metabolomics Training Centre</b><br><i>Dr Cate Winder</i>               |   |
|       | 09.30 – 10.30 | <b>Lecture : Introduction to metabolomics and analysing complex biological samples</b><br><i>Professor Warwick Dunn</i>        |   |
|       | 10.30 – 10.45 | Break  |   |
|       | 10.45 – 11.40 | <b>Lecture : Overview of instrumentation and their potential in metabolite identification</b><br><i>Professor Warwick Dunn</i> |   |
|       | 11.40 – 12.45 | <b>Lecture : Tools for mass spectral interpretation</b><br><i>Professor Warwick Dunn</i>                                       |   |
|       | 12.45 – 13.30 | Lunch  |   |
|       | 13.30 – 16.00 | <b>Group 1 : Lab session : Q Exactive (Instrument set-up, DDA and DIA method set-up)</b><br><i>Dr Cate Winder</i>              | <b>Group 2 : Lab session : LTQ Orbitrap Elite (MS/MS, MS<sup>n</sup>, optimizing methods for difficult structural elucidation)</b><br><i>Dr Lukáš Najdekr</i> |
|       | 16:00 – 16:15 | Break  |   |
|       | 16.15 – 17.30 | <b>Computer workshop : Instrument software and searching mass spectral libraries</b><br><i>Dr Ralf Weber</i>                   |   |

|       |               |   |   |
|-------|---------------|---|---|
|       | 09.15 – 10.45 | <u>Group 1</u> : Lab session : LTQ Orbitrap Elite (MS/MS, MS <sup>n</sup> , optimizing methods for difficult structural elucidation)<br><i>Dr Lukáš Najdekr</i> | <u>Group 2</u> : Lab session : Q Exactive (Instrument set-up, DDA and DIA method set-up)<br><i>Dr Cate Winder</i>   |
|       | 10.45 – 11.00 | Break   |   |
|       | 11.00 – 12.00 | <u>Group 1</u> : Lab session : LTQ Orbitrap Elite (MS/MS, MS <sup>n</sup> , optimizing methods for difficult structural elucidation)<br><i>Dr Lukáš Najdekr</i> | <u>Group 2</u> : Lab session : Q Exactive (Instrument set-up, DDA and DIA method set-up)<br><i>Dr Cate Winder</i>   |
|       | 12.00 – 12.30 | Lunch   |   |
| Day 2 | 12.30 – 13.30 | <u>Group 1</u> : Lab session : Q Exactive (Instrument set-up, DDA and DIA method set-up)<br><i>Dr Cate Winder</i>   | <u>Group 2</u> : Lab session : LTQ Orbitrap Elite (MS/MS, MS <sup>n</sup> , optimizing methods for difficult structural elucidation)<br><i>Dr Lukáš Najdekr</i> |
|       | 13.30 – 15.00 | <u>Group 1</u> : Lab session : LTQ Orbitrap Elite (MS/MS, MS <sup>n</sup> , optimizing methods for difficult structural elucidation)<br><i>Dr Lukáš Najdekr</i> | <u>Group 2</u> : Lab session : Q Exactive (Instrument set-up, DDA and DIA method set-up)<br><i>Dr Cate Winder</i>   |
|       | 15.00 – 15.15 | <b>Lab session : Review identification of unknown metabolites</b><br><i>Dr Cate Winder</i>  |   |
|       | 15.15 – 15.30 | Break   |   |
|       | 15.30 – 16.30 | <b>Computer workshop : Using Mass Frontier</b><br><i>Professor Warwick Dunn</i>   |   |
|       | 16.30 – 17.15 | <b>Q&amp;A : Tips and tricks from the experts and question session</b><br><i>Professor Warwick Dunn &amp; Dr Cate Winder</i>                                    |   |
|       | 17.15 – 17.30 | <b>Feedback survey</b><br><i>Mr David Epps</i>  |   |