

# Automated Approaches in Modern Chromatography and Mass Spectrometry

From method development to data visualisation



The 2013 Chromatographic Society Spring Meeting 10<sup>th</sup> April 2013  
The Discovery Centre, Merck Sharp and Dohme, Hoddesdon, Herts.

“ A one day symposium and workshop on recent advances in software assisted and automated approaches for chromatography and mass spectrometry. This meeting will focus on the various software and approaches that facilitate improvements in workflow; from method development, data processing and visualization, to statistical analysis and pattern recognition. ”

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**Thermo**  
S C I E N T I F I C



# Programme

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## Session 1

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8.40	Coffee and Registration
9.20	Welcoming Comments
9.30	Sarah Perry - Thermo Fisher Scientific Gold Sponsor Talk : "The Real Life Application of Automated Instrument Data Management – A Forensic Case Study"
10.00	Roman Szucs – The impact of structural similarity on the accuracy of retention time prediction in liquid chromatography
10.30	Coffee
11.00	Patrik Petersen - Modelling of analytical (U)HPLC: An important element in the QbD toolbox
11.30	Prof Frederick Lynen (Gent) – Automated chiral and achiral selectivity tuning through combined stationary and mobile phase optimization approaches in LC
12.00	Manufacturers Intro
12.15	Lunch and Exhibition; all exhibitors Gold to Bronze

## Session 2

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13.30	Mark Earll (Syngenta) – Semi-automated processing of LC/GC-MS data with open source software
14.00	Prof Frank Pullen – MSMS prediction is it luck? Can a deeper understanding of 3D ionic structure help de-mystify this process?
14.30	Adrian Dunn (GSK) – Experiences in automating System Suitability
15.00	Vendor Workshops

## Parallel sessions (20 - 30 mins)

### Gold and Silver Sponsors

16.00	Tea, Closing remarks and Raffle
16.30	End of Meeting

# Registration Form

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Please complete the form below and send with a cheque made payable to the "Chromatographic Society". Electronic registration and credit card payment facilities will be available shortly; please see further mailings or refer to our website for updates.

Early registration is strongly advised as numbers will be limited and registrations should be received with full remittance by 1st April 2013.

## Registration (including all sessions, exhibition, refreshments and lunch)

Member of Chromsoc/BMSS/RSC C & E Group and EuSSS	£100 (inc. VAT)
Non Member	£150 (inc. VAT)
Non Member plus 1 year Chromatographic Society Membership	£140 (inc. VAT)
Student	£50 (inc. VAT)

Please register me for "Automated Approaches in Modern Chromatography and Mass Spectrometry"

A remittance of £ ..... is enclosed as registration for attendance at the meeting.

Cheques should be made payable to the "Chromatographic Society".

Block Capitals Please.

Name: .....

email: .....

Address: .....

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Telephone: .....

Fax: .....

I have special dietary requirements .....

I would like travel directions ( )

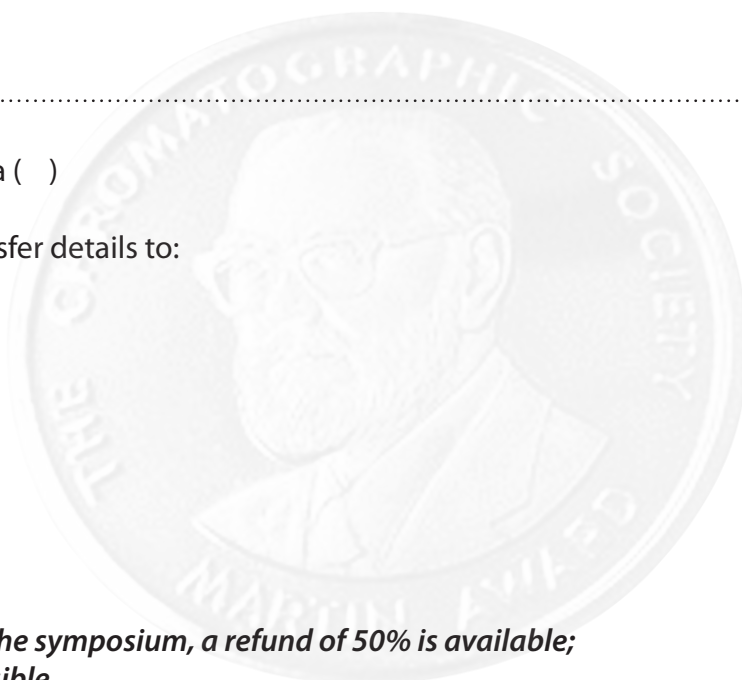
I would like details of accommodation in the area ( )

Please return this form with cheque or bank transfer details to:

Matthew Gilmour  
Senior Conference Executive  
Meeting Makers  
Block 4, Unit 4, Kelvin Campus  
West of Scotland Science Park  
2317 Maryhill Road, Glasgow, G20 0SP

### ***Cancellation policy:***

***For delegate cancellations up to 3 weeks before the symposium, a refund of 50% is available; for cancellations after this time, no refund is possible.***



# Directions

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Situated just north of London, Hoddesdon can be easily reached from the A10 and M25.

## By Car

Address for Sat Nav: EN11 9BU

By Road from London

- Take the A10 north (M25 Jnc 25) and leave at the signposted Hoddesdon junction after 5.5 miles
- At the top of the slip road turn right, which takes you onto the A10 link road
- At the bottom of the hill, turn left at the first roundabout into Amwell Street
- Turn left at the next roundabout (after 100 yards) into Hertford Road (B1179)
- MSD is located on the left just over the top of the hill (after approximately 0.5 miles)

## By Train

Destination station: Broxbourne

If travelling by train from London, take the train from Liverpool Street station or Tottenham Hale station to Broxbourne. A taxi from Broxbourne station to MSD Offices will cost approximately £6.00.

## By Air

Stanstead and City Airports are a half hour taxi ride from Hoddesdon, with London Luton and London Heathrow only an hour away.

## Hotels

Please contact Matthew Gilmore at Meeting Makers ([matthew@meetingmakers.co.uk](mailto:matthew@meetingmakers.co.uk))