CCDC ユーザミーティング 2019

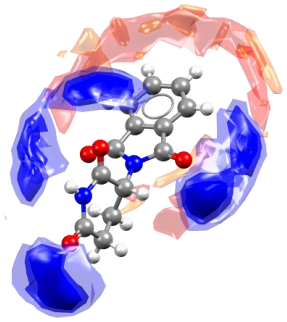
‘Going for Growth’ UGM 2019

主催：Cambridge Crystallographic Data Centre，化学情報協会

CSD は，The Cambridge Crystallographic Data Centre (CCDC)が運営する世界最大の有機低分子の結晶構造データベースです．1965 年に結晶構造を集め始め，構造化学における金字塔として本年 100 万件目の構造を収録いたしました．CCDC では，CSD に蓄積された構造情報を基に医薬分子の設計のみならず，材料開発に注目した製品開発にも取り組んでおります．今回のユーザ会では，CSD 1M のデータをどのように生かすか，基本となる CSD-System およびアップグレード版の CSD-Discovery と CSD-Materials の基本機能や活用法をご紹介いたします．

日時：2019 年 10 月 28 日(月)　10:00 - 17:00
会場：化学情報協会 中居ビル 6 階 講習会室 (東京都文京区)
参加費：無料 (事前登録が必要です)

プログラム



9:45 - 10:00　**Registration**

10:00 - 10:15　**Welcome and Introductions** (化学情報協会)

Chair (Jonathan Betts, Director of Business Development)

10:15 - 10:35　**Session 1. Advancing Structural Science in Japan**

◆1M Structures and beyond (Jürgen Harter, CEO)

10:35 - 11:00　**Session 2. The Power of Data - CSD 1M and Machine Learning**

◆How the CSD is being used in AI/Machine Learning (Andrew Maloney & Jonathan Betts)

11:00 - 14:30　**Session 3. Solutions Update - Tools and Services to Power Digital Transformation**

◆New solutions for making R&D more efficient (JB)

◆A Million Crystal Structures: From Data to Knowledge (Andrew Maloney & Francesca Stanzione)

[12:00 - 13:00 昼食]

◆How the CSD can aid Drug Design – Introduction and Application Examples of CSD-Discovery tools (FS)

CSD-Discovery suite provides valuable insights from the fully curated crystallographic structures in the CSD that can inform the design, development and identification of new and/or better pharmaceutical products. Knowledge derived from the CSD data is extremely relevant to drug discovery since the small molecule crystal structures in the CSD, including FDA approved drugs and drug-like molecules, resemble the geometry and interactions observed in protein-ligand complexes.

This presentation will provide an overview of the CSD-Discovery capabilities, including:

- Protein-ligand docking using GOLD
- Assessing protein-ligand interaction preferences using SuperStar
- Mining structural databases, including protein-ligand using CSD-CrossMiner.

◆Solid Form Informatics for Pharmaceuticals and Fine Chemicals: Knowledge-based development and risk assessment (AM)

- How companies use CSD-Materials tools to make development more efficient, reducing risk and the cost of failure.

[14:30 - 14:40 休憩]

14:40 - 15:00 **Session 4. Product Roadmap**

◆2019 Developments and 2020 Plans covering development themes, new products and enhancements for making R&D more efficient (Jürgen Harter)

15:00 - 15:40 **Session 5. Customer Feedback** (All)

★事前にご質問いただいた内容にお答えします．当日の飛び入り質問も歓迎です．

15:40 - 16:00 **Summary and Close** (Chair)

16:00 - 17:00 **Networking & Demo** (自由参加)

★聞きそびれたこと，個別相談，デモ等，会場にて承ります．

お問い合わせ先：化学情報協会　科学データ情報室　桜井<crystal★jaici.or.jp>

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[Speakers]

Jürgen Harter (JH): Jürgen has joined the CCDC in July 2018 as Chief Executive Officer and brings two decades worth of life sciences, information technology and business experience. His executive leadership expertise is extensive, paired with commercial acumen, a strong technical background and broad business skills, gained in organisations such as Horizon Discovery, Exco InTouch, PerkinElmer Informatics, CambridgeSoft, Abcam and Biowisdom. He holds a PhD in organic chemistry from the University of Cambridge and carried out his postdoctoral research at the Unilever Centre for Molecular Informatics. He cares passionately about digital transformation, big data, knowledge management, automation, scientific and business intelligence. He has successfully delivered many complex solutions and projects (ERP / CRM / ELN / LIMS / mHealth platforms) spanning a range of business functions on an enterprise-wide level, and has worked with most of the Top 20 pharmaceutical companies. He has a wide global network in the biotech, pharma and chemical industry sectors. This is combined with many active links to information management and software development companies.

Jonathan Betts (JB): Jonathan has over 20 years' experience in software sales and technology commercialisation in life sciences, healthcare and research markets. He has worked in sales leadership and customer success roles building teams with a relentless focus on delivering value to customers. Prior to joining CCDC he cofounded and built a SaaS business with a global customer community, taking it through multiple funding rounds to profitability and a successful trade exit. His qualifications include a PhD in gene structure and regulation and an MBA in strategic management.

Andrew Malolney (AM): Andrew obtained his degree in Materials Chemistry from the University of Edinburgh in 2011. He then remained in Edinburgh to undertake a PhD with Prof. Simon Parsons and Dr. Pete Wood (CCDC), studying intermolecular interactions in organic and inorganic systems. His thesis work included expanding the PIXEL method to include transition metals, increasing the number of CSD structures that could be analysed in this way, for which he was awarded the 2016 Fraser and Norma Stoddart PhD Prize. Andy's research interests include crystal engineering through the analysis and prediction of multi-component systems, polymorphism and intermolecular interactions using a combination of knowledge-based and computational methods. He is particularly interested in studying the differences in crystal packing between single and multi-component systems as well as the effect of high Z'.

Francesca Stanzione (FS): Francesca's research interests lay where applied mathematics, scientific computing and modeling of biological phenomena meet. She dedicates her work to design and model high-fidelity physical systems in order to define the properties and the dynamics of the biological systems. This approach finds its outcome on advancing the integration of computational methods with the chemistry, biology and medicine of drug targets. She works in the Discovery Chemistry group. Duties include validation of new software, applications, and scientific support of the CCDC's suite of Life Sciences software products (Hermes, GOLD, CSD-CrossMiner). Also involved in outreach activities such as giving talks and workshops and in the development of teaching material for the Life Sciences and Small Molecules software products (CSD systems: Mercury, ConQuest, Mogul, IsoStar).