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REVIEW: SCS-SYNGENTA SYMPOSIUM 2013: FRONTIERS IN FLUORINE CHEMISTRY

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On October 24, 2013, over 170 chemists came together for the ‘Frontiers in Fluorine Chemistry’ one-day symposium, hosted at Syngenta’s Research and Development (R&D) Center in Stein, Switzerland. Building on the success of the first joint symposium between the Swiss Chemical Society (SCS) and Syngenta during IYC2011, this sold-out event attracted chemists from academia and industry alike to share top quality science, exchange ideas and enhance scientific networks.

In 2011, the SCS-Syngenta partnership was formed to provide the regional chemical sciences community with a platform for communicating the latest advances in selected fields, as well as to demonstrate Syngenta’s interest in top quality research and knowledge sharing. “We, as a global company focusing on research and innovations, like to be ‘the place to be’ when it’s about the exchange of know-how and knowledge between industry and academia. And we have a very strong tradition in this,” commented Dr. **Gerardo Ramos**, Head of Syngenta Crop Protection R&D at Syngenta.

The second SCS-Syngenta Symposium held recently brought together top chemists from leading universities and companies from across Switzerland, as well as neighbouring regions of France and Germany. It was a full day of cutting-edge lectures from internationally renowned speakers, and a post-graduate and industrial poster session discussing various aspects of theoretical, mechanistic and applied fluorine chemistry.

The popularity of the event reflects the importance of fluorinated compounds, in life sciences (crop protection, pharmaceuticals, diagnostics, and animal health), material science (*e.g.* Teflon and liquid crystal displays) and energy (*e.g.* lithium ion batteries). Fluorine is the 13th most abundant element on Earth, and half of which is used in the steel industry to lower the melting point of smelts. And although there are only a handful of natural products that contain fluorine, that is not the case for new active ingredients. Around 30% of new pharmaceuticals and approximately half of all new agrochemicals contain at least one fluorine atom or fluorine-containing substituent.

Morning session – Chair: Prof. Peter K ndig (University of Geneva, Swiss Chemical Society President)

The program began with a scene-setting lecture from Dr. **Guillaume Berthon**, team leader in insecticide chemistry at Syngenta; he gave a brief history and a general overview of the importance of fluorine in the design of biologically active compounds, allowing all subsequent lecturers to dive straight into their research.

Dr. Berthon explained how the nature of the polarized C–F bond, which is stronger than the C–H bond, makes compounds more resistant to oxidative metabolism, can act as a conformational lock (bringing favourable membrane permeability) or probe (increasing bioavailability), can increase receptor binding affinity, influences log P and affects pK_a. Usually a few of these five aspects

are exploited in the design of a particular molecule for its desired effect.

The first of the plenary lectures was given by Prof. **Antonio Togni** from ETH Z rich, discussing the variety of trifluoromethylation reactions that can be carried out using hypervalent iodine reagents developed by his group. Work focused on heteroatom substrates, and in particular phosphorus, with application in the preparation of a new class of trifluoromethylated ligands. Mechanistic aspects were debated on the radical nature of the intermediates.^[1]

Next Dr. **Emmanuel Magnier** from Versailles University, France, presented his work on sulfonium salts and sulfoximines as versatile tools for fluoroalkylation. He presented a simplified procedure for synthesizing sulfonium salts,^[2] which could serve as electrophilic, radical or nucleophilic species. Improved syntheses of sulfoxamines were also disclosed, used routinely as electrophilic reagents, as well as novel applications as ligands and in biological studies.^[3]

Prof. **David O’Hagan** from St. Andrews University, UK, concluded the morning session by discussing the identification, characterisation and exploitation of fluorination enzymes. The rarity of organofluorine natural products reflects the abundance and use of fluorination enzymes. Fluorinase, which is a slow enzyme in biocatalysis, is being developed for use in PET imaging, to catalyze the formation of ¹⁸F–C bonds in substrates to be used as tracers.^[4]

Afternoon session – Chair: Dr. Alain De Mesmaeker (Principal Fellow, Syngenta Crop Protection R&D, Research Chemistry)

Prof. **Ryan Gilmour** from the University of M nster, Germany, began the afternoon session with a brief account of his connection with Syngenta: “Syngenta gives a lot back to the scientific community – to education – to people like myself.” He went on to describe his work exploiting fluorine as a chemically inert steering group in acyclic conformational control. Known as the Gauche effect, the β -effect of the highly polarized C–F bond gives a predictable 60° angle for α -substitution or acts as a conformational lock. This was exploited to design new catalysts in hetero- and homogeneous catalysis, enhancing the activity of the catalysts or probing mechanisms in organocatalysis.^[5]

Dr. **Stefan Abele** from Actelion Pharmaceuticals, Switzerland, explained some of the challenges of scale-up in manufacturing pharmaceuticals and agrochemicals, where synthesis routes must meet very stringent requirements. Currently large-scale fluorination methods are very limited compared to the number of techniques being developed for small scale. New and modified fluorination methods to make fluoronaphthyridines were disclosed, which are key intermediates for active ingredients at Actelion and elsewhere.

Prof. **Santos Fustero** from Valencia University, Spain, highlighted some of his methods using transition metals and organofluorine molecules in organic synthesis. Examples included asymmetric synthesis of fluorine isoindolines and isoquinines,^[6] and a novel preparation of fluorinated cyclopentenone derivatives that can be used in the formal synthesis of α -cuparenone.^[7]

Prof. **Peer Kirsch** from Merck KGaA, Germany, provided an overview of the application of fluorinated compounds for liquid



crystal design in organic electronics, molecular nanomaterials and biosciences. The behaviour and application of liquid crystals for LCD applications depends both on aromatic and aliphatic fluorine compounds, and Dr. Kirsch's team has been investigating both. For example, hypervalent sulphur fluoride substituted aromatics have been synthesized to induce varying degrees of polarity, which will influence the behaviour of the final liquid crystal material.^[8]

Prof. **Jinbo Hu** from the Shanghai Institute of Organic Chemistry (SIOC), concluded the scientific program sharing his developments of novel fluoroalkylating reagents. Through systematic investigation of seemingly unfavourable fluorine effect of α -fluoro carbanions in nucleophilic reactions, novel reactions have been designed. Additionally, this effect was also

used to promote fluorinated carbene chemistry to give rise to several novel fluoroolefinations.^[9]

Dr. **Andrew Plant**, Head of Chemistry Crop Protection R&D at Syngenta, wrapped up the symposium and said: "We were treated to a day of top quality science from academia and industry, enriching our knowledge of fluorine chemistry, expanding our scientific networks, stimulating new ideas and forging new collaborations." Three posters prizes were then awarded to David Grassi (University of Geneva), Sébastien Alazet (University of Lyon), and Dr. Christoph Taeschler (Lonza) for their poster contributions.

Prof. **Peter Kündig**, President of the Swiss Chemical Society (SCS) and Professor at University of Geneva, Switzerland was equally enthusiastic about the outcome of the joint

symposium: "This symposium was impressive: outstanding scientists and excellent speakers made the symposium to a full house, and a perfectly organized event that was exciting to the very end. We were glad to collaborate again and look forward to 2015!" The SCS-Syngenta symposium 2015 is now being developed and more information will be available by early 2015 on the SCS-Syngenta website.

The SCS-Syngenta symposium organizing committee is Dr. Andrew Plant (Head of Chemistry, Syngenta Crop Protection R&D), Dr. Alain de Mesmaeker (Principal fellow, Syngenta Crop Protection R&D, Research Chemistry), Dr. Jérôme Cassayre (Head of Insecticide Chemistry,



Syngenta Crop Protection R&D), Dr. Mathilde Lachia (Team Leader, Syngenta Crop Protection R&D, Research Chemistry), Dr. Sarah Sulzer (Team Leader, Syngenta Crop Protection R&D, Research Chemistry) and Prof. Peter Kündig (University of Geneva, Swiss Chemical Society President).

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Symposium website: <http://www.syngenta.com/country/ch/de/Forschung/forschungstein/symposium/Pages/Symposium.aspx>

More photos: <https://vimeo.com/78603929>

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CHIMIA will be devoting a special issue in the context of the SCS-Syngenta Symposium 2013: Frontiers in Fluorine Chemistry in 2014, issue 6, which will be organized by the guest editor Prof. Ryan Gilmour.

A WARM WELCOME TO OUR NEW MEMBERS!

Fabio Di Lena, Rorschach – Vanni Doffini, Zürich – Galina Dulcevscaia, Bern – Thomas Hofstetter, Lenzburg – Edjere Oghenekohwiroro, Neuenhof – Patrick Rupper, St. Gallen – Sachiko Tsukamoto, Kumamoto (JP).



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Nanoflow-HPLC-MS: Praktische Grundlagen beim Arbeiten mit kleinen Flussraten	Dübendorf	24.04.2014	TR-13
Validieren von Analysenverfahren I, Grundlagen	Dübendorf	06.05.2014	QS-8
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Introduction à la chromatographie en phase liquide (HPLC)	Genève	04.03.2014	LC-1f
Introduction à la chromatographie en phase gazeuse (GC) et panorama général	Genève	06.03.2014	GC-1f
Analyse structurale de (bio)molécules par spectrométrie de masse	Lausanne	19.–20.03.2014	MS-5f
Validation de méthodes I	Genève	27.03.2014	QS-1f
Validation de méthodes II	Genève	28.03.2014	QS-2f
Choix technologiques en GC et développements de méthodes quantitatives	Genève	01.04.2014	GC-2f
Introduction à la GC/MS	Genève	03.–04.04.2014	MS-1f
Troubleshooting, entretien et applications de la GC, y compris avec des techniques complémentaires	Genève	08.04.2014	GC-3f
Introduction à l'HPLC	Genève	09.–11.04.2014	MS-4f
Choix technologiques et développement de méthode en HPLC	Genève	29.04.2014	LC-2f
Principes de base en méthodologie – calculs statistiques	Genève	06.05.2014	AA-5f

Es freut uns, Ihnen das Weiterbildungsprogramm 2014, das wir zusammen mit dem Centre de Compétence en Chimie et Toxicologie Analytiques (CCCTA) realisiert haben, vorzustellen.

Einzelmitglieder der folgenden Fachverbände können unsere Kurse zum vorteilhaften Mitgliedertarif besuchen:

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Falls Sie sich für unsere Veranstaltungen interessieren, erreichen Sie uns unter Telefon **058 765 52 00** oder Fax **058 765 58 01** oder mailen Sie an verena.schmid@eawag.ch. Online-Anmeldung im Internet unter: www.scg.ch/das

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