

Berita IKM - Chemistry in Malaysia

September 2020





Articles

- The Arctic Monitoring and Assessment Programme
- Emerging Pollutants: The Threat to Water Security
- Reductionism and Metabolomics
- Practicing Organic Chemistry in Malaysia

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Please address all communications to: Berita IKM Editorial Board Chairperson Institut Kimia Malaysia Wisma IKM, 127B, Jalan Aminuddin Baki, Taman Tun Dr Ismail, 60000 Kuala Lumpur Tel: 03-7728 3272 Fax: 03-7728 9909 Website: http://www.ikm.org.my Email: zuriatiz@gmail.com / ikmhq@ikm.org.my

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Message from the President

IKM on the Recovery Mode

As Malaysia enters into its recovery mode on the control of the COVID-19 pandemic, the Malaysian economy is slowly recovering from the downturn and proceeds to enter into positive territory by next year. IKM is in a similar situation and we are expected to fully recover by the end of 2020.

1. COVID-19 pandemic and the MCOs

The COVID-19 pandemic in Malaysia seems to be entering the final phase. Since August, new COVID-19 cases are hovering around single digit and the lower end of double digit of not more than 20. More than half of the new cases are from Malaysians coming back from overseas and the rest are local transmission from some clusters. I believe that with strict control and enforcement of SOP, we would be able to win the battle against COVID-19 soon.

2. IKM on the recovery mode

Starting August 2020, we are reactivating some of our programmes and activities.

First is LMIC Examination Refresher Course which prepares students for the LMIC Examination at the end of the year. The Course started in July and finished by end of August. The LMIC Examinations 2020 will be held from 19 – 21 September 2020 at University of Malaya, Kuala Lumpur.

We are also restarting our Professional Centre courses in August. Unfortunately, a few of the courses have to be cancelled but we are going full steam starting September.

We also conducted our 53rd Annual Meeting General, 53AGM, on 25th July 2020 and elected the new Council for 2020/2021. There is a report on the 53AGM in this issue of the Berita.

Fortunately, we are going ahead with Kuiz Kimia Kebangsaan Malaysia, or K_3M , which will take place on 5th November 2020. I am pleased to announce that we have close to 30,000 students taking part this year. This is more than the numbers last year. Our next big social event will be Malam Kimia 2020 which will take place on 4 December 2020 at the Berjaya Times Square Hotel, Kuala Lumpur.

Unfortunately, our two scientific meetings, the International Congress on Pure & Applied Chemistry (ICPAC) and the 20th Malaysian International Chemistry Congress (20MICC), both supposed to be held in Kota Kinabalu, Sabah, have to postponed to 2021.

3. 2021 onwards

We are going full steam ahead in 2021. The usual programmes and activities such as AGM, Refresher Course, Professional Centre programmes, K_3M and the branches activities including Karnival Kimia Malaysia, or K_2M , will be back to normal. We shall also organise ICPAC KK and 20MICC in Kota Kinabalu, Sabah, in early July 2021. LabAsia 2021 will be held from 19 – 21 October 2021 in Kuala Lumpur Convention Centre, Kuala Lumpur.

By 2021, we also expect the Chemists Rules 2020 to be ready. This is the first time that we have made amendments to the Rules since our inception in 1967. The new rules are quite comprehensive and covers six major areas. Once approved by the Honourable MOSTI Minister, it will be distributed to our members.

All IKM programmes and activities require the involvement and support of IKM members in order for us to achieve our objectives. We hope to mobilise all IKM members to work together towards making IKM a strong, and influential professional scientific organisation in Malaysia recognised by the chemistry community all over the world.

Thank you and with best wishes.

Datuk ChM Dr Soon Ting Kueh President, Institut Kimia Malaysia Date: 01st September 2020

by Lars Otto Reiersen, Ramon Guardans, and Leiv K. Sydnes

fter World War II, the Cold War generated significant barriers between the East and the West, and this affected all sorts of cooperation, including research and scientific collaboration. However, as the political situation in the Soviet Union started to change in the 1980s under the leadership of Mikael Gorbachev, the environment for international collaboration in many areas gradually improved.

This became quite visible in the Arctic, and the reason for this has often been ascribed to a visionary speech given by Gorbachev in Murmansk (Russia) in 1987 where he called for development and implementation of a new policy with a number of political goals, including:

- a Northern Europe free of nuclear weapons;
- reduction of military activity in the region and promotion of military trust;
- cooperative development of Arctic resources and opening up of the north-eastern sea route to international shipping;
- development of a comprehensive plan, including a monitoring program, to protect the Arctic environment.

This invitation was guickly picked up by the Finnish government, which challenged Canadian authorities to take the lead and launch a process to implement some of the proposals made in the Murmansk speech. This generated a lot of diplomatic activity among the eight Arctic states (Canada, Denmark, Finland, Iceland, Norway, Sweden, the Soviet Union, and the United States), and many initiatives were explored and discussed. At a meeting in Rovaniemi (Finland) in 1989, it was concluded that there was no international structure with the capacity to coordinate effective environmental cooperation in the Arctic, and it was therefore decided to develop an international body that would be in charge of and coordinate a program to monitor the environmental status and development in the Arctic (Stone, 2015). Such a body would need a solid political platform, and this gradually emerged and led first (1991) to the development of the Arctic Environmental Protection Strategy (AEPS) and subsequently (1996) to the formation of the Arctic Council (AC). This Council is led by the ministers of foreign affairs from the Arctic countries and is today the key political body for the Arctic.

With the AEPS agreement in place, the Arctic Monitoring and Assessment Programme (AMAP, www. amap.no) was launched with the aim of implementing the AEPS. In practical terms, the task was to monitor and assess the levels, trends, and effects of pollutants and climate change on the Arctic ecosystem and the people living there, especially the indigenous peoples. The work was coordinated by a secretariat located in Oslo (Norway), first working as part of AEPS, but from 1996 under the umbrella of the Arctic Council.

From the outset, AMAP was given a wide mandate, namely to study the trends and effects of anthropogenic pollutants in all compartments of the Arctic environment *irrespective of their sources*. The lack of any source restriction was very important because it included contaminants of both civilian and military origin. Based on scattered studies from the 1970s and 80s, the program was specified to focus on persistent organic pollutants (POPs), heavy metals, radionuclides, acidification of land and freshwater, petroleum hydrocarbons, and climate change, and at the same time looking-up for emerging issues.

The AMAP approach and method

In November 1991, the AMAP Task Force met for the first time, and at this meeting, Rules of Procedure and variables essential for the assessment were approved.





Reproduced with permission from Chemistry International Vol 42 (2), Apr-June 2020, page 8-14 It was also decided that the monitoring should be coordinated with existing international programs and based on standardized methodologies. And finally, only results published in scientific journals with an independent peer-review system in place, or new data collected in accordance with an adopted strict quality assurance/quality control (QA/QC) system for planning, sampling, extraction, analyses, and data handling.

An important task in the establishment of AMAP was capacity building to make sure that the QA/QC system could be, and indeed was, followed. In some cases, no approved methodology existed for the analysis of specific compounds of interest, e.g. for some of the POPs, and in such cases, experts in POP analysis were asked to develop and publish approved methods that were then adopted as AMAP methodology. In order to improve the quality of the analyses, international inter-calibration exercises were also implemented. In cooperation with Canada, AMAP established two new inter-calibration systems for POPs, one for human-blood samples and another for various samples from Arctic animals, and when in place, laboratories had to achieve an acceptable intercalibration score to become approved AMAP laboratories for such analyses.

In 1994 AMAP decided to start the work with a comprehensive report about the work carried out and the main results. A team of about 100 scientists and experts nominated by the Arctic countries, observing countries, international organizations, and representatives for the Arctic indigenous peoples (permanent participants) carried out the task and produced a 860page assessment report, AMAP Assessment Report (AAR), which was published in 1998 after a thorough peer-review process, first a "friendly" process to make sure that the scientists that had provided the data accepted the assessment and then an international independent peer review. In addition, a layman-style publication, Arctic Pollution Issues: A State of the Arctic Environment Report (SOAER) (AMAP, 1997), written in plain language to be suitable for politicians and the public, was published and translated into eight languages, including the Saami language. The geographical area covered by AMAP is shown in Figure 1.

When AMAP started the work, it was rather seldom that scientists would report results back to the people living in the area where the samples had been collected. However, early on AMAP adopted this practice, particularly on issues related to human health which were done in close cooperation with local health-care personnel and local indigenous organizations.

AMAP outcome

Radioactivity

In 1994, AMAP established an expert group with specialists from Russia, Norway, Sweden and Finland, to perform an assessment of radioactive "hot spots" in North-West Russia. The 1995 report from the group documented threats from several sources and recommended several actions for cleanup. In January 1996, the report was presented to the International Atomic Energy Agency (IAEA) in Vienna, and the following years a significant amount of work was carried out to clean-up contaminated sites and improve the security in operation of nuclear power plant at Kola Peninsula. Also, all except one of the 198 Russian nuclear submarines taken out of service since in 1994 have been decommissioned, nuclear waste storage sites cleaned up, and several hundred lighthouses previous driven by radioisotope thermonuclear generators have been replaced by solar power devices.

134Cs in star reindeer lichen, Bq/kg dw



Figure 2. Levels of radioactive cesium observed at an Arctic location in Finland due to releases from Chernobyl and Fukushima. (AMAP, 2016. AMAP Assessment 2015: Radioactivity in the Arctic.)

Later assessments have confirmed that traces of radionuclide depositions from testing of atomic weapons and the Chernobyl accident still can be detected in the Arctic (AMAP, 2009 & 2015). It has also been documented that the ¹³⁷Cs in the Barents Sea in the 1970s did not come from Soviet Union, but from the Sellafield reprocessing plant in the UK, and it was also proved that radioactive iodine came from Cap de la Hague in France. Based on these observations Nordic countries put political pressure on the UK to stop the discharges, and over the years the situation has changed to the better. The accident at Fukushima, Japan (2011) affected mainly marine areas around Japan, but traces have been detected in the Arctic marine environment (Figure 2). Another contaminated area is the sea around the Thule airbase in Greenland; here there is still plutonium equivalent to one nuclear bomb present (www.amap.no).

Acidification and Arctic Haze

In the 1970s, acidification of land and freshwater due to atmospheric emission of SO₂ was high on the environmental political agenda in Europe and North America and this parameter was included in the AMAP program as well. AAR 1998 documented some ecosystem effects due to acidification in northern Scandinavia, especially on forest, but this was not due to longrange transportation from central Europe; the effect was rather caused by impact from some large smelters in the northwest part of the Soviet Union. The second report on acidification, published in 2006, showed that the atmospheric concentration and deposition of acidifying chemicals had decreased significantly, and further monitoring and assessment of acidification under AMAP was therefore put to a hold.

Persistent Organic Pollutants (POPs)

Monitoring of POPs was a key objective in AMAP from the very beginning. An important reason for that was the results from a major Canadian investigation, performed in the 1980s, of the levels of some metals and POPs, such as PCBs and toxaphene, in the diet, blood, and breast milk of Inuits; it documented clearly levels of PCBs comparable to or above those found for populations in urban and industrialized sites in Canada (Stone, 2015). This study was followed up in 1990, when the Canadian federal government announced a new environmental program, the "Northern Contaminate Programme", directed towards monitoring contaminants in the food consumed by indigenous people living in the Arctic; the results from this study confirmed the results from the '80s.

In the beginning of the 1990s the only international agreements that could possibly deal with POPs were the Basel Convention (1989) on chemical waste, and the Geneva Convention on Long-Range Transboundary of Air Pollution (LRTAP) (1979), a regional agreement covering Europe and North America. Monitoring in the Canadian Arctic had been initiated under both conventions, but when the AMAP initiative started to materialize, a major well-coordinated international program involving several Arctic countries was launched under the auspices of the AMAP umbrella.

The collective aim of this monitoring program was to address several important questions: How are POPs



moving from their sources to the Arctic? Are POPs accumulating in organisms, ecosystems, and people? Is the POP input mostly attributable to atmospheric long-range transport? Results quickly emerged and at an AMAP international conference in 1997, new results on POPs documented that some of the levels found in Arctic animals were comparable to effect levels found in laboratory studies.

The results presented by AMAP made headlines globally and had quickly a significant impact. In 1997, the Governing Council of the United Nations Environmental Program (UNEP) decided to establish an International Negotiating Committee (INC) with the mandate to develop and propose a legally binding instrument for launching international actions to regulate and curb the use of 12 specific POPs. Based on input from an international group of experts and the scientific community at large, progress was gradually made, and in 2001 the negotiations were completed. The outcome was the Stockholm Convention (SC), which has been presented in detail in a previous issue of this magazine (Fiedler et al., 2019). Today this global convention has listed some 30 groups of substances and 183 parties are signatories, with the notable exceptions of the USA and Greenland! An important innovation in the SC was the evaluation instrument, which is applied to assess the progress made by the parties to the convention in their work to reduce their use and release of POPs.

On the basis of this work, a Global Monitoring Plan (GMP) on POPs was published in 2004, and later updates have definitely contributed positively to reduce the use of these compounds (Daniel *et al.*, 2018). The latest AMAP and GMP reports on POPs have documented a positive trend for some of the compounds of concern in the sense that their levels have been reduced both in Arctic ecosystems and in humans living in the region, see Figure 3. This can in part be attributed to reduced use and emissions caused by stricter regulations, enhanced awareness, and changed diets, that also may have affected intake on intake of vitamins from traditional food, *e.g.* sea mammals.

It has been noted that specific regulations can lead to significant progress relatively quickly, but the time lag between early warning and effective implementation of regulations can also be 30-40 years (Guardans, 2012). A serious concern today is that new substances are released from new sources, and some of these compounds behave like some of the classical POPs. The increasing presence in the Arctic of new POPs and new substances that behave like POPs is of emerging concern, see Figure 4.

Chemicals of Emerging Arctic Concern

- Per-polyfluorinated compounds (PFCAs, PFSAs, etc.)
- Brominated flame retardants (BDE-209, HBCD, DPTE, etc.)
- Organophosphate-basedflame retardants and plasticisers (TnBP, TCEP, TCPP, TDCPP, etc.)
- Phthalates
- Short-chained chlorinated paraffins
- Siloxanes
- Pharmaceuticals and personal care products
- Polychlorinated napthalenes
- Hexachlorobutadiene
- Current used pesticides (Difocol, Pentachlorophenol/anisole, etc.)
- Mono-dibutylins
- PACs (e.g. nitro-PAHs, hydroxyl-PAHs, alkyl-PAHs)
- PCB11 from smelting
- Halogenated natural products (naturally formed BDEs, OH-BDEs, MeO-BDEs, brominated dioxins, etc.)
- Microplastics

Figure 4. Chemicals of emerging Arctic concern; new POPs and products that behave like POPs. (AMAP Assessment 2016: Chemicals of Emerging Arctic Concern)

Heavy metals

At the outset AMAP focused on heavy metals, but the first assessment (AMAP, 1998) clearly demonstrated that the metal problem was mainly associated with mercury (Hg) and lead (Pb). For lead, analyses of



Figure 5. The variation of lead (Pb) in ice core from Greenland reflecting global emissions, especially due to the use of leaded gasoline from 1947 to 2000). Analyses of Ice cores can tell the story of global emissions of gases and metals, several 100k years back in time. AMAP, 2005. AMAP Assessment 2002: Heavy Metals in the Arctic

ice cores documented a variation reflecting its levels in the atmosphere, where it was deposited through industrial emissions and the use of leaded gasoline (Figure 5). Today, the main Pb threat to humans in the Arctic is as fragments in birds and animals shot with homemade lead bullets. AMAP therefore recommended stopping the use of such bullets and switching to steel bullets for hunting in the Arctic, but this regulation has not been easy to implement in routine hunting activities.

As far as mercury is concerned, the Hg problem in the Arctic is predominantly due to coal-burning power plants in South-East Asia, see Figure 6. Few filters, if any, can trap mercury from gaseous emissions mercury and thereby prevent it from entering the atmosphere and ultimately end up in the Arctic. The consequences of such a release were observed especially in the Faroes Islands where negative effects on humans have been detected. For instance, exposure during pregnancy has been shown to be irreversible. For other examples and more details, see the AMAP human health reports from 2003, 2009 and 2015.

The use and handling of mercury are regulated by the Minamata Convention, which is a global, legally binding document that entered into force in 2017. The results from the AMAP monitoring mentioned above indeed contributed to speed up the international negotiations leading to the convention (Platjouw *et al.*, 2018). This paper indeed describes the evolutionary process in which scientific knowledge, herded by an intergovernmental, regional forum, was involved and formed the basis for the agreement.



Figure 6. Global emissions of mercury. (UN-Environment. Global Mercury Assessment 2018)

Climate change

Climate issues were on the AMAP agenda from the start, and the first climate assessment was published as part of the AMAP 1998 report. This led to international cooperation, particularly with International Arctic Science Cooperation (IASC), and the Conservation of Arctic Flora and Fauna (CAFF) working group of the Arctic Council, which broadened the scope of the next assessment. Arctic Climate Impact Assessment (ACIA), published in 2005. This assessment brought both the global implications of a melting Arctic and the Arctic Council into the spotlight. There were several reasons for that: on the negative side, the report documented a "Meltdown of the Arctic", which means reduced snow and ice cover, thawing of the permafrost, global Sea Level Rise (SLR), etc; and on the positive side, new opportunities related to Arctic shipping (cargo and tourism) and accessibility of new resources such as minerals, oil, and gas. A political consequence was also observed: EU and several countries, including China, India, and Singapore, far away from the Arctic requested observer status in the Arctic Council.

These events made climate change a top priority for AMAP. Over the last decade several AMAP reports have documented the ongoing climate change and outlined the effects on Arctic ecosystems and communities, the impact on human health within the region, and climate feedbacks from the Arctic to lower latitudes. Two AMAP reports on Snow, Water, Ice and Permafrost in the Arctic (SWIPA) have significantly influenced the work of the Intergovernmental Panel on Climate Change (IPCC), for instance the results of the latest modelling of the expected temperature increase in the Arctic even if the Paris agreement is fully implemented (see Figure 7). The figure shows how much warmer Arctic areas may become and thereby trigger an enormous melting of snow and ice with the consequence the global sea level will rise 0.5-2 m by 2100 depending on where you are on the globe. For development of local and regional adaptation strategies in the North and elsewhere on the globe, it is important to use detailed seasonal scenarios to highlight the future situations at the sites in question, as Figure 8 illustrates.

It is well established that increased emission of CO₂ also leads to increased acidification of the world oceans. However, the AMAP assessment has documented that in parts of the Arctic oceans, this process is faster than anywhere else due to a combination of several factors, including the larger storage capacity of CO₂ in cold water than warm water, and much lower buffering capacity for acidity in Arctic surface water (less saline).



Figure 7. Projected air temperature using the three scenarios representative concentration pathway (RCP) 2.5, (close to a future +1.5 °C world), RCP 4.5 (close to a future +2.5 °C world) and RCP 8.5 (business as usual); to the left over the Northern hemisphere; in the middle over the Northern Hemisphere north of 60°N; to the right the increase in November-March North of 60°N (Overland et al., 2018).

Over the years, AMAP has also documented that the Arctic environment and the people living there are threatened by several stress factors, which include pollutant, climate change, and a variety of human activities. In 2017, AMAP published three assessments regarding "Adaptation Actions in a Changing Arctic", analyzing combined effects of several stress factors and their influence on potential adaptation strategies to be developed and implemented within the Arctic region. An interesting observation was that for many people living in the Arctic the climate change was not seen as the most serious threat; the most important was, not surprisingly, to have a job, secure income and enough clean food for tomorrow, a clear signal to decision makers that have to satisfy short-term needs (economic and food security) in a long-term sustainable fashion (prevent climate change).

Stratospheric ozone depletion

In the first AMAP report there is a chapter on Climate change, Ozone and Ultraviolet radiation, which summarizes the long-term climatic changes on the basis of paleoenvironmental data and more recent instrumental records. It is interesting that ozone depletion is discussed because there has been much less attention to the Arctic ozone hole than the Antarctic analogue, conceivably because the depletion has been much less pronounced in the Arctic. The reason is believed to be due to differences in the stratospheric dynamics around the two poles, which are a function of temperature, aerosol contents and structural features, and the presence of anthropogenic chemicals such as chlorofluorocarbons (CFCs). CFCs play a significant role in depleting stratospheric ozone (the Ozone Layer). Over the last couple of decades CFC emissions have been considerably reduced by regulation and control introduced during the implementation of the Montreal Convention. Ozone has therefore gradually received less attention in the AMAP Monitoring Programme.

Some reflections

The scientific cooperation under AMAP has been in operation for more than 25 years with support from the governments of the Arctic Council member states, local communities in the member states, and observing countries and organizations. The results provided by AMAP have been used to provide food advice to communities in the Arctic to avoid high exposure of pollutants to humans, especially during pregnancy, and to inform international organizations like UNEP, LRTAP, and WHO about developments that calls for international regulations and actions to reduce emissions of toxic and polluting chemicals. It is also noteworthy that the AMAP program has led to increased

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scientific cooperation among the Arctic states, which in turn has played an important role in reducing the political and military tension that was so visible in the North some 30 years ago.

Several outcomes of the work made by AMAP and the experience gained in the process might be of use in other regions of the world that face similar problems with pollution and climate change, for instance in Himalaya, Africa, and South America. Some important points are as follow:

- Promoting a stable and solid scientific community that can operate independent of political influence in its daily monitoring and assessment work has shown to yield valuable and respected results.
- Scientific results should be used to create policy-relevant recommendations based on science.
- Funding must be secured for the work and that of a professional secretariat.
- Programs should be completely based on inclusive, transparent, predictable, and long-term processes and include, if possible, all relevant scientific disciplines.
- Scientists and institutions that deliver scientific data of high quality must be given due credit.
- Indigenous people and local knowledge must be included; this may be very beneficial for the design of monitoring programs.

Lars-Otto Reiersen <lars.o.reiersen@uit.no> is senior advisor to the Rector at the University of Tromsø, the Arctic University of Norway. Former executive secretary for Arctic Monitoring and Assessment Programme (AMAP).

Ramon Guardans <ramon.guardans@soundplots.com> is and advisor on POPs to the Ministry of Ecological Transition (MITECO) Madrid, Spain. Serving since 2006 as cochair of the SC Global Monitoring Plan on POPs. Leiv K. Sydnes <leiv.sydnes@uib.no> is professor emeritus at Department of Chemistry, University of Bergen, Norway. He was president of IUPAC 2004-2005 and chaired the IUPAC CHEMRAWN committee in 2008-2015. In the 1990s, he was engaged in several environmental investigations in the Arctic.

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Urban agriculture

Urban agriculture is becoming more popular across developed countries. Almost half (48%) of all households in metropolitan areas are now growing some form of edible produce.

Most lead contamination is a result of the historical use of lead in petrol and lead-based paint (now phased out) and previous industrial emissions. Scientists and regulators are well aware of these legacy issues, but the general public remains underinformed about the potential risks.

Lead levels above health limits in urban backyard soils

Many studies published today reveals that 40% of major cities homes soil contain lead above the international health guideline of 300 ppm (mg/kg).

This presents a hazard because soil lead can adhere to or get absorbed into edible plants. An additional pathway of exposure occurs when contaminated soil dust enters homes and is accidentally ingested. Lead is a potent neurotoxin that affects childhood development.



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Rouillon, M., Taylor, M. P., & Dong, C. (2017). Reducing risk and increasing confidence of decision making at a lower cost: in-situ pXRF assessment of metal-contaminated sites. *Environmental Pollution*, 229, 780-789.

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53rd IKM Annual General Meeting

The 53rd IKM Annual General Meeting (AGM) was held on 25 July 2020 at Berjaya Times Square Hotel, Kuala Lumpur. IKM President, Datuk ChM Dr Soon Ting Kueh welcomed members to the 53rd AGM of IKM. A total of 149 members attended the AGM. The 53rd AGM initially scheduled to be held on 28 March 2020 was postponed to 25 July 2020 because of Movement Control Order (MCO) imposed by the Government and COVID-19 pandemic. The President presented PowerPoint slides describing IKM activities and achievements for the term 2019/2020. The year 2019 was described as a busy, fruitful and rewarding year for IKM. IKM Hon. Secretary, Assoc Prof ChM Dr Juan Joon Ching, presented the PowerPoint slides of the Annual Report.

IKM Hon. Treasurer, ChM Steven Tea Hing San presented the Annual Statement of Accounts and Auditor's Report for 2019. A Resolution by IKM Council to contribute RM50,000.00 to government's Tabung COVID-19 was unanimously supported by the members present at the AGM. Datuk ChM Dr Soon Ting Kueh informed that the IKM Law Hieng Ding Foundation registration is pending approval from the Registrar of Companies (ROC). A meeting was held with Attorney General's Chamber Officials on 23 July 2020 to finalize the contents of Chemists Rules 2020. The amendments are expected to be gazetted by end of the year. Malam Kimia and Presentation of IKM Awards 2020 will be held on 4 December 2020 at Berjaya Times Square Hotel, Kuala Lumpur.

The highlight of the AGM was the election of 6 Council members to fill vacancies created by retired Council members. The AGM ended at 6.03 pm. Immediately after the AGM, 312th Council meeting was held to elect principal office bearers for 2020/2021 term. This was followed by appointments of committee/section Chairpersons.



Elected Council Members

	<u>Term</u>
ChM Dr Hj Mas Rosemal Hakim Mas Haris	2020 - 2023
Datuk ChM Dr Soon Ting Kueh	2020 - 2023
ChM Chang Hon Fong	2020 - 2023
Assoc Prof ChM Dr Juan Joon Ching	2020 - 2023
Prof ChM Dr Mansor bin Ahmad @ Ayob	2020 - 2023
ChM Dr Yvonne Choo Shuen Lann	2020 - 2021



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The Council Members for 2020/2021

Committees & Chairpersons for 2020/2021

Administration & Finance		
Administration & Finance Committee	Assoc. Prof ChM Dr Juan Joon Ching & ChM Dr Malarvili Ramalingam	
Malam Kimia 2020 Organizing Committee	Assoc. Prof ChM Dr Juan Joon Ching	
ICPAC Kota Kinabalu 2021 Organizing Committee	Datuk ChM Dr Soon Ting Kueh	
20th Malaysian International Chemistry Congress (MICC) 2021 Organizing Committee	Prof ChM Dr Mansor Ahmad	
Benevolent Fund Committee	DCP(R) Dato' ChM Dr Yew Chong Hooi	
Publications		
Berita IKM: Chemistry in Malaysia Editorial Board Datin ChM Dr Zuriati Zakaria		
Malaysian Journal of Chemistry Editorial Board	Datin ChM Dr Zuriati Zakaria	
Professional Affairs & Development		
Professional Affairs Committee Prof ChM Dr Ho Chee Cheong		
Membership Committee	Tuan Haji ChM Mohamed Zaini Abdul Rahman & Datuk ChM Dr Soon Ting Kueh	
Examination Board Prof ChM Dr Ho Chee Cheong		
IKM Professional Centre Development Committee	ChM Chang Hon Fong	
Investigation Committee	DCP(R) Dato' ChM Dr Yew Chong Hooi (Chairman) Assoc. Prof ChM Dr Juan Joon Ching ChM Dr Hj Mas Rosemal Hakim Mas Haris	

Committees & Chairpersons for 2020/2021

Disciplinary Committee Laboratory & Quality Assurance Committee	Tuan Haji ChM Mohamed Zaini Abdul Rahman (Chairman) Datuk ChM Dr Soon Ting Kueh Datin ChM Dr Zuriati Zakaria Prof ChM Dr Yang Farina Abdul Aziz ChM Dr Malarvili Ramalingam <i>Laboratory Excellence Award</i> ChM Chang Hon Fong &	
	ChM Li Hui Ling	
	ChM Dr Hj Mas Rosemal Hakim Mas Haris	
IKM HQ & Branches		
IKM HQ	Datuk ChM Dr Soon Ting Kueh	
IKM Northern Branch Committee	ChM Dr Hj Mas Rosemal Hakim Mas Haris	
IKM Southern Branch Committee	ChM Yap Fei Ching	
IKM Sarawak Branch Committee	ChM Dr. John Chan Sung Tong	
IKM Sabah & FT Labuan Branch Committee	ChM Dr Jenny Lee Nyuk Len	
IKM Perak Branch Committee	ChM Khairul Hadi Bin Haji Abd Raof	
IKM Terengganu Branch Committee	ChM Teo Chook Kiong	
IKM Pahang Branch Committee	Assoc. Prof ChM Dr Chong Kwok Feng	
Academic & Inc	lustrial Sections	
Inorganic & Bioinorganic Chemistry Section	Prof ChM Dr Yang Farina Abdul Aziz	
Analytical Chemistry Section	ChM Dr Malarvili Ramalingam	
Organic & Biomolecular Chemistry Section	tion Datin ChM Dr Zuriati Zakaria	
Physical & Theoretical Chemistry Section	Prof ChM Dr Mansor Ahmad	
Polymers & Materials Chemistry Section	Prof ChM Ts Dr Chan Chin Han	
Environment & Green Chemistry Section	Assoc Prof ChM Dr Juan Joon Ching	
Industrial Chemistry Section	ChM Dr Yvonne Choo Shuen Lann & Assoc Prof ChM Dr Juan Joon Ching	
Food Chemistry Section	Datin ChM Maimonah Sulaiman	
Forensic Chemistry Section	DCP(R) Dato' ChM Dr Yew Chong Hooi, Datin ChM Maimonah Sulaiman & ChM Halimah binti Abdul Rahim	
Malaysian Young Chemists Network	Assoc Prof ChM Dr Juan Joon Ching	
Chemistry Educa	tion & Community	
Chemistry Education Committee – K ₃ M	Datuk ChM Dr Soon Ting Kueh	
Community Chemistry Committee – CATIS & Chemistry Festival	ChM Dr Hj Mas Rosemal Hakim Mas Haris & ChM Dr Yvonne Choo Shuen Lann	

Chemistry ^{*in*} Malaysia

Kuiz Kimia Kebangsaan Malaysia (K3M) 2020

K3M 2020 Question Setting Technical Committee Meeting was held on 16-19 July 2020 at Hotel Hatten Malacca. The Chairman, Dato' ChM Dr. Mohd Jamil, welcomed the committee members and thanked them for their contribution towards K3M. Datuk ChM Dr Soon Ting Kueh congratulated the newly appointed members.

Committee members for the term 2020 – 2022

Chairman:	Prof Dato' ChM Dr Mohd Jamil Maal
Co-Chairman:	Datuk ChM Dr Soon Ting Kueh
Secretary:	Datin ChM Dr Ng Soo Boon
-	ChM Dr Sa'adah Masrukin
Committee	Datin ChM Dr. Zuriati Zakaria
Members:	Prof ChM Dr. Mansor Ahmad
	ChM Li Hui Ling
	ChM Dr. Ng Kim Hooi
	Assoc. Prof ChM Dr. Ng Chew Hee
	Prof ChM Dr. Sharifuddin Md Zain
	Cikgu Ong Poh Tin
	Cikgu Yau Kim Tan
	Cikgu Wan Noor Afifah Wan Yusoff
	Cikgu Tan Sze Chuan
	Cikgu Wong Choy Wan
	Cikgu Chong Pei Si
	Cikgu Lim Kuok Chen
	Cikgu Suziyana Hassim
	Cikqu Lee Saw Im

Two sets of questions, for O-level and A level, were compiled successfully. Each set of quizzes includes 40 questions covering Organic Chemistry, Inorganic Chemistry, Physical Chemistry and current COVID-19 issues. K3M 2020 will be held at participating schools on 5 November 2020 and the closing date for registration is 15 September 2020.





Sept 2020

The Chemistry of



Behold Some of the Molecules Responsible for the Distinct Fragrance of Malaysia's National Dish!

2-acetyl-1-pyrroline

2AP (in short) is the molecule that accounts for the desirable aroma of fragrant rice and the delightful flavour of Pandan (screwpine) leaves.

by Or Gronne Choo Shnen lanr

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Independence Day

Zingerone

A significant contributor to ginger's flavour. It is formed when ginger is cooked breaking down gingerols (molecule present in fresh ginger) into zingerone.

HO

110

Delta-Lactones

Delta-Lactones are the main molecules that makes up the flavour and smell of coconut milk, coconut oil and coconut meat.

Nasi Lemak (Literally translates into "Rice" "Fat") is made up of 2 key ingredients mainly rice and coconut milk (The Fat). It is usually served with a dollop of spicy sambal,

fried anchovies, cucumbers and peanuts.

The next time you indulge yourself with a plate of Nasi Lemak, be reminded that the combination these molecules makes up the mouth-watering, appetite stimulating aroma of the dish.

For More Info:

Not forgetting, Chemistry is all around us.



IKM Refresher Course for LMIC Examination

The 12th IKM Refresher Course for those who intend to sit for the IKM LMIC Examination was held from 4 July 2020 to 23 August 2020 at IKM Professional Centre, Taman Tun Dr Ismail, Kuala Lumpur. The course is based on the syllabus of IKM Part I Examination and was conducted by experienced instructors. A total of 20 participants attended this course. IKM President, Datuk ChM Dr Soon Ting Kueh presented attendance certificates to the participants on the last day of the course. The LMIC Examinations will be held from 19-21 September 2020 at the Department of Chemistry, University of Malaya, Kuala Lumpur.



Week	Date	Day	Module	Instructor
1	4 July 2020	Saturday	Physical Chemistry	Prof ChM Dr Ramesh T Subramaniam
	5 July 2020	Sunday	Analytical Chemistry	ChM Shanmuga Kittappa
n	18 July 2020	Saturday	Inorganic Chemistry	Prof ChM Dr Leong Loong Kong
2	19 July 2020	Sunday	Analytical Chemistry	ChM Shanmuga Kittappa
2	25 July 2020	Saturday	Organic Chemistry	Assoc Prof ChM Dr Khoo Kong Soo
3	26 July 2020	Sunday	Analytical Chemistry	ChM Shanmuga Kittappa
4	8 August 2020	Saturday	Inorganic Chemistry	Prof ChM Dr Leong Loong Kong
4	9 August 2020	Sunday	Physical Chemistry	Prof ChM Dr Ramesh T Subramaniam
Б	15 August 2020	Saturday	Physical Chemistry	Prof ChM Dr Ramesh T Subramaniam
5	16 August 2020	Sunday	Organic Chemistry	Assoc Prof ChM Dr Khoo Kong Soo
C	22 August 2020	Saturday	Inorganic Chemistry	Prof ChM Dr Leong Loong Kong
U	23 August 2020	Sunday	Organic Chemistry	Assoc Prof ChM Dr Khoo Kong Soo



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Emerging Pollutants: The Threat to Water Security

Yang Farina^{1,2}, Nurfaizah Abu Tahrim^{1,2}, and Nurlin Abu Samah³ ¹Centre for Water Research and Analysis (ALIR), ²Department of Chemical Sciences

Universiti Kebangsaan Malaysia

³Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang







Water, water everywhere but not a single drop from the tap. Such a scenario occurs more and more frequent. It is estimated that the world's population living in water stressed countries will increase from less than one billion people in the mid-1990s to four billion people in 2050. Another global phenomenon that will cause an impact on water security is the urbanisation of the population. In 2014 about 54% of the world's population lived in cities and is expected to increase to 66% in

2050 (Jensen and Hu, 2018).

Increase in population especially in cities will create a greater demand for safe potable water. It would be prudent for any country to achieve long term water security in ensuring sustainability of water resources for potable water. Under the Economic Transformation Plan (ETP), Malaysia is geared to be a high income nation befitting a developed nation. However, this vision will be hampered if our water security issues are not addressed. In a study conducted in Malaysia, it was reported that the annual rainfall is about 973 billion cubic metres (BCM). However, out of this there are loses of 414 BCM due to evaporation, 496 BCM to surface runoff, and another 63 BCM goes to groundwater recharge. The demand for water by the population is predicted to be 17.2 BCM in 2020 and 18.2 BCM in 2050. Hence, the effective rainfall is estimated to be 74 BCM which is roughly guadruple the amount needed by Malaysians. It is thus worrisome that despite the apparent abundance of water, Malaysia suffers from seasonable water shortages. States such as Perlis, Kedah, Pulau Pinang, Selangor and Melaka are water deficit states where crisis in potable water shortages have led to water rationing in 2014 and 2015 (Sharizaila et al, 2016). The irregularity and unpredictable changes in rainfall due to climate change coupled with high population densities and/or extensive agricultural activities in these regions have led to water demands exceeding the carrying capacity of the respective river basins. Changes in weather patterns, for example the El-Nino phenomenon caused no rainfall in the catchment areas between January and March 1998. In 2014, another severe drought hit the west coast causing water level of major dams to go below the critical level (Rasyika, 2018). The problems of unpredictable and changes in rainfall patterns are further exacerbated by the increasing pollution of our rivers. Culminations of all these factors have caused threats to sustaining continuous potable water to homes. In a year many areas are faced with water cuts that can last for days. Hence it is no surprise that the consumers are anxious when the taps go dry which has become a normal incidence occurring a few times in a year.

If we study the statistics from the Environmental Quality Reports for the year 2013 and 2014, out of the 473 rivers monitored, the percentage of clean rivers has dropped from 58% to 52%, slightly polluted rivers have increased from 37% to 39%, while polluted rivers have also increased from 5% to 9%. The main source of pollutants is from point sources such as ammoniacal nitrogen, biological oxygen demand and suspended solids. However, in the last few years we have witnessed increasing incidences of industrial pollutants that has caused water treatment plant closures. Thus it is worrying to note that despite all the regulations available, cases of illegal dumping of industrial waste is still rampant. The occurrences of these pollutants also signifies the state of our rivers.

The pollution of Malaysian rivers has caused a lot of alarm among the members of the public. There have been a few high profile cases which have caused anxiety among the general public. One such example is the recent Sg Kim Kim incident in September 2019, when a toxic gas emanating from a concoction of highly volatile organic compounds resulted in the hospitalization of hundreds of people. The case of Cameron Highlands was highlighted a few years ago, when the drinking water was found to contain banned pesticides (Abdullah et al. 2015). The Langat Basin has attracted a lot of attention too. There are a total of 4 major water treatment plants situated on the Langat and Semenyih rivers which are Semenyih (687 MLD), Langat (449 MLD), Cheras Bt 11 (27 MLD) and Bukit Tampoi (32 MLD). In 2016 there were 4 major shutdowns which were due to the presence of an unknown industrial pollutant which emitted a strong odor. The closure of the Semenyih Treatment Plant two years ago was due to the illegal disposal of a fire retardant which contaminated Sg Semenyih. The Semenyih Water Treatment Plant (WTP) faced closures because of odour in October and December 2019 which affected more than 300 000 households. Air Selangor received 1143 complaints on odour in water in early October 2019 after the treatment plant resumed operations. Bad odour from ammonium pollution was also the cause for 90 percent of plant shut downs in Johor. Other polluters such as wastewater, detergents, oil spills, muddied flow due to floods, deforestation and quarrying have caused the shutting down of treatment plants and disrupted water supply in other parts of the country. The latest to face a shutdown due to the presence of strong odour emanating from illegal dumping of solvent is the Sungai Linggi Treatment Plant on the 10th of June 2020. In the latest incident on the 3rd of September 2020, 4 water treatment plants on Sungai Selangor



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were shut down because of the presence on odorous chemicals.

The presence of industrial pollutants in our rivers marks a growing concern on the presence of emerging pollutants. These emerging pollutants even though present in small quantities is a constant threat to the provision of safe potable water. What are emerging pollutants? Let us look at the various definition on what is deemed as an emerging pollutant.

Houtman (2010) defined emerging contaminants as belonging to three categories of compounds:

- i) compounds newly introduced into the environment,
- ii) compounds that have been around for long but has only been detected because of the development of new analytical techniques and
- iii) compounds that have been in existence for a longer time but have only been recently recognised as having adverse effects on ecosystems or humans.

Sauvé and Desrosiers (2014) defined emerging pollutants (EPs) a:

i) "true or really new" emerging contaminants, new compounds or molecules that were not previously known or that just recently appeared in the scientific literature,

- ii) contaminants of emerging interest which were known to exist but for which the environmental contamination issues were not fully realized or apprehended, and
- iii) emerging issues about "old" contaminants, i.e., situations where new information is jostling our understanding of environmental and human health risks related to such legacy contaminants. Hence, emerging pollutants are chemical or natural materials, manufactured or made by man, that are present in various environmental media, whose toxicity is capable of altering the metabolism of living being.

The Norman Network (2016) defined EPs as substances detected into the environment but currently not included in routine environmental monitoring programmes and which may be candidate for future legislation due to its adverse effects and/or persistency.

The Norman Network has identified more than 1000 compounds which falls under the definition of EPs and it includes, gathered in 16 classes (algal toxins, anti-foaming and complexing agents, antioxidants, detergents, disinfection byproducts, plasticizers, flame retardants, fragrances, gasoline additives, nanoparticles, perfluoroalkylated substances, personal care products, pharmaceuticals, pesticides, anticorrosives).

Contaminant	Description
Pharmaceuticals	Pharmaceuticals are not fully utilized by the human body as well as animal and thus end up in the sewage. The compounds such as antibiotics, analgesics, antidiabetic drugs, lipid modifying agents etc. These compounds are not completely removed by the sewer- age and water treatment. The well documented health effect of these pharmaceuticals are on fish. There are still no known published work on the health impacts towards hu- man.
Personal Care Prod- ucts	Personal care products (PCPs) are substances used for health, beauty and cleaning purposes which includes disinfectants, fragrances, insect repellents, preservatives and UV filters, among others. Some of these substances are endocrine disruptors and may impact on the endocrine system in humans and animals such as the reproductive system.
UV Filters	Organic UVB filters (3-(4'-methylbenzylidene) <u>camphor</u> and octocrylene are utilized in hair and skin products to filter off the harmful effect of ultraviolet rays. These substances are endocrine disrupting substances that interferes with the reproductive system.
Endocrine disruptors	Impacts the endocrine system in the human body. Negative effects of EDCs include breast cancer, infertility and animal hermaphroditism.
Hydrocarbons	High toxicity, mutagenicity and carcinogecity.
Illicit drugs	Cocaine, morphine, amphetamine, and MDMA have potent pharmacological activities and their presence as complex mixtures in water may cause adverse effect on aquatic organisms and human health.
Food additives	Synthetic organic pollutants, including sweeteners, antioxidants, etc. Sweeteners are quite soluble in water and are found mostly in wastewater. Antioxidants, on the other hand, are not water soluble and found in groundwater.
Metabolites	Some pharmaceuticals is transformed into other metabolites when it enters the water system.
Fire Retardants	May cause odour in water.
Pesticides	Found in areas involved in intense farming such as Cameron Highlands. Some banned pesticides may be traced back current usage.

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Peña-Guzmán (2019) classed emerging pollutants into 10 different contaminants; pharmaceuticals, personal care products, UV filters, endocrine disruptors, hydrocarbons, illicit drugs, food additives, metabolites, fire retardants and pesticides and its description is given in the table below.

In Malaysia various research groups have studied these emerging pollutants. A complete review of the work by Malaysian scientist is currently being written. Of these emerging pollutants the compounds most studied are pharmaceuticals, personal care products and endocrine disruptors. Besides these emerging pollutants there is another big class of pollutant known as micro-plastics that is causing a huge impact on the marine system.

The threat of odorous chemicals is another group of compounds that are constantly threating the safe running of water treatment plants. This is another area of research that needs to be studied in detail. A multi-disciplinary approach would be needed to solve this problem that is a threat to water security in Malaysia.



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Reductionism and Metabolomics



ChM Dr Intan Safinar Ismail, FRSC Department of Chemistry, Faculty of Science, Universiti Putra Malaysia Email: safinar@upm.edu.my

Introduction

Many a time I have been asked whether my field of expertise has changed. Some even removed my name under the natural products chemistry group, just due to

the word 'metabolomics' that I associated my works with. I think it is appropriate to seize this opportunity to share some of my research using metabolomic tools that might shine a light on a better understanding of what metabolomics is about.

I am still very much a natural product chemist who just decided to jump onto a wagon of metabolomics band. The interest in obtaining compounds, either new or known, does not waver. I still could taste the brief moment of euphoria in discovering an entity that can erase the long-hour of sieving through a matrix of compounds. More so when the compound possesses a biological activity. Even more so when the compound's role is made meaningful from viewing through a system-wide window, which is what metabolomics offers. It was not an easy choice to take on learning a new way to perceive natural products when the conventional reduction method has been imprinted in oneself. Yet, however hard it was at first, there was something enticing and subsequently a lot of things beautiful about metabolomics.

Natural products chemistry was formally introduced to me in 1993. Like many other natural product chemists, which most of the time the subject is a plant worked on through the usual steps of harvest, extraction, fractionation, and purification. It is mostly about wading through the unknown, sometimes unseen, pitfalls, but with a tinge of luck, a pure compound might be new, better with a novel skeleton is isolated. Bioassayguided fractionation in pursuing the bioactive unknown is the famous choice. Some fall in love with natural products chemistry, others cannot endure the frustration of doing tedious tasks, and ending up with many things that do not work. Those who endure are prone to be the experts in chromatographic and spectroscopic techniques.

However, strategies for the identification of bioactive constituents from a crude plant extract have been changing over the past years. Even though the reductionist approach, particularly the use of bioassayguided fractionation, remains the most popular approach currently in practice, this method fails to deliver holistic information on the therapeutic (or toxic) potential of the various chemical constituents within a crude extract. This is due to its inability to identify the effects of synergism or antagonism, which are widely considered as the most important attribute of a medicinal plant preparation.

Metabolomics as a tool

Metabolomics as a global and comprehensive analytical tool could overcome this disadvantage by examining the structural diversity present in an extract. This tool is not recent. The somewhat similar application of metabolomics can be traced back to the ancient Indians in 6AD,¹ when tiny insects like ants were the diagnostic tool to prove that someone had diabetes. Sounds weird, but come to think of an ant analyzing the whole sample is conceptually similar to having a modern analytical instrument, such as a Nuclear Magnetic Resonance (NMR) or a Mass spectrometer (MS), detecting sugar in a urine sample.

Metabolomics measures the 'downstream products' of multiple genes, proteins, and environmental interactions which makes it a good reporter of an organism's phenotype or physiology.² However, the number of metabolites that need to be tracked at the same time is high, since the overall metabolic profile can be astronomical, although one or more secondary metabolites can be unique to a plant. Hence, making the identification of a highly complex matrix through metabolomics is a difficult task.

Analogously, the metabolomics approach is like diving into an ocean full of creatures. If one is equipped with a befitting instrument(s) to get the desired catch, the approach is victorious. The maze to be conquered is the same, the option is either a conventional or metabolomics technique. The ease, if you perceive it as ease, is the possible absence of the purification step either at some stage or even throughout the metabolomics research.

Regardless of either to profile or fingerprint the metabolome (a collection of all small molecule metabolites or chemicals that can be found in a cell, an organ, or an organism), the metabolomic data are representative of unassigned signal peaks. Hence, metabolomics needs a powerful database of collective single entities to make the correct interpretation and chemical assignment of a system such as a plant. It is common to see the reported identified metabolites in metabolomic findings be regarded as having putative identities, not as confirmed data.

No single analytical tool can measure all metabolites. Thus, acknowledging what is desired to be measured is crucial. Enhancing the identification of the metabolites could be achieved by having another complementary set of analytical data (LCMS for NMR or vice versa) or/and secondary information i.e. 2D-NMR, MS/ MS, and a MS molecular network. A further step for the identity confirmation can be made through the reductionist approach of purifying the desired metabolite and putting it through the necessary spectroscopic methods i.e. Fourier-transform infrared spectroscopy (FTIR), ultraviolet-visible spectrophotometry (UV-Vis), MS, and NMR. A comprehensive set of spectroscopic data on a compound is the weighty establishment of structure.

Hence, these two approaches, reductionism and

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metabolomics should not be observed as scientific contenders. Instead, they should be deployed synergistically to achieve the global aim of deciphering the significance of natural products for society. When reductionism is blind to many windows, metabolomics is capable of a far wider view through its holistic eyes. Meanwhile, reductionism can create and populate the data on individual metabolites that are needed to provide a more accurate view of metabolomic diversity. Thus, these two analytical tools must be seen as complementary technologies that can act synergistically to enhance drug discovery from complex natural matrices or metabolite modifications as the matrix changes due to the exogenous stimuli.

Metabolomics studies

Let me share some of my research to provide a broad overview of how metabolomics can be applied in studies. This might also clarify the reason why these two approaches, reductionism and metabolomics, should be utilized cooperatively to harmonize natural product research. My first embarkment using metabolomics was a study of the leaves of a local herb, Andrographis paniculata Wall. (family Acanthaceae) and its changes, interpreted using attenuated total reflection (ATR)-FTIR targeting on the two major compounds andrographolide and neoandrographolide, based on harvesting ages, as well as the times. The spectra from each accession exhibited differences that were discriminated against and clustered into groups through Multivariate Data Analysis (MVA) of Orthogonal Projections to Latent Structures Discriminant Analysis (OPLS-DA).³ These findings could be useful as a guide as to what time and age of A. paniculata should be harvested to optimize the targeted major diterpene lactone intensities.

This first experience taught me well on the selection of the subject related to the analytical tool to be utilized. While ATR-FTIR was a simple instrument to use, however, its low sensitivity exhibited results that were difficult to interprete as there were minimal observable variations between the different samples. When the sensitivity of the analytical platform is as low as FTIR, a targeted study is a better choice. The two major metabolites of *A. paniculata*, andrographolide and neoandrographolide, were employed as a spectral guide, as they are specifically well-reported belonging to the plant. Hence, the prior spectral data on the metabolites augmented the FTIR interpretability.

Metabolomics studies can be used for targeted or untargeted investigation. An untargeted study is a comprehensive analysis of all the measurable analytes in a sample, including many unknowns. For a targeted study, the measurement is of chemically characterized and biochemically annotated metabolites.⁴ The choice of either a targeted or non-targeted depends on the objective(s) of the study, and will be reflected through the experimental design. In any metabolomic study, designing the experiment is the prime part. The core aspect to scrutinize in design is how to produce highconfidence level statistical data. Among the drawbacks in the statistical analysis of metabolomics data are the difficult interpretability and poor reproducibility of the identified clusters. The worst case scenario is the unreliable results based on a poor understanding of the complicated data. Bad results are from bad data input that is led by mostly failure in the experimental design, if not the filtering of noise from the results leading to false positives.

The typical main steps in a natural product research program utilizing metabolomics are: a) taxonomic and agronomic details of the plant which govern the harvesting step, b) preparation of the sample including drying method, extraction, and storage, c) spectroscopic data acquisition, d) multivariate data analysis, e) identification of the metabolites which can lead to the nomination of chemicalmarker, and f) biological activity acquisition and analysis (this part may be absent in chemistry-focused research). When a natural product study includes a biological assay, the bioassay results will also be analyzed via MVA in correlation with the chemical data. A biomarker is determined when a biological system, such as a cell, an organ, or an organism is used. Through the use of metabolomics tools in studies combining chemistry and biology, a holistic view of the occurred perturbation in a biological sample can be interpreted via the chemical changes detected by the applied analytical platform.

The common online accessible metabolomic databases, such as HMDB (http://www.hmdb.ca), METLIN (http://metlin.scripps.edu), and KEGG (http:// www.kegg.jp) are exhaustively referred to for the identification of metabolites. However, the bulk of the data from these sources relate to primary metabolites. Due to the nature of the secondary metabolites, some of which can be generally shared across many species, but some of which are specific to a species, the collective secondary metabolites data cannot be cited for all plant families. Over the past few decades, the list of secondary metabolites from Arabidopsis thaliana has continuously expanded. This model species is as numerous and diverse as those of other plant taxa despite its small stature, short life-cycle, and highly reduced genome.⁵ The studies on isolating and identifying the secondary metabolites from A. thaliana are the conceptual example of building up compound data of a plant. However, a metabolite database on the Malavsian local plants is absent, which impinges on the identification step of the metabolomics research workflow. It can obviously be perceived from my reported studies of repetitive identification on mostly the primary, and lacking on the secondary metabolites.

After the first experience with FTIR, I decided to explore the use of NMR as the analytical platform in looking into the effect of Orthosiphon stamineus Benth. (Lamiaceae) leaves in the nephrotoxic rat model. The research was started with the selection of the drying method for the leaves as the biological properties of the tea were thought to be in direct correlation with the primary and secondary metabolite composition, which in turn largely depends on the choice of drying method. The effects of three commonly used drying methods, i.e. shade, microwave, and freeze-drying, on the metabolite composition and the antioxidant activity of O. stamineus leaves were investigated using proton NMR (¹H NMR) spectroscopy combined with multivariate classification and regression analysis tools. 1D-NMR or ¹H NMR is the first analysis option to view the metabolite differences between the sample groups. Shade-dried leaves were identified to possess the highest concentrations of bioactive secondary metabolites, such as chlorogenic acid, caffeic acid, luteolin, orthosiphol, and apigenin, followed by the microwavedried samples. Freeze-dried leaves had higher concentrations of choline, amino acids leucine, alanine and glutamine, and sugars such as fructose and \Box -glucose, but contained the lowest levels of secondary metabolites.⁶

Metabolite profiling, coupled with MVA, is important to decide on the best drying method related to the focused metabolites. A Principal Component Analysis (PCA) is always the first choice of a MVA plot. Yet, the drying method is not the only first crucial phase, harvesting age, and time, as shown in the study A. panic*ulata,* are critical aspects to be determined, along with the harvesting method. For a freeze-dried sample, the material has to be snap-frozen in liquid nitrogen as soon as the plant part is acquired. A supplement of ice cubes will be helpful when the distance between the cultivation area and laboratory is far. Another point is the recording of all pertinent environmental parameters including the Global Positioning System (GPS) coordinates, and the agronomic and meteorological data of the cultivation plot of the plant.

O. stamineus, which is a popular medicinal plant used in traditional Chinese medicine owing to its diuretic effects and for renal system disorders, was further studied for its possible protective activity in cisplatininduced nephrotoxicity. The ¹H NMR profile of the rat urine samples showed marker metabolites suggesting involvement of the TCA cycle, disturbed energy metabolism, altered gut microflora, and BCAA metabolism pathways. It was observed that the orally administered 50% aqueous ethanolic, shade-dried leaf extract caused significant changes (p < 0.05) in the levels of several biomarkers, namely leucine, acetate, hippurate, lysine, valine, 2-oxoglutarate, 3-HBT and acetoacetate, resulting in an ameliorative effect.⁷ This study exhibited the importance of solvent in extracting the desired metabolites. A range of different polarity solvents is commonly used to extract the respective metabolites. Methanol is a universal solvent used to obtain a global metabolite representation of a wide polarity range. However, fractionation of the methanol extract based on used solvent polarity can be as a step to divert from a non-targeted investigation to a targeted one.

Orthosiphon stamineus is also a herb known in ethnomedicine for treating diabetes mellitus (DM). A ¹H NMR-based urine metabolomics analysis was used to identify the metabolic protective mechanism of the plant in a streptozotocin (STZ)-induced DM model in rats. The same set of *O. stamineus* leaf samples used for the nephrotoxicity study were employed in this DM model. Hence, a plant extract can be utilized in more than a biological assay model. From these two disease models of nephrotoxicity and diabetes, the results pattern were different, wherein the 50% aqueous ethanolic, shade-dried leaves gave the nephrotoxic ameliorative effect, while the microwave-dried 100% water extract caused a reversal of DM comparable to that of 10 mg/kg bw glibenclamide.⁸ In contrast, the microwavedried leaves from any solvent extract were observed to be harmful to the nephrotoxic rats. These two models provided scientific evidence against the general assumption that a medicinal plant preparation could remedy many illnesses.

The project on O. stamineus has awakened me further on the importance of how to obtain reliable data. Unlike MS, which is a dynamic analytical method, NMR is a rather stagnant and universal platform. However, the marriage of these two platforms that complement each other will produce more confident data. The research on another Malaysian herb, Clinacanthus nutans Lind. (family Acanthaceae), utilized both analytical methods H NMR and Liquid Chromatography-Mass Spectroscopy (LCMS) in revealing the biochemical outcomes of metabolic dysregulation in serum associated with physiological sickness behavior following lipopolysaccharide (LPS)-induced neuroinflammation in rats. Parameters of rat behavior related to sickness were tracked using device software (SMART 3.0.1). The acquired and accumulated data were analyzed using MVA with the SIMCA Software package (version 13, Umetrics AB; Umeå, Sweden). The pattern trends of the related groups were documented using PCA and OPLS analysis.

A moderate correlation was observed between the spectral metabolite profile of the serum and the cytokine levels of the OPLS regression model. The study revealed the existence of high levels of proinflammatory cytokines, namely IL-1 α , IL-1 β , and TNFa in the LPS-induced rats. The C. nutans treatments lowered IL-1 β significantly better than the positive control. dextromethorphan. Interestingly, the control drug and plant treatments exhibited upregulation of the antiinflammatory cytokines IL-2 and IL-4. Hence, this study showed that a metabolomics approach was successfully applied to discover the mechanistic role of a medicinal plant in controlling the neuroinflammatory conditions through the modulation of complex metabolite interactions in the rat brain. The results denoted that the metabolomics approach is a reliable tool to disclose the relationship between central neuroinflammation and the systemic metabolic and physiological disturbances which could be used for future ethnophar-macological assessments.⁹

Since Clinacanthus nutans, locally known as Belalai Gajah or Sabah snake grass, is a medicinal plant being traditionally used for its diuretic effects, other than treating skin rashes, insect and snake bites, diabetes mellitus, and fever, a study was conducted on this plant in a cell-nephrotoxic assay. Again, both ¹H NMR and LCMS-coupled with MVA, were employed to characterize the metabolic variations of intracellular metabolites, and the compositional changes of the corresponding culture media in rat- (NRK-52E) and humanrenal proximal tubular cells (PCS-400-010). The NMR and LCMS analysis highlighted the main metabolites which differentiated the cisplatin-induced group from the extract in both cell lines extract, and their corresponding media. The altered pathways perturbed by cisplatin nephrotoxicity on the cells included changes in amino acid metabolism, lipid metabolism, and glycolvsis.¹⁰ Accordingly, the use of a metabolomics tool resulted in the identification of the perturbed metabolites leading to an understanding of the possible mechanism involved.

The last research that I would like to share is on the utilization of the metabolomics approach in the possible quality control of stingless-bee honey. The official standard for the quality control of honey is currently based on physicochemical properties. However, this method is time-consuming, cost-intensive, and does not lead to information on the origin of the honey. The raw stingless bee honeys were classified by the bee species origins using a NMR-LCMS-based metabolomics approach in combination with chemometrics tools. The honey samples could be classified into three different groups based on the bee species origins, namely, Heterotrigona itama, Geniotrigona thoracica, and Tetrigona apicalis. D-Fructofuranose (H. itama honey), α - and β -D-glucose, D-xylose, (G. thoracica honey), and L-lactic acid, acetic acid, L-alanine (T. api*calis* honey). They were identified by the ¹H NMR data, and the diagnostic ions of UHPLC-QTOF MS, and were characterized as the discriminant metabolites or putative chemical markers. It could be suggested that the quality of the honey in terms of origin and purity can be rapidly determined using classification technique based on the bee species origins via the metabolomics approach.11

Conclusion

Studies employing metabolomics as a research tool yield information-rich data sets that offer important insights into many chemical, biological, and biochemical phenomena. The examples given here have shown that metabolomics can be applied in many fields of studies, and not limited to chemistry. The clear inadequacy, that should be addressed by a collective effort, is to build databases on the metabolites of the local flora and fauna. Reductionism and metabolomics approach should be orchestrated and executed together for the future advancement of natural products chemistry.

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Introduction

Organic chemistry a major branch of chemistry field which focuses on the study of structures, properties, and reactions of carbon-containing

compounds. Natural organic compounds found abundantly in nature are the backbone of the living organisms, while the synthetic organic compounds are important commodities with huge economic importance. Organic compounds are materials that we interact and have daily close contact, and have many important applications such as in the field of medicine, agricultural, manufacturing industry, food industry, etc. The medicines to treat the common cold to the antidotes for the most venomous venoms are organic compounds. In the comfort of our home, the active ingredients responsible for the aroma of the lovely jasmine flower to the spicy curry are organic compounds. The most treasured commodities in the world such as petroleum. rubber, palm oil, etc are organic compounds. Hence, organic chemistry is one of the most important field of study to improve our life and nature around us.



Becoming an Organic Chemist

Organic chemist typically carry-out research and development work either in a research institution or commercial laboratory setting. Introductory organic chemistry is taught in the pre-university programme, while the main organic chemistry syllabus is taught to undergraduate university students. Advanced organic chemistry is taught at the post-graduate level with majoring in specialize organic chemistry topic. To become an organic chemist, a person needs to complete the chemistry programme/course and obtained a relevant bachelor degree. In Malaysia, most of the organic chemists either work in the institution of higher learning as a chemistry lecturer/researcher or private industry in the R&D and/or QA/QC laboratory. Besides, due to the importance of the organic compounds in the living organism, good mastering of organic chemistry is required to becoming a medical doctor, veterinarian, dentist, pharmacologist, and pharmacist.

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Research in Organic Chemistry

ymchoo@um.edu.my

Practicing Organic Chemistry in Malaysia Dr. Yeun-Mun Choo Chemistry Department, University of Malaya, Kuala Lumpur, Malaysia

> Organic chemistry research in Malaysia focuses on two main topics, i.e. organic synthesis and natural product chemistry, with intended product applications in the pharmaceutical, pesticides, food supplements, and cosmetics industry. A classic example of developing drugs for pharmaceutical is penicillin. Penicillin is an important antibiotic first isolated and characterized from the common mold Penicillium rubens. Due to the drug-resistance phenomenon displayed by harmful bacteria, organic chemist subsequently has developed the 2nd and 3rd generation penicillin to address this problem. Penicillin is still in use today as an antibiotic. With the current critical transmission of the COVID-19 virus, the role of the organic chemist is once again being called upon to the forefront. The basic knowledge of hand-sanitizer making among organic chemists is

put to good use during the initial hand -sanitizer shortage period, which has led the organic chemists to make the hand-sanitizer in the lab. The race to discover the treatment for COVID-19 has resulted in many organic chemists going back to the laboratory to synthesize new compounds and isolate new natural compounds to test as potential COVID-19 inhibitors.

Challenges in Organic Chemistry

Although each field has its challenge, organic chemistry faces much more challenges than other chemistry fields. One of the major challenges is the high operation cost and expensive consumables associated with the running of an organic chemistry laboratory. A common organic chemical can easily cost up to RM1000 per gram. These fine chemicals are often classified under the hazardous chemical list

and/or control chemical which makes it harder to transport/import into the country. Organic chemistry laboratory requires much more safety fixture such as fume-hood and PPE to cope with the usage of these hazardous chemicals. In addition to the high cost of chemicals and laboratory fixtures, the instrumentation requires for the study of the structures and properties of organic chemical compounds are often very expensive, i.e. NMR, LCMS, etc. These high-tech expensive instrumentations can only be afforded by the top Institutions and hence, hampering the progress of research in the smaller institutions in Malaysia. The lack of interest among young students to study organic chemistry is another major challenge. It is well known that the young students are have diminishing interest to study



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STEM subjects, and even lesser students are taking up an interest in organic chemistry. The organic chemistry laboratory often associated with the stigma of being smelly, messy, and long working hours is another a discouraging point for the young students. While the student's complaint on organic chemistry being a hard subject is due to the lack of understanding of the underlying concept and theory of organic chemistry.

Future of Organic Chemistry

The sustainability of organic chemistry in Malaysia would be hinging on two main points. The funding for organic chemistry research and the ability to attract new talents. Collaboration and networking among Malaysia organic chemists to share resources such as chemicals and facilities would provide a more effective and sustainable research en-

vironment under the current limited research funding scenario. Introducing organic chemistry to the student at a younger age would be able to stir the interest and curiosity of the young's mind, and instil the love of the subject and reduce the stigma that organic chemistry is smelly and hard. This can show the younger student the practicality and usefulness of organic chemistry in their daily life, and deeper their understanding of the subject.





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Celebrate 45 Years of Ion Chromatography Innovation

lon chromatography is one of the most widely used separation techniques of analytical chemistry with applications in fields such as medicinal chemistry, water chemistry and materials science.

For ion analysis, nothing compares to the Thermo Scientific[™] Dionex[™] ion chromatography (IC) system. Today, we mark 45 years of Thermo Scientific Dionex IC celebration with innovative technology. We are committed to ensuring that our IC systems continue to be future-ready, helping laboratory professionals be more productive, be safer with less chemical handling and maximize their resources.



Thermo Scientific[™] Dionex[™] ICS-6000 HPIC[™] System

Key technological advancements for IC

In recent years, Thermo Fisher Scientific's key technological advancements for IC includes eluent generation, reagent-free IC and hyphenated IC:

- a. Eluent generation (EG) Eluent generation is an electrolytic process that allows the production of high purity eluents for ion chromatography, and is a part of Reagent-Free Ion Chromatography[™] (RFIC[™]).
 - Watch the video to understand why some methods use carbonate eluent and some uses hydroxide eluent, what are the differences and how this was developed. The video is at thermofisher.com/role-of-eluent-generation
 - Read this Analyte Guru blog post which provides information on why continuously regenerated trap column can keep your eluent cleaner, provide better baseline and background to your ion chromatograph. This blog post is at thermofisher.com/eluent-generation-technology

- b.Reagent-free ion chromatography (RFIC) Eliminate eluent preparation errors with RFIC. Check out our Dual EG technology and learn how you no longer have to manually prepare hydroxide and sodium acetate to analyze oligosaccharides. Learn more about our advancements in EG and RFIC at thermofisher.com/ion-chromatographyinnovations
- c. Hyphenated IC Consider hyphenating your ion chromatography system to gain an abundance of information instead of just using conductivity or amperometry as your IC detection. Hyphenate with an inductively coupled plasma mass spectrometry (ICP-MS) to speciate transition metals to decipher toxic versus non-toxic; utilize mass detection by hyphenating IC with a mass spectrometry system (IC-MS) to maximize the ability to detect and quantify unexpected co-elutions of components and to confirm trace components. Learn more about hyphenated IC at thermofisher.com/IC-MS

Ion Chromatography Symposium - 45 Years

Coming up as part of our 45th ion chromatography anniversary celebration, Thermo Fisher Scientific will organize the inaugural Ion Chromatography Symposium - 45 years in October 2020.

This virtual forum will enable customers across Asia to exchange knowledge and engage in discussions with presenters such as Joachim Weiss, PhD, an international expert in analytical chemistry.

Dr. Weiss is the International Technical Director for Dionex Products at Thermo Fisher Scientific. He is renowned for his decades of experience and many significant contributions to ion and liquid chromatography. In 2015, he was awarded the Maria Sklodowska Curie Medal of the Polish Chemical Society for his achievements in separation science.

Register your interest early for this free virtual ion chromatography forum as we are expecting participants across more than 12 locations throughout Asia to join us. All participants at the "live" Ion Chromatography Symposium - 45 years will receive a certificate of attendance from Thermo Fisher Scientific.

Scan the QR Code or visit thermofisher.com/apj-ic45







Knowledge Exchange

Thermo Fisher Scientific, the world leader in serving science, is sharing knowledge with chemists, researchers, scientists and other laboratory professionals in Malaysia through virtual conferences and webinars. Check out these opportunities to connect, learn and exchange knowledge with experts worldwide!



On-demand webinar: Making trace element analysis effortless using the right instrumentation

Trace elemental analysis covers a range of applications that have vastly differing analytical requirements and need different types of instruments.

This webcast will provide you with the knowledge needed to choose the right tool for your elemental analysis, including atomic absorption (AA), inductively coupled plasma-optical emission spectroscopy (ICP-OES) and ICP-mass spectrometry (ICP-MS).

On-demand webinar: Isotope fingerprints for environmental investigations

The natural and synthetic materials have a fingerprint, a unique chemical signature that allows them to be identified and differentiated from one another.

In this presentation we explain how stable isotope fingerprints of carbon, nitrogen, sulphur, oxygen and hydrogen are used to identify the origin of air, soil and water pollution. Data will be shown to illustrate how isotope fingerprints offer conclusive answers on questions associated with where pollution came from.

Scan the QR Code or visit **thermofisher.com/asktheexpert** to register:



Pharma 4.0

Specially for Asia's pharmaceutical manufacturing industry, Thermo Fisher Scientific has developed a virtual learning series with thought leaders from across the world to discuss:

- · Recent developments
- Future trends
- Challenges
- Solutions

This is an invaluable opportunity for Asia's participants in industry, academia and regulatory to learn in order to further the development and manufacturing of pharmaceutical and biotechnology products.

Virtual Learning Series

This virtual learning series comprises two days of presentations – Day 1 on Small Molecules, Day 2 on Large Molecules – by renowned experts including:

- Dr. Ajaz Hussain, The National Institute for Pharmaceutical Technology & Education
- Mr. Peter Van Broeck, Janssen Pharmaceuticals
- Mr. Martin Warman, University of Strathclyde
- Mr. Jared Auclair, Biopharmaceutical Analysis & Training Lab
- Professor Pauline Rudd, A*STAR

Live Video Forums

Complementing the virtual learning series are three roundtable Live Forums covering different topics. These are:

- · Lab of the Future,
- Emerging Technologies, and
- · Regulatory and Quality Challenges.

A 'Certificate of Attendance' will be provided to all registered attendees to the virtual learning series and "live" video forums.

Scan the QR Code or visit **thermofisher.com/pharma4-0** to register:





Knowledge Exchange

Thermo Fisher Scientific, the world leader in serving science, is sharing knowledge with chemists, researchers, scientists and other laboratory professionals in Malaysia through virtual conferences and webinars. Check out these opportunities to connect, learn and exchange knowledge with experts worldwide!

During this period when countries around the world are busy with the pandemic, Thermo Fisher Scientific is focusing on strengthening knowledge exchange and learning sessions among local and international scientists, chemists, and laboratory professionals.

Thermo Fisher Scientific's Senior Commercial Director for Chromatography and Mass Spectrometry in Asia Pacific and Japan (APJ) Mr. Rich Youn explains in detail about these opportunities for discussions and learning sessions in the region.

In today's environment, what are the key challenges faced by Asia's scientific community and how can these be addressed?

Asia's challenges are impacted by mega trends around the world which include aging population, digitalisation and the adoption of emerging technologies such as artificial intelligence and the Internet of Things.

For instance, in the pharmaceutical industry, we see that as the population ages, governments focus on making healthcare accessible, leading to a decrease in the prices of drugs and causing pressure on the costs of drug production. At the same time, the pharmaceutical industry is experiencing a transformation towards Pharma 4.0 which leverages technologies for connectivity, digitalisation and artificial intelligence for the development and manufacturing of pharmaceutical and biotechnology products.

Against this backdrop, Thermo Fisher Scientific is working closely with thought leaders around the world to facilitate knowledge sharing sessions within the scientific community. For example, we have virtual learning series and live video forums to bring participants from more than 12 locations across Asia to meet and discuss pertinent issues such as regulatory and quality challenges, emerging technologies and transformation to the laboratory of the future. Together as one with the scientific community, we can progress for the greater good of society.

In 2020 as countries continue to deal with the pandemic, how is Thermo Fisher Scientific helping the scientific community?

The public is expecting unprecedented progress from the scientific community. Our new instruments and software can power discovery, improve productivity, and enable breakthroughs across a variety of applications. These include proteomics and protein analysis, untargeted small molecule profiling, biopharma characterization, screening and quantitation in food safety, and environmental analysis and toxicology.

In 2020, we have launched several new instruments and software for the industry. The key ones for the region's omics, biopharma and pharma industries include the Thermo Scientific Orbitrap



Exploris 240 mass spectrometer for scientists working on proteomics, metabolomics, biopharmaceutical characterization and small-molecules, the Thermo Scientific Orbitrap Exploris 120 mass spectrometer for scientists working across small molecule applications, the Thermo Scientific Vanquish Core HPLC systems as a productivity-enhancing solution for routine laboratories and the Thermo Scientific Proteome Discoverer 2.5 software to offer artificial intelligence (Al) technology to proteomics scientists.

How else is Thermo Fisher Scientific helping people in Asia?

For the medical industry, having high quality, high efficacy and safe drugs are especially important. Thermo Fisher Scientific focuses on helping customers to ensure that drugs that are developed and manufactured in the region meet the highest scientific and regulatory goals.

One way that we do this is through pro-active sharing of our application notes with the scientific community. For instance, one of our application notes is based on real drinking water samples to help lab professionals test for NDMA levels.

N-Nitrosodimethylamine (NDMA) is a member of a large class of N-nitrosamines. NDMA has attracted wide attention as being highly hepatotoxic and a known carcinogen in lab animals.



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Application Note: Porcine gelatin peptide detection in cosmetic products and food confectionery using a TSQ Altis triple quadrupole mass spectrometer with Vanquish HPLC for halal testing application

This application note is to establish a sensitive, fast, accurate and robust method using a LC-MS/MS for the detection of porcinebased gelatin in cosmetic and food confectionery products.

The authors explained that adulteration of cosmetic and food products has become a growing concern in the 21st century as manufacturers seeking financial gains often substitute expensive ingredients with cheaper alternatives.

Contamination of products through the introduction of foreign ingredients during the manufacturing process can also contribute to questionable products being purchased by the end consumer. Such incidences are a huge problem as the authenticity of a labelled product can no longer be guaranteed, especially for consumers with health, ethical, or religious concerns. An example would be the requirement that products consumed or used by the Muslim population are halal and do not contain any non-halal ingredients, especially anything from a porcine source.

Porcine-based products are not only a major source of meat in the global food supply chain, the other non-edible parts of the animal such as the skin and bones are also processed into a very flexible chemical agent called gelatin.

Gelatin consists of a mixture of peptides and proteins obtained from the permanent hydrolysis of collagen, the major protein in animal skin and bones. Although it can be derived from various animal by-products, it is primarily sourced from pork due to economic reasons.

Known as one of the most flexible food and chemical modifiers, gelatin is translucent, colourless, brittle, and flavourless in terms of its physical properties.

The multiple functions of gelatin includes stabilizing, binding, thickening, emulsifying, plasticizing and foaming, resulting in a wide area of application including food processing, pharmaceutical, cosmetics, photography, and printing.





Such wide applications for gelatin especially in a variety of food and cosmetic products are a huge cause of concern for the Muslim consumers. These concerns lead to the need for effective testing methodologies to detect porcine gelatin in various products.

Currently, there are two techniques that have been established for the detection of porcine gelatin.

The first technique is by polymerase chain reaction (PCR), which is frequently used in species determination through the identification of animal DNA present in the sample. The second commonly used technique is a protein-based method known as ELISA (enzyme-linked immunosorbent assay).

Unreliability of existing testing protocols has elevated the need for a reliable, sensitive, simple and accurate test for the detection of porcine gelatin.

As such, in this application note, the authors developed a testing procedure focusing on the use of triple quadrupole LC-MS/MS technology that can rapidly identify the presence of porcine gelatin through the combination of UHPLC fast separation and SRM-based targeted approach for a highly sensitive and robust solution.

Scan the QR code to download this application note:





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