



# 2025

Best Practices for Non-Targeted Analysis working group

Annual Report

**2025 Steering Committee:**

Sara Nason, Chair

David Schiessel, Vice-Chair

James McCord, Past-Chair

Stephan Baumann, Treasurer

Sonja Klee, Secretary

Gabby Black, Operations Liaison

Anna Robuck, Technical Liaison

## A Note from the Chair:



Hello everyone, and thank you for your interest in the Best Practices for Non-Targeted Analysis working group (BP4NTA). It has been my pleasure to serve as the 2025 chair of the organization. BP4NTA is special to me because it has provided me the opportunity to work with fantastic colleagues on influential projects that are important for the greater scientific community, but also have led to key improvements in my own research program. It has been a place to interact with like minded colleagues at all different career stages who are employed in government, industry,

and academia. It is important to me that the organization continues to both promote high quality NTA work and provide opportunities for collaborative projects and networking.

While BP4NTA welcomes members from across the globe, it was founded and continues to draw heavy participation from members based in the US. Employees of US federal agencies founded BP4NTA, have served as BP4NTA leadership, and have been some of our most influential members. As such, shutdown and changes that have happened in the 2025 US government have impacted BP4NTA activities and participants. In particular, the loss of the US EPA Office of Research and Development has been a huge blow to non-targeted analysis and BP4NTA, as well as the scientific community at large. While the changes, shutdown, and uncertainties have affected some projects and collaborations, BP4NTA has nonetheless been able to continue as an active and effective organization, with members from industry and academia stepping up to help keep things going. If anything, the changes in the U.S. federal government make the efforts of those of us who are relatively unscathed even more important, as there is great need for leadership in producing high quality scientific results that drive innovation and protect public and environmental health.

In this document you will find descriptions of major activities for the year as we have continued our transition to becoming a fully formed non-profit organization and worked to produce high quality scientific content that promotes and improves non-targeted analysis (NTA) studies using mass spectrometry.

Scientific achievements I would like to highlight include:

- Publication of the manuscript developed by the BP4NTA Stakeholder Outreach Committee: “Communicating with Stakeholders to Identify High-Impact Research

Directions for Non-Targeted Analysis”

<https://doi.org/10.1021/acs.analchem.4c04801>

- The first full year of work completed by the GC-NTA subcommittee
- Completion of a working draft of the NTA Study Planning Tool with four completed examples from various fields
- Initiation of a new subcommittee focused on Extractables and Leachables
- Hosting of 8 webinars featuring talks by NTA practitioners from various fields
- Dr. Christine Fisher accepting the Kathy T. Peter Memorial BP4NTA Outstanding Service Award

I look forward to this work continuing into 2026, as manuscripts from the GC-NTA and Study Planning Tool groups near completion and the Extractables and Leachables committee gets fully up and running.

Administratively, this was the first year that BP4NTA was self-supporting with paid memberships providing the funds to support our online resources. We made some key upgrades to our organizational infrastructure that will make our organization more efficient and sustainable with less volunteer effort required for administrative tasks. While this work takes place outside the view of most BP4NTA members, I want to acknowledge the impact it has had. Specific highlights include:

- Updates to the BP4NTA homepage at [nontargetedanalysis.org](http://nontargetedanalysis.org)
- Transferring hosting of BP4NTA events to our own zoom platform
- Setting up an automated system for email management
- Adopting a new membership platform to allow members to more easily manage their online accounts
- Successfully filing taxes for the first time as a non-profit organization
- Moving webinar recordings to be hosted on our own website

Overall, I would like to thank our members for a great year of BP4NTA progress. Thank you for the opportunity to chair the organization. I look forward to continuing my participation in BP4NTA and supporting the great work that happens here.

Sincerely,



Sara Nason, Ph.D.  
2025 BP4NTA Chair  
Associate Scientist, Connecticut Agricultural Experiment Station

## Monthly Meetings:

Month	Topic	Presenter	Presentation Title
January	Metabolomics	Alexander Aksenov, University of Connecticut	Illuminating the Dark Matter of Metabolomics Through Molecular Community Networking
February	PFAS	Benjamin Place, US National Institute for Standards and Technology	The NIST Per- and Polyfluoroalkyl Substances Interlaboratory Study – Exercise 1
March	<i>BP4NTA Update Meeting</i>		
April	qNTA	Jaanus Liigand, Quantem Analytics	Make your MS Analysis Quantitative Without Analytical Standards
May	PFAS	Carsten Baessmann, Bruker	Monitoring emerging contaminants like PFAS beyond regulatory requirements using trapped-ion-mobility QTOF MS in combination with newly developed non-targeted workflows.
June	<i>BP4NTA Update Meeting</i>		
July	PFAS	Carrie McDonough, Carnegie Mellon University	Work on PFAS detection using high-resolution mass spectrometry (HRMS), ion mobility spectrometry (IMS), and FluoroMatch
August	Extractables & Leachables	David Weil, Agilent	Challenges and Best Practices for Extractable and Leachable Nontargeted Analysis
September	Exposomics	Jeremy Koelmel and team, Yale School of Public Health	Non-Targeted Analysis in Exposomics: Global Perspectives from the NEXUS International Survey.
October	<i>BP4NTA Update Meeting</i>		
November	Extractables & Leachables	Michael Rush, Edwards Lifesciences	Challenging the Database: Improving RRF Reliability in Chemical Characterization
December	<i>BP4NTA Update Meeting</i>		

# Technical Committee Activities:

## Study Planning Tool

**Co-chairs:** Benjamin Place, Niti Shah

**Background:** Originally formed as the Standards Committee in 2022, the group worked to identify areas of non-targeted analysis that need standardization and noted that the design of NTA studies need to be more consistent to enable comparison of results (and eventually standardization or harmonization of methods). In 2023, the committee started work on the Non-Targeted Analysis Study Planning Tool (NTA-SPT) to guide NTA practitioners with the systematic development of non-targeted analysis studies.

**Membership:** The SPT Committee has 31 active members.

**Current Activities:** Over the past two years, the SPT Committee has been actively working on the development of the study planning tool. These efforts include engaging with stakeholders and other non-targeted analysis organizations (mQACC and the Lipidomics Standard Initiative) to identify collaborations and align any concurrent efforts in the space of NTA study design.

**Upcoming Activities and BP4NTA Involvement:** SPT Committee is completing the final version of the NTA-SPT along with example cases and an accompanying manuscript. It is intended that these materials will be submitted to the BP4NTA consensus process in the first quarter of 2026. We look forward to being able to present these materials to BP4NTA and to bring this new tool to NTA practitioners around the world!

## GC-NTA

**Co-chairs:** Anna Feerick, Seth Newton

**Background:**

**Membership:** The GC-NTA Committee has about 50 active members.

**Current Activities:** We have been working on a perspective journal article on the state of GC-NTA and the path forward for the field, and the committee facilitated a presentation at the ICNTS 2025 conference about the GC-NTA work.

## Extractables and Leachables

**Co-chairs:** Michal Rush and Jasmine Yuan

**Background:** The E&L Technical Subcommittee was officially launched with its first meeting on October 28, 2025. Since then, the group has met regularly, including the November 25 session focused on agenda-setting and collaboration priorities. Our meetings are on the 4<sup>th</sup> Tuesday of each month (excluding this upcoming December) at 9 AM MTN time. Reach out to Michael at [mailto:Michael\\_Rush@edwards.com](mailto:Michael_Rush@edwards.com) or Jasmine as <mailto:JYuan10@ITS.JNJ.com> for more information/meeting invite.

**Membership:** The subcommittee includes representatives from manufacturers, CROs, mass spectrometry vendors, and more, creating a diverse and global participant base. We have 16 members at the end of 2025.

**Current Activities:**

- **Conference Engagement:** Members presented at PharmaED E&L West and E&L Europe, sharing insights on chemical characterization and non-targeted analysis. We brought our experiences at these conferences and shared them as conference reports to members who were unable to attend.
- **Collaborative Initiatives:** Planned to enhance the BP4NTA literature library by curating a list of E&L publications for different applications (e.g., food contact, biocompatibility) and explored best practices for spectral identification and data processing workflows.
- **Networking and Knowledge Sharing:** Established recurring meetings and open calls for interest via platforms like LinkedIn to broaden participation and foster technical collaboration.

**Upcoming Activities and BP4NTA Involvement:** We are looking to post some E&L datasets as challenges for us to explore various aspects of data processing, acceptance criteria, and spectra identification. If the BP4NTA broader community have interests in contributing or other applications for this type of data, please contact us! We are also trying to get the word out about our subcommittee. As you know, E&L covers a lot - from medical devices such as bandages to brain implants, combination products with pharmaceuticals, food contacting materials, and more - so we want to ensure our work to define and establish best practices accommodates the various materials and test articles! Please spread the word about our BP4NTA E&L Technical Subcommittee!

## PFAS

**Co-chairs:** Jackie Bangma, Jeremy Koelmel

**Current Activities:** Monthly meetings were paused in early 2025, but given the broad interest in PFAS NTA, the PFAS committee could be re-started to focus on a manuscript or presentation goal with member interest. Please reach out to Jackie Bangma ([bangma.jacqueline@epa.gov](mailto:bangma.jacqueline@epa.gov))

## Education

**Co-chairs:** Brittany Saleeby

**Current Activities:** Meetings were held in the spring, and the committee worked to collect source material for educational efforts while supporting website updates

**Upcoming Activities and BP4NTA Involvement:** The committee has looked into setting up an institution-agnostic course platform or learning management system to share course materials and host interactive demos, and seeks to build momentum on this in 2026.

## Stakeholder Outreach

**Co-chairs:** Sara Nason and James McCord

**Current Activities:** We celebrated the final publication of our manuscript, “Communicating with Stakeholders to Identify High-Impact Research Directions for Non-Targeted Analysis”

<https://doi.org/10.1021/acs.analchem.4c04801>, which was released in January 2025. The committee was officially disbanded following publication.

## External Collaborations

### mQACC: Metabolomics Quality Assurance and Quality Control Consortium

**BP4NTA leads: Christine Fisher and Alli Phillips.** Several collaborative meetings were held this year to discuss a potential joint publication. The potential publication would outline the roles of our respective organizations as well as other groups in the -omics and high-resolution mass spectrometry space and identify how to best address needs in the scientific community separately and through collaboration. This effort was disrupted by US federal government limitations affecting those in both groups and is on hold while other similar efforts (listed below) develop.

Additionally, Ben Place presented the NTA Study Planning Tool (SPT) at an mQACC meeting in July 2025 and there is potential interest in future evaluation and/or use of the SPT by mQACC. However, this is not being included in the initial publication of the SPT.

### PRISM: Precise Reporting in Small Molecules

**BP4NTA leads: James McCord, Alli Phillips.** This is a multi-organization effort, led by Rick Dunn and the Metabolomics Society, focused on organizing reporting standards for small molecule analysis. Participants include the Metabolomics Society, BP4NTA, mQACC, NIH, the Lipidomics Standard Initiative (LSI), and Metabolomics Standards Initiating in Toxicology (MERIT). This effort had a lot of momentum in early 2025, but is moving forward slowly.

### (LSI) Lipidomics Standards Initiative

**BP4NTA leads: Christine Fisher, Alli Phillips, and Ben Place.** LSI hosts an excellent reporting checklist on their online platform, and members of the SRT team reached out to discuss potential collaboration. Subsequently, LSI and the BP4NTA SPT committee have discussed developing an online version of the SPT, potentially to be developed and hosted on the LSI web platform. This is being considered as part of SPT phase 2 and will be further pursued after initial SPT publication.

## Presentations on behalf of BP4NTA

1. Presentation: Benjamin Place **“The Best Practices for Non-Targeted Analysis (BP4NTA) Working Group” AOAC International Annual Meeting**, August 2025, San Diego, CA.

**Abstract:** Non-targeted analysis (NTA) is a type of analytical technique with the purpose of identifying chemicals in a material without the use of a priori knowledge regarding the chemical composition of the material. As novel methods using NTA approaches rapidly emerge, the Best Practices for Non-Targeted Analysis (BP4NTA) Working Group formed to address the need for harmonization across research communities. The presentation will discuss all facets of BP4NTA, from formation in 2017 to its current goals. Over the past 8 years, BP4NTA has become an international, nonprofit organization consisting of members from academia, government (state, federal US, and non-US), and industry with a range of NTA experience. Initial efforts within BP4NTA aimed at harmonization of language and methods through the creation of the informative website with NTA Reference Content. Numerous other outcomes have been generated, ranging from manuscripts and tools to engagement activities with varied stakeholders involved in the development of NTA workflows and use of the data. Examples include the NTA Study Reporting Tool, guidance on understanding performance metrics for non-targeted analysis and proposing a roadmap for the high-impact research directions for NTA. In addition, BP4NTA has identified opportunities fulfill an educational in training and supporting researchers that are new to NTA. Moving forward BP4NTA endeavors to identify new collaborative opportunities with other scientific communities using non-targeted approaches, develop new tools that further enhance transparency and reproducibility of non-targeted analysis, and to establish best practices for scientists using non-targeted approaches.

2. Presentation: Sara Nason **“The Best Practices for Non-Targeted Analysis Working Group: Supporting and Expanding the NTA Community” the International Conference on Non-Targeted Screening**, October 2025, Erding, Germany and virtual.

**Abstract:** The Best Practices for Non-Targeted Analysis working group (BP4NTA) was founded in 2018 with a goal of improving the quality of non-targeted analysis (NTA) through communication and consensus. Over the past 7 years, BP4NTA has expanded to over 250 members across 6 (sub)continents and has published many NTA resources including the Study Reporting Tool, comprehensive online reference content, and manuscripts on

assessing NTA performance and creating a chemical space tool. Most recently, we published a manuscript featuring focus group and survey results from a variety of stakeholder groups where NTA is expected to provide future value. We identified barriers to NTA use including concerns about data quality, lack of data processing tools, and lack of knowledge among both laboratory analysts and data end users. Additionally, we proposed four priorities for expanding NTA use and increasing NTA data quality:

1. Education and training materials;
2. QA/QC frameworks and study design guidance;
3. Accessible compound databases and libraries; and
4. NTA linkages with toxicity and fate information

These priorities drive current BP4NTA activities, which include the development of a Study Planning Tool, an Education Committee, and technical groups focused on key topics in NTA such as GC-HRMS, PFAS, and extractables and leachables. We are also engaged with external collaborators to promote communication amongst related fields such as metabolomics, lipidomics, and exposomics. As the field of NTA expands and improves, BP4NTA will continue to promote high quality science and serve as a networking center for NTA practitioners.

3. Presentation: Anna Feerick **“Gas Chromatography and Non-targeted Analysis: Struggles and Successes” the International Conference on Non-Targeted Screening**, October 2025, Erding, Germany and virtual.

**Full author list:** Feerick, A., Bade, J., Bauman, S., Begley, A., Ayala-Cabrera, J., Chen, Y., Clifton, M., Reis de Carvalho, A., Franchina, F. A., Franklin, E., Froment, J., Hayes, J., Hanozin, E., Klee, S., Koelmel, J., Kralles, Z., Letzel, T., McDonough, C., McGlynn, D., McNeil, B., Nieto, S., O'Connor, C., Rostkowski, P., Saleeby, B., Stein, S.E., Sunyer-Caldú, A., Geer Wallace, A., Williams, A., Yee, L., Young, T., Newton, S.

**Abstract:** Gas chromatography, combined with high-resolution mass spectrometry (GC-HRMS), is uniquely suited for detecting volatile and semi-volatile compounds within complex samples. Despite this unique chemical coverage, GC-HRMS remains underutilized compared to liquid chromatography-HRMS (LC-HRMS) as a separation and ionization technique for non-targeted analysis (NTA). To understand this discrepancy, we have performed a critical review of the use of GC-HRMS for NTA (GC-NTA), from instrumentation specifics to criteria for compound identification. Within this review, we evaluate the key developments that have advanced NTA using LC-HRMS (LC-NTA),

compare GC-NTA with specific LC-NTA advantages (such as versatility, soft ionization, broad analyte range, and sample preparation), and highlight the unique advantages of GC-NTA. We perform a detailed review on many of the key steps in GC-NTA workflows, with the goal of understanding the current state of the science: how GC-NTA data is collected, processed, and analyzed to obtain useful information. The review also plots a path forward for the GC-NTA community by synthesizing lessons from LC-NTA development, addressing critical gaps identified in the GC-NTA state of the science review, and reducing barriers to GC-NTA adoption into more NTA studies. We finish by identifying critical knowledge gaps caused by the paucity of GC-NTA applications. In conclusion, we argue that GC-NTA can and should become as widespread as LC-NTA as it covers a complimentary chemical space and, while there are significant challenges to be faced, they are not insurmountable. The views expressed do not represent agency policy.

4. Presentation: Alli Phillips “**Standardizing Reporting in Non-Targeted Analysis with the Study Reporting Tool**” **Society for Environmental Toxicology and Chemistry North America Meeting**, November 2025, Portland, OR.

**Abstract:** Non-targeted analysis (NTA) is rapidly becoming a powerful tool used in many research disciplines. The rapid rise in NTA use has led to inconsistent scientific reporting, which creates challenges for peer-review and threatens the reproducibility of key scientific findings. Under the leadership of Dr. Katherine Peter, the Best Practices for Non-Targeted Analysis (BP4NTA) working group developed the NTA Study Reporting Tool (SRT) to address the need for standardized reporting criteria in untargeted exposomics. The SRT is the first easy-to-use tool for rigorous evaluation of NTA reporting practices and is available for download as an Excel or interactive PDF file on the BP4NTA website ([www.nontargetedanalysis.org/srt](http://www.nontargetedanalysis.org/srt)). It is organized by NTA study chronology and contains 13 sub-categories for scoring that cover all aspects of study design; data acquisition, analysis methods, and outputs; and quality assurance/quality control metrics. The SRT uses a color-coded, 4-level scoring system to evaluate research reporting quality and reserves space for reviewers to explain their rationale for assigned scores. Designed with ease-of-use in mind, the SRT contains examples of information that might be reported in each sub-category. Sub-category headings are hyperlinked to reference content on the BP4NTA website, providing detailed background information for users less familiar with certain subject matter. Since its initial publication in 2021, the SRT has been updated several times based on user feedback and to expand its relevance to multi-omic workflows. The SRT has been viewed over 3,500 times, downloaded 1,400 times, and cited 120 times, demonstrating its value and current application in the NTA community. Efforts are underway to interlink the SRT with BP4NTA's

Study Planning Tool (SPT), a companion guide for NTA study design and execution, and to connect with other -omic working groups (i.e., Metabolomics Quality Assurance & Quality Control Consortium [mQACC], Metabolomics Society, International Lipidomics Society [ILS]) around consensus-based reporting standards and tools for untargeted mass spectrometry applications. Dr. Katherine Peter was the driving force behind the SRT's conception and initiated many of the ongoing efforts and collaborations to expand its impact.

## Finances

Starting Balance (January 1, 2025): \$2,552.28

Approved Expenses (December 16, 2025): \$1,424.41

Total Income (December 16, 2025): \$1,429.55

Ending Bank Balance (November 5, 2025): \$1,514.98

Ending PayPal Balance (December 16, 2025): \$1,297.82

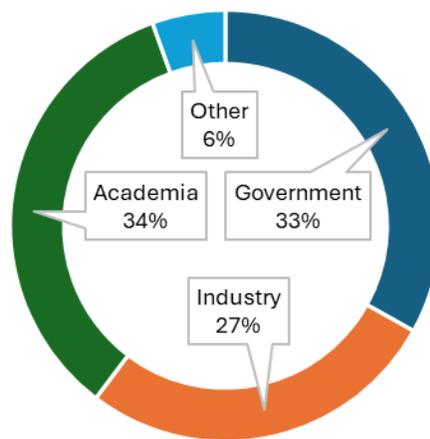
Total Balance (December 16, 2025): \$2, 812.80

Funds are distributed between our Wells Fargo bank account and our PayPal account. Approved expenses included the purchase of the goods awarded for the Kathy T. Peter Memorial BP4NTA Outstanding Service Award, website hosting fees, subscriptions for online membership management, email management, and Zoom, and purchase of custom pins for distribution at the Kathy T. Peter memorial session at the SETAC North America meeting.

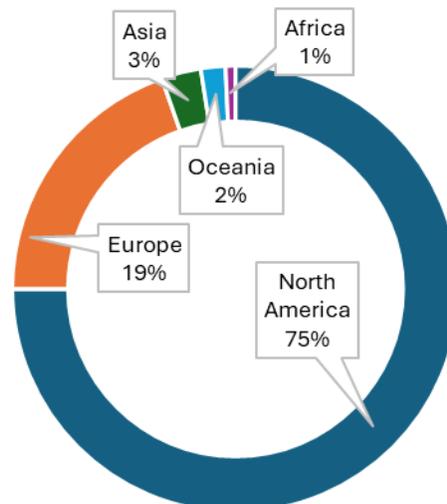
## Membership

As of December 10, 2025, there are 317 member accounts on our website. Active paid memberships include 12 Gold Members, 16 Full Members, and 5 Discount Members. The remainder are free accounts. Paid memberships support BP4NTA infrastructure, and paid membership is required to vote in elections, hold office, and participate in the BP4NTA consensus process. Technical difficulties with membership renewals have led to a drop in paid memberships, but updates are in progress to facilitate that process. Graphs below are accurate as of October 17, 2025.

### Sector Affiliation



### Geographic Distribution



## Steering Committee Activities

Month	Decisions & Topics
January	<ol style="list-style-type: none"> <li>1. Official start of an annual BP4NTA report</li> <li>2. Clear annual goals for each steering committee member</li> <li>3. Charter finalization</li> <li>4. Start a Website Update</li> <li>5. BP4NTA guided session at ICNTS (International Conference for NonTarget Screening)</li> </ol>
February	<p><b><i>US Federal Situation starting to effect BP4NTA</i></b></p> <ol style="list-style-type: none"> <li>1. Switch from EPA MS Teams channel to independent channel</li> <li>2. Try to do a quarterly review of goals</li> <li>3. Start discussions about membership benefits for paying members</li> <li>4. BP4NTA Calendar</li> </ol>
March	<ol style="list-style-type: none"> <li>1. Start of own BP4NTA Zoom Account</li> <li>2. BP4NTA first tax submission and financial review</li> <li>3. BP4NTA award provided to Christine Fischer- (O'Donnell)</li> </ol>
April	<ol style="list-style-type: none"> <li>1. Full shift of BP4NTA activities &amp; documents from EPA MS Teams account</li> <li>2. Option of NEXUS collaboration</li> <li>3. Written guideline for BP4NTA activities &amp; product</li> </ol>
May	<ol style="list-style-type: none"> <li>1. <b>Guests</b> presentation: NEXUS presents to BP4NTA steering committee &amp; discussions collaboration option</li> </ol>
June	<ol style="list-style-type: none"> <li>1. Recruitment for 2026 BP4NTA steering committee election</li> <li>2. E&amp;L Subcommittee Request</li> <li>3. Review of "NEW BP4NTA Activities" document</li> <li>4. <b>Guests:</b> Benjamine Place (NIST) as SPT Chari: SPT Review 1 -&gt; Consensus Process Request by Steering Committee</li> </ol>
July	<ol style="list-style-type: none"> <li>1. Membership Renewal Process Start</li> <li>2. Kathy Honoring Pins no BP4NTA product. Steering committee agreed on supporting this activity (incl. payment)</li> <li>3. Approved Consensus Process Policy</li> <li>4. Approved shift of July Webinar</li> <li>5. Approved BP4NTA promotion of ICNTS scholarships</li> </ol>
August	<ol style="list-style-type: none"> <li>1. Website Updates</li> <li>2. Election Recruitment: 3 great candidates were contacted</li> </ol>
September	<ol style="list-style-type: none"> <li>1. Election Recruitment: 3 volunteers defined for freeing positions</li> <li>2. Website Updates</li> <li>3. Option of AOAC collaboration</li> <li>4. Non-technical aspects of NTA underrepresented currently. Approved to underline this topics importance via webinar presentation</li> <li>5. Start of Annual Report Preparation (deadline before December Webinar)</li> </ol>
October	<ol style="list-style-type: none"> <li>1. <b>Guests:</b> Upcoming Steering Committee Members &amp; decision of positions for each new member</li> <li>2. Website Update</li> </ol>

November	<ol style="list-style-type: none"> <li>1. Approved E&amp;L Subcommittee</li> <li>2. Approval of an Anti-Trust Statement for BP4NTA</li> <li>3. Approval of the acceptance of non-renewed members for election participation</li> </ol>
December	<ol style="list-style-type: none"> <li>1. Website Update &amp; first official email from new email list, recordings finally available via member account on website</li> <li>2. Certification and onboarding process of new steering committee members</li> <li>3. Annual Report Status</li> <li>4. Review &amp; Summary of BP4NTA 2025 Steering Committee activities</li> </ol>

Overall:

- Process to move BP4NTA forward as a fully functional, self-reliant organization
- Improvement of membership benefits
- Collaboration with other communities
- New activities and products for BP4NTA