

# Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations



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## Deliverable D7.1: CINDI-3 Campaign Planning Document



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## List of acronyms

AIOFM	Anhui Institute of Optics and Fine Mechanics, Hefei, China
AIRYX	Airyx GmbH
ABOM	Australian Bureau of Meteorology, Melbourne, Australia
AUTH	Laboratory of Atmospheric Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece
BIRA	Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Brussels, Belgium
CESAR	Cabauw Experimental Site for Atmospheric Research
CINDI	Cabauw Intercomparison of UV-Vis DOAS Instruments
CNR-ISAC	Consiglio Nazionale delle Ricerche - Istituto di Scienze dell'Atmosfera e del Clima, Bologna, Italy
DOAS	Differential Optical Absorption Spectroscopy
DS	Direct sun
ESA	European Space Agency
Evora	Institute of Earth Sciences (ICT), University of Evora, Evora, Portugal
FOV	Field of View
FRM4DOAS	Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations
FWHM	Full Width at Half Maximum
INTA	Instituto Nacional de Técnica Aeroespacial, Madrid, Spain
ISRF	Instrumental Spectral Response Function
IUPB	Institute of Environmental Physics (IUP), University of Bremen, Bremen, Germany
IUPH	Institute of Environmental Physics, Heidelberg University
LATMOS	Laboratoire Atmosphère, Milieux, Observations Spatiales, Guyancourt, France
LBLICK	Luftblick Og
LMU	Ludwig Maximilian University of Munich, Germany
MAX-DOAS	Multi-Axis DOAS
MPIC	Max Planck Institute for Chemistry, Mainz, Germany
NIER	National Institute of Environmental Research, Incheon, South Korea
NDACC	Network for the Detection of Atmospheric Composition Changes
PGN	Pandonia Global Network
PKNU	Pukyong National University, Busan, South Korea
UNAM	Universidad Nacional Autónoma de México, Mexico
UOM	University of Melbourne, Australia
RAL	Rutherford Appleton Laboratory Space
RSS	Remote Sensing Site
SUWON	University of Suwon, Hwaseong-si, Republic of Korea
SWING	Small Whiskbroom Imager for atmospheric composition monitoring
UOT	Department of Physics, University of Toronto, Toronto, Canada

USTC

University of Science and Technology of China, Hefei, China

WNW

West Northwest

# 1 Introduction

Introduced in the late seventies (Noxon, 1975), passive UV-visible spectrometry has since been widely developed and used for routine remote sensing of atmospheric trace gases in both the stratosphere and troposphere. While original studies exploited zenith-sky twilight observations, more recent instruments focus on using additional observations geometries (direct-sun and MAX-DOAS) to derive information on various tropospheric species including NO<sub>2</sub>, formaldehyde (HCHO), BrO, glyoxal, IO, HONO and SO<sub>2</sub>. Multi-axis DOAS measurements (MAX-DOAS), scanning the sky vertically at several elevation angles between horizon and zenith, allow deriving vertically resolved information on these gases as well as on aerosols (e.g., Wagner et al., 2004; Frieß et al., 2006).

With the advent of satellite-based atmospheric composition instruments such as GOME, SCIAMACHY, OMI, GOME-2, TROPOMI, GEMS and the recently launched TEMPO mission, the need for operational validation relying on traceable and quality-controlled ground-based fiducial reference measurements (FRMs) has grown steadily, resulting in a considerable increase in the number of instruments. A particularly successful example of such a development is the PGN (Pandonia Global Network) which, for about a decade, operationally deploys a continuously growing fleet of Pandora instruments worldwide.

While operational monitoring calls for harmonization of both instruments and data retrievals methods, research activities aiming at improving measurement techniques and extending the range of possible applications imply the continuous development and operation of a large variety of instrumental designs. The need to assess the consistency of existing UV-Vis instruments operated in large-scale infrastructures such as the Network for Detection of Stratospheric Composition Changes (NDACC), PGN or the pan-European ACTRIS research infrastructure (RI) has led to the regular organisation of formal intercomparisons gathering as many different instruments as possible. The first Cabauw Intercomparison of NO<sub>2</sub> measuring Instruments (CINDI) was organised in 2009 under the auspices of ESA, NDACC and the EU GEOMON project to provide an assessment of the status of the capabilities for NO<sub>2</sub> monitoring. Seven years after CINDI, the CINDI-2 campaign, held in September 2016, gathered 36 instruments from 24 different institutes resulting in a major assessment of the overall consistency of these systems for the measurement of several key atmospheric trace gas data products (NO<sub>2</sub>, HCHO and O<sub>3</sub>). Conclusions and recommendations arising from CINDI-2 and subsequent related studies were taken on-board for improving and standardising UV-Visible MAX-DOAS measurements, e.g. within the ESA-funded FRM4DOAS centralised data processing system which provides a service for MAX-DOAS data processing within NDACC and ACTRIS.

In the continuity of CINDI-2, the CINDI-3 intercomparison, which is being held under the umbrella of ESA, NDACC and ACTRIS, primarily aims at characterising the level of consistency between UV-Vis DOAS instruments operated worldwide and used for satellite validation and science investigations on atmospheric composition variability and trends. It also aims at a better understanding of the measurement technique and data evaluation approaches. As in previous intercomparison campaigns of the same type (see Kreher et al., 2020 and references therein), a semi-blind intercomparison protocol is adopted., i.e.:

- a) The data acquisition schedule applied by the participants is strictly prescribed to coordinate the timing and geometry of each individual measurement as exactly as possible, so that the same air mass could be measured by all instruments with good synchronisation.
- b) For each data product, a set of retrieval settings and parameters is prescribed. These are mandatory for participation in the semi-blind exercise.

- c) All slant column data sets measured during the previous day are submitted to an independent campaign referee every morning. At daily meetings in the afternoon, comparison results of the slant column measured the previous day are displayed anonymously, i.e. without assignment to the different instruments.

In comparison to CINDI-2, CINDI-3 incorporates a series of new activities and focused work, as detailed below:

- Airborne deployment: in conjunction with ground-based measurements performed on the Cabauw site, the BN-2 aircraft from the Belgian Coast Guard equipped with the SWING NO<sub>2</sub> whiskbroom imager and NO<sub>x</sub>, NO<sub>2</sub> and O<sub>3</sub> in-situ sensors will be operated for a series of 6-7 flights planned over Cabauw and the Rotterdam areas. The aim is to better document the spatial variability of NO<sub>2</sub> around the site and its impact on remote-sensing measurements. The synergy with mobile measurements systems available for the campaign will be fully exploited.
- On-site calibration: each instrument will undergo a set of calibration tests to be performed on-site according to a calibration protocol.
- Target species: in comparison to CINDI-2, three additional species (CHOCHO, HONO and BrO) will be included in the semi-blind slant column intercomparison.
- FRM4DOAS on-site data processing: in parallel to data evaluations performed by individual groups, the FRM4DOAS centralised processing system will be run on spectra measured by each instrument and the resulting slant columns and vertical columns will be intercompared, providing an alternative picture on the consistency of the reported measurements.
- O<sub>3</sub> measurement focus: while previous CINDI campaigns had a primary focus on NO<sub>2</sub> measurements, CINDI-3 will add a second focus on ozone measurements, both in terms of total columns and vertical profile information. This activity will be supported by Brewer and tropospheric ozone lidar measurements.

This document presents the overall schedule and plans for the semi-blind intercomparison exercise. Details and instructions are provided for:

- data acquisition
- slant column retrieval settings
- output file format for both static and mobile DOAS measurements
- semi-blind intercomparison protocol

## 2 Schedule

The schedule of the CINDI-3 campaign is represented graphically in Figure 1. It starts on 21<sup>st</sup> of May 2024 with one week dedicated to instrument installation, testing and various calibration activities. This is followed by three weeks of intensive measurements. This period includes two full weeks of semi-blind intercomparison according to a protocol like the one defined for previous UV-Vis intercomparison campaigns (see Kreher et al., 2020, and references therein). Upon necessity (e.g. in case of persisting bad weather conditions during the nominal intensive measurement phase), the semi-blind intercomparison can be extended until the 16<sup>th</sup> of June at the latest. If not required, this additional week will be used for extra measurements addressing science topics to be agreed on during the campaign. The latter activities could also be extended in a last week of measurements ending on 21<sup>st</sup> of June 2024.

## MAY 2024

SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY
19	20	21	22	23	24	25
Whit Sunday	Whit Monday	Build-up/preparation	Build-up/preparation	Build-up/preparation	Build-up/preparation	Build-up/preparation
26	27	28	29	30	31	1
Build-up/preparation	Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase	

## JUNE 2024

SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY
26	27	28	29	30	31	1
						Intensive phase
2	3	4	5	6	7	8
Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase
9	10	11	12	13	14	15
Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase	Intensive phase
16	17	18	19	20	21	22
Intensive phase	Optional extension	Optional extension	Optional extension	Optional extension	Optional extension	Site cleanup
23	24	25	26	27	28	29
Site cleanup	Site cleanup	Site cleanup	Site cleanup	Site cleanup	Site cleanup	

**Figure 1:** Schedule of the CINDI-3 campaign. The intensive phase includes a minimum of two full weeks of semi-blind intercomparison with possible extension until 16 June depending on the weather conditions.

### 3 Campaign setup



Like for CINDI-2, the local organisation of CINDI-3 is managed by KNMI under the lead of Arnoud Apituley (photo). To allow for optimal synchronisation of the measurements, all the spectrometers participating in the intercomparison exercise are installed near each other on the remote-sensing site (RSS) of the CESAR station (see Figure 2). To achieve this, containers are temporarily installed for the campaign period. The rationale behind this setup is to arrange the instruments to minimise ambiguity in air masses observed simultaneously by all spectrometers. Combined with the adoption of a strict data acquisition protocol (see section 6), this arrangement minimizes the impact of fast changes in the local concentration of measured gases (e.g. NO<sub>2</sub>) on the comparisons.

The setup envisaged for CINDI-3 is like the one adopted for CINDI-2. Considering the large number of systems to be accommodated, two rows of containers will be deployed. The bottom row of containers is predominantly used to host 1-D MAX-DOAS and zenith-sky instruments while the second row is deployed on top of the first one, with the stacked double containers providing additional height. All 2-D MAX-DOAS systems should be installed on the roof of the top-level containers allowing for more flexibility on the azimuth scan settings and avoiding any risk of interference with the 1-D systems.

Like for CINDI-2, all the 1-D MAX-DOAS instruments will use the same azimuth viewing direction of 287° (i.e. approximately WNW) which provides an unobstructed view to the horizon. This direction is also the preferential direction used by the 2-D MAX-DOAS systems (see section 6).



**Figure 2:** The CINDI-2 container layout at the CESAR Remote-Sensing Site (RSS). The picture shows the organisation of the MAX-DOAS instruments on two superposed rows of containers.

**Coordinates of the site:**

Measurement Tower: 51.97038 °N, 4.92625 °E

Remote Sensing Site: 51.96800 °N, 4.92900 °E

## 4 Participating instruments

The UV-Vis DOAS instruments registered for participation to the CINDI-3 campaign are listed in Table 1 and Table 2. Most of them are two-dimensional MAX-DOAS systems scanning the sky in both elevation and azimuth. In some cases (e.g. Pandora instruments), direct-sun observations can also be performed. Next to 2D-MAXDOAS systems, also one-dimensional MAX-DOAS systems performing elevation scans in one fixed azimuthal direction are deployed and 4 zenith-sky systems.

In Table 3, we also provide a list of the mobile DOAS systems that will be used for various purposes during the campaign. Note that a complete set of instrumental data sheets with more detailed information on each system can be found on the campaign data repository (<https://knmi.data.surfsara.nl/index.php/login>).

**Table 1:** One-dimensional MAX-DOAS spectrometers participating to the CINDI-3 campaign. The first column lists the identification numbers that were assigned by the local organisation (KNMI) to the various instruments. These numbers uniquely identify each instrument and should be used throughout the campaign, e.g. for data reporting (see section 8).

#	Institute acronym	Instrument PI	Instrument type	Elev FOV (°)	Spectral range	ISRF FWHM (nm)	Det. Temp (°C)
01	UOM	Rob Ryan	SkySpec-1D	0.3	300-460 nm	0.6	20
02	ABOM	Rob Ryan	SkySpec-1D	0.3	300-460 nm	0.6	20

03	KNMI	Ankie PETERS	SkySpec-1D	0.3	300-460 nm	0.6	20
04	KNMI	Ankie PETERS	Mini-DOAS Hoffmann	0.45	290-433 nm	0.6	25
				0.4	400-600 nm	0.5	25
05	MPIC	Thomas Wagner	Tube-DOAS	0.6	300-460 nm	0.65	20
06	UOT	Ramina Alwarda	SkySpec-1D	0.3	300-460 nm	0.6	20
07	SUWON	Hyeong-Ahn Kwon	SkySpec-1D	0.3	300-460 nm	0.6	20
14	LMU	Mark Wenig	SkySpec-1D	0.3	300-460 nm	0.6	20
26	IUPB	Kai Krause	Rapid DOAS	n/a	305-550 nm	0.8	RT*
08	LATMOS	Andrea Pazmino	SAOZ	10	270-640 nm	1.37	RT
09	LATMOS	Andrea Pazmino	Mini-SAOZ #1	8	270-820 nm	0.71	RT
10	LATMOS	Andrea Pazmino	Mini-SAOZ #2	8	270-820 nm	0.75	RT
11	EVORA	Daniele Bortoli	SPATRAM-1	2.0	300-400 nm	0.5	-20
					400-600 nm	0.65	
17	AIOFM	Yuhan Luo	2D-MAXDOAS	0.5	290-420 nm	0.55	25

\* Room temperature

**Table 2** : Two-dimensional MAX-DOAS spectrometers.

#	Institute	Instrument PI	Instrument type	DS (Y/N)	Elev FOV (°)	Spectral range	ISRF FWHM (nm)	Det. T (°C)
15	AIOFM	Ang Li	2D-MAXDOAS	N	0.5	290-450 nm	0.85	25
16	AIOFM	Pinhua Xie	2D-MAXDOAS	N	TBD	290-420 nm	0.35	25
18	AUTH	Dimitris Karagkiozidis	PHAETHON	Y	1	280-539 nm	0.55	10
19	AUTH	Dimitris Karagkiozidis	DELTA	Y	0.8	305-523 nm	0.85	-50
						335-385 nm	0.4	
20	BIRA	Alexis Merlaud	2D-MAXDOAS	Y	0.5	304-383 nm	0.35	-50
						402-543 nm	0.5	
21	BIRA	Alexis Merlaud	SkySpec-2D	Y	0.3	296-459 nm	0.5	20
						408-553 nm	0.6	
22	BIRA	Gytha Mettepenningen	SEMPAS	N	0.3	TBD	0.6	-50
23	BIRA	Cedric Busschots	NO <sub>2</sub> camera	N	0.04	430-470 nm	0.6-0.8	~0
24	ISAC	Elisa Castelli	SkySpec-2D	Y	0.3	300-405 nm	0.45	20
						405-565 nm	0.6	
25	IUPB	Kai Krause	2D-MAXDOAS	N	1	305-390 nm	0.5	-35
						406-579 nm	0.85	
27	IUPB	Kai Krause	IMPACT	N	0.8	TBD	0.5	-30
28	IUPH	Udo Frieß	SkySpec-2D	Y	0.3	296-459 nm	0.5	20
						408-553 nm	0.6	
29	IUPH	Udo Frieß	PMAX-DOAS	N	0.26	285-565 nm	1.3	-28
30	INTA	Monica Navarro	RASAS-III	N	0.5	422-539 nm	0.6	-30
32	AIRYX	Johannes Lampel	SkySpec-2D	Y	0.3	299-409 nm	0.45	20
						408-554 nm	0.56	
33	RAL	Ka Lok Chan	SkySpec-2D	N	0.3	310-410 nm	0.45	20

						405-550 nm	0.6	
34	KNMI	Ankie Piters	Pandora-1S	Y	1.5	280-540 nm	0.6	15
35	LBLICK	Alexander Cede	Pandora-1S	Y	1.5	280-540 nm	0.6	15
36	LBLICK	Alexander Cede	Pandora-1S	Y	1.5	280-540 nm	0.6	15
37	LBLICK	Alexander Cede	Pandora-1S	Y	1.5	280-540 nm	0.6	15
38	LBLICK	Alexander Cede	Pandora-1S	Y	1.5	280-540 nm	0.6	15
39	USTC	Cheng Liu	SkySpec-2D	N	0.3	310-410 nm 405-550 nm	0.45 0.6	20
40	PKNU-NIER	Gyeong Park/ Hyunkee Hong	AQ-Profiler	N	2.2	280-795 nm	0.5	20

**Table 3** : Mobile DOAS instruments.

#	Institute acronym	Instrument PI	Instrument type	Elev FOV (°)	Spectral range	ISRF FWHM (nm)	Det. Temp (°C)
14	LMU-RAL	Mark Wenig/ Ka Lok Chan	SkySpec-1D (in car-DOAS configuration)	0.3	300-460 nm	0.6	20
50 51	IUPB	Kai Krause	Car-DOAS (double channel system, zenith + adjustable elev.)	10	305-550 nm	0.8	20
52	MPIC	Steffen Ziegler	Tube-DOAS #1 (1D scanner)	0.6	300-460 nm	0.65	20
53	MPIC	Steffen Ziegler	Tube-DOAS #2 (1D scanner)	0.6	300-460 nm	0.65	20
54	BIRA	Alexis Merlaud	Aeromobil (double channel system, zenith + 30° elev.)	2.5	195-755 nm	1.15	RT
55	BIRA	Michel Van Roozendaal	Bike-DOAS (zenith only)	5.0	280-547 nm	0.6	RT
56	UNAM	Claudia Rivera Cardenas	Car-DOAS (zenith only)	n/a	356-510 nm	0.6	RT
	VT	Elena Lind	Pandora-1S (operated on MAMS)	1.5	280-540 nm	0.6	15

## 5 Semi-blind Intercomparison Referee



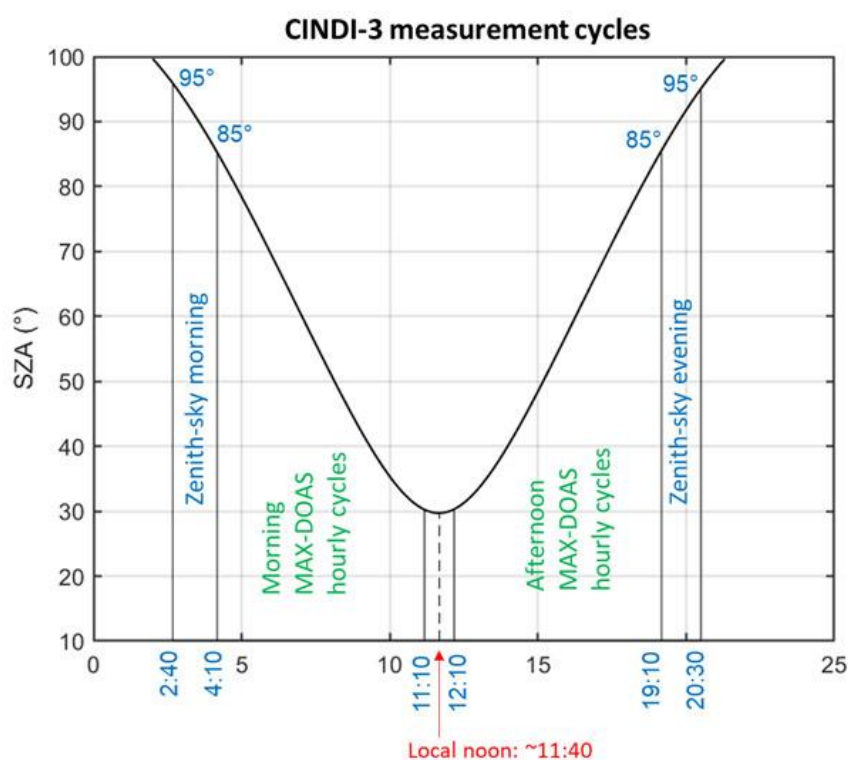
The CINDI-3 semi-blind intercomparison exercise will be coordinated by Karin Kreher (BK Scientific, photo) assisted by Martina M. Friedrich (BIRA-IASB). Karin Kreher has over 20 years of experience in UV-Visible remote-sensing trace gas retrieval and is acting as co-chair of the NDACC UV-Vis working group. She was referee of the CINDI-2 intercomparison campaign (Kreher et al., 2020) and was involved in several of the NDACC/NDACC intercomparison campaigns since the early nineties. Martina M. Friedrich has developed the MMF MAX-DOAS vertical profiling code and has extensive experience in DOAS measurements and data analysis.

The roles of the CINDI-3 referee, and her assistant are to (1) interface with the participating groups and support them in their data reporting tasks, (2) manage on-site data collection, (3) organise daily meetings and report on campaign progress, and (4) coordinate the writing of a peer-review publication on the intercomparison results.

## 6 Data Acquisition Protocol

Based on experience gained from previous intercalibration campaigns, it has been shown that the level of agreement achievable between MAX-DOAS sensors depends on the level of spatial and temporal synchronization between the different instruments. This issue is particularly critical for tropospheric NO<sub>2</sub> comparisons, given the high variability of this pollutant.

CINDI-3 therefore adopts a data acquisition protocol similar to the one developed with success during the CINDI-2 campaign in 2016 (see Kreher et al., 2020), i.e. all instruments will be setup on the same observation platform (a set of containers deployed on the Remote-Sensing Site of the Cabauw Observatory) and arranged in such a way that the same air masses can be observed by all of them (see Section 3). To further constrain the synchronicity of the measurements, a strict protocol on the timing of the spectral acquisition is imposed.



**Figure 3:** Mean diurnal variation of the solar zenith angle (SZA) at Cabauw during the CINDI-3 period (21 May – 21 June 2024). The different measurement periods are indicated below the curve. Time is given in UTC.

The settings for MAX-DOAS and zenith-sky DOAS data acquisition are described below. They are similar to those used for CINDI-2, but not identical. Main changes address:

- The change of the season: CINDI-3 will take place in late May – early June, i.e. close to the summer solstice, resulting in longer days and higher sun elevation at noon.
- An additional focus on direct-sun measurements, which were not part of the semi-blind intercomparison during CINDI-2
- Azimuth scans limited to a fixed elevation angle (provisionally 2°)

- A better overlap between the different systems (1D & 2D MAX-DOAS, SAOZ)
- One free sequence of 10' every hour, allowing for non-standard measurements, e.g. elevation scans in different azimuths, almucantar scans, etc

Like for CINDI-2, the reference azimuth direction to be used for comparison of 1D and 2D systems is 287° North, i.e. the west-north-westerly direction. The convention for the azimuth angle is 0° for North, 90° for East, etc.

We also keep distinguishing between twilight (morning and evening) and daytime conditions, for which separate data acquisition protocols are prescribed. According to the geometry of the solar position during the campaign (see Figure 3), the daytime period is set between 4:10 UTC and 19:10 UTC. During this period, we define 7 hourly cycles in the morning, one noon cycle and 7 hourly cycles in the afternoon.

## 6.1 Zenith-sky twilight observations

This protocol holds for all instruments contributing to the zenith-sky NDACC-type intercomparison of stratospheric measurements at twilight.

For measurements at sunrise, 45 acquisitions shall be recorded with a duration of 120s each, the first one starting at 02:40:00 UTC and the last one starting at 04:08:00 UTC.

For measurements at sunset, 41 acquisitions shall be recorded with the same accumulation time (120s), the first one starting at 19:10:00 UTC and the last one starting at 20:30:00 UTC.

## 6.2 Dark current measurements

Half an hour after the end of the sunset sequence of zenith-sky observations, i.e. starting at 21:00:00 UTC, record a set of dark current measurements covering the full range of exposure times used during the day.

## 6.3 MAXDOAS and zenith-sky observations during the day

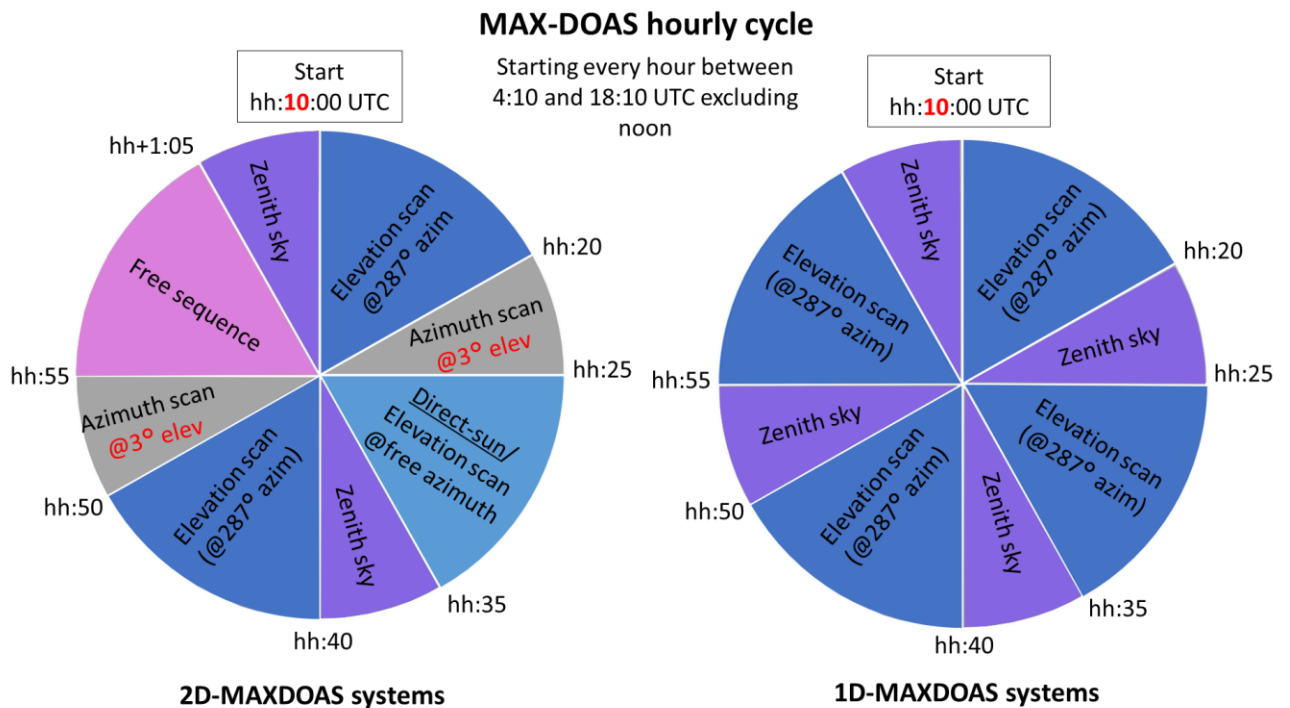
For daytime observations starting at 04:10:00 UTC and ending at 19:09:59 UTC the following hourly sequences shall be followed:

- For 1D-MAXDOAS systems (pointing azimuth direction: 287°):
  - 4 elevation scans of 10 minutes each, alternating with 4 sequences of 5 minutes each for zenith-sky measurements.
  - Elevation scans consist of the following angles: -2, 1, 2, 3, 4, 6, 8, 15, 30, 90°
  - Duration of each single acquisition: 1 minute.
- For 2D-MAXDOAS systems:
  - 2 elevation scans of 10' in the reference pointing azimuth of 287°, elevation scans consist of the following angles: -2, 1, 2, 3, 4, 6, 8, 15, 30, 90°
  - After each of these elevation scans, one azimuthal scan of 5' at a fixed elevation angle (provisionally 2°) using a predefined set of azimuth angles. The angles used during CINDI-2 were: 45, 95, 135, 195, 245, 287, 355°. Up to 10 angles can possibly be included in the total sequence of 5' (using an acquisition time of 30 sec), however the time needed to move the scanner back to the reference azimuth direction at the

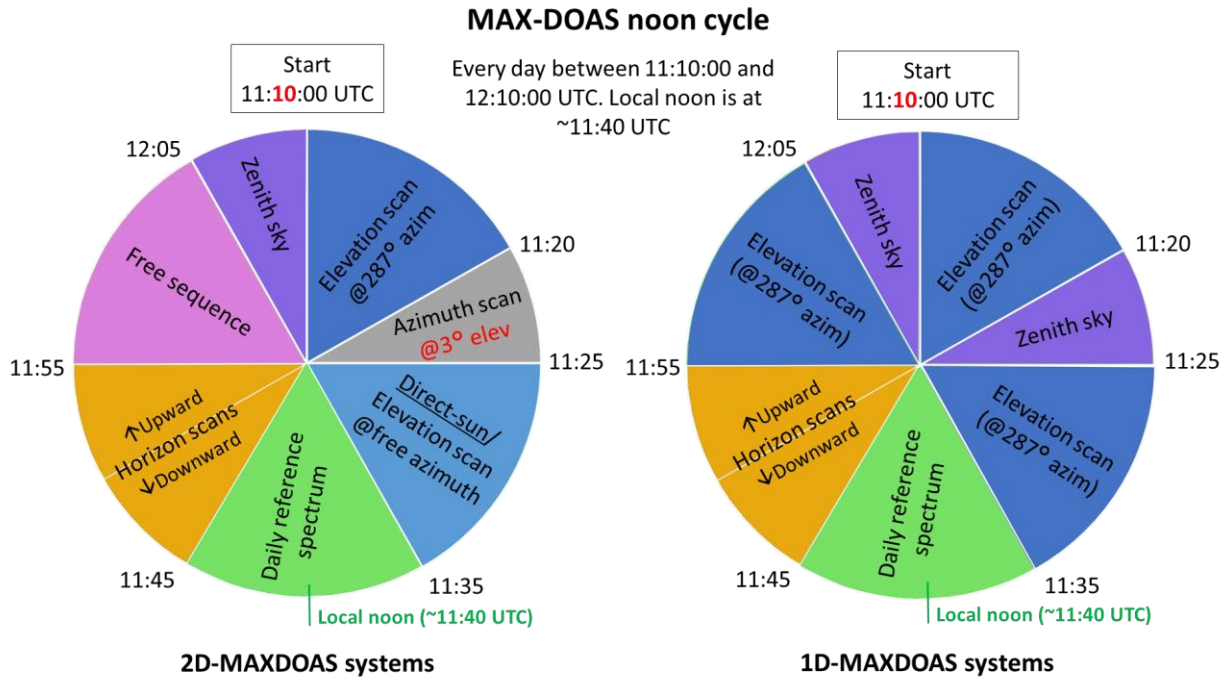
end of the sequence must be taken into account, which might be a limiting factor for some instruments.

- 2 sequences of 5' for zenith-sky measurements.
- 1 sequence of 10' for direct-sun measurements (for instruments equipped with a sun-tracker), or an elevation scan at a free azimuth angle.
- 1 sequence of 10' reserved for free measurements.
- Duration of each single acquisition in zenith mode and during elevation scans: 1 minute.
- For azimuth scans and direct-sun measurements, use an acquisition time of 30 sec.
- For zenith-sky DOAS systems:
  - Zenith measurements of one minute (acquisition time) shall be performed during the whole day from 04:10:00 UTC to 19:09:59 UTC.

These data acquisition schemes are described in tabular form in Table 4 and Table 5, and graphically in Figure 4 and Figure 5.



**Figure 4: Graphical representation of the CINDI-3 data acquisition hourly cycles for 1D- and 2D-MAXDOAS systems.**



**Figure 5:** Graphical representation of the CINDI-3 data acquisition noon cycle for 1D- and 2D-MAXDOAS systems.

**Table 4:** Data acquisition scheme for daytime conditions at the following UTC times (hh in the Table): 04, 05, 06, 07, 08, 09, 10, 12, 13, 14, 15, 16, 17, 18h.

TIME (UTC)	2D-MAXDOAS		1D-MAXDOAS	Zenith
	Azimuth(°)	Elevation (°)	Pointing direction : 287°	
hh:10:00	287	-2	-2	90
	287	1	1	90
	287	2	2	90
	287	3	3	90
	287	4	4	90
hh:15:00	287	6	6	90
	287	8	8	90
	287	15	15	90
	287	30	30	90

	287	90	90	90
hh:20:00	<b>Azimuthal scan</b> at fixed elevation (3°) with 30 sec integration time per acquisition		90	90
			90	90
			90	90
			90	90
			90	90
hh:25:00	<b>Direct-sun measurements</b> with 30 sec integration time per acquisition.  For 2D-MAXDOAS instruments not equipped with a suntracker, start with a zenith-sky acquisition and perform elevation scan in free azimuthal direction.		-2	90
			1	90
			2	90
			3	90
			4	90
hh:30:00			6	90
			8	90
			15	90
			30	90
			90	90
hh:35:00	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
hh:40:00	287	-2	-2	90
	287	1	1	90
	287	2	2	90
	287	3	3	90

	287	4	4	90
hh:45:00	287	6	6	90
	287	8	8	90
	287	15	15	90
	287	30	30	90
	287	90	90	90
hh:50:00	<b>Azimuthal scan</b> at fixed elevation (3°) with 30 sec integration time per acquisition		90	90
			90	90
			90	90
			90	90
			90	90
hh:55:00	<b>Free acquisition sequence</b>  Can be filled with direct-sun measurements, almucantar scans or elevation scans in free azimuthal directions. In the latter case, start with a zenith-sky acquisition.		-2	90
			1	90
			2	90
			3	90
			4	90
(hh+1):00:00			6	90
			8	90
			15	90
			30	90
			90	90
(hh+1):05:00	287	90	90	90
	287	90	90	90
	287	90	90	90

	287	90	90	90
	287	90	90	90

**Table 5:** Data acquisition scheme for noon conditions between 11:10:00 UTC and 12:10:00 UTC. It includes a zenith-only acquisition sequence between 11:35:00 and 11:50:00 UTC and a horizon scan between 12:05:00 and 12:44:00 UTC.

TIME (UTC)	2D-MAXDOAS		1D-MAXDOAS	Zenith
	Azimuth(°)	Elevation (°)		
11:10:00	287	-2	-2	90
	287	1	1	90
	287	2	2	90
	287	3	3	90
	287	4	4	90
11:15:00	287	6	6	90
	287	8	8	90
	287	15	15	90
	287	30	30	90
	287	90	90	90
11:20:00	<b>Azimuthal scan</b> at fixed elevation (3°) with 30 sec integration time per acquisition		90	90
			90	90
			90	90
			90	90
			90	90
11:25:00	<b>Direct-sun measurements</b> with 30 sec integration time per acquisition.		-2	90
			1	90

	For 2D-MAXDOAS instruments not equipped with a suntracker, start with a zenith-sky acquisition and perform elevation scan in free azimuthal direction.			
			2	90
			3	90
			4	90
11:30:00			6	90
			8	90
			15	90
			30	90
			90	90
11:35:00	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
hh:40:00	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
11:45:00	287	Horizon scans between -5° and +5° above the horizon with a step of 0.2° between -2 and +2° and a step of 1° outside this range. 10s per acquisition. If time allows, perform a double scan up and down.		90
	287			90
	287			90
	287			90
	287			90
11:50:00	287			90

	287			90
	287			90
	287			90
	287			90
11:55:00	<b>Free acquisition sequence</b> Can be filled with direct-sun measurements, almucantar scans or elevation scans in free azimuthal directions. In the latter case, start with a zenith-sky acquisition.		-2	90
			1	90
			2	90
			3	90
			4	90
12:00:00			6	90
			8	90
			15	90
			30	90
			90	90
12:05:00	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90
	287	90	90	90

## 7 Target species and slant column retrieval settings

The semi-blind intercomparison exercise focuses on data products of relevance for satellite validation and NDACC operation continuity. These products are listed in Table 6. Note that it is not mandatory to provide results for all data products. Depending on the specific characteristics of their instrumentation, participants are free to contribute only a subset of the data products. This will be communicated to the campaign referee ahead of the comparison exercise.

**Table 6:** Data products to be included in the semi-blind intercomparison exercise.

Data product	Abbreviation	Fitting range
NO <sub>2</sub> (VIS range)	NO2VIS	425.0 – 490.0 nm
NO <sub>2</sub> (alternative VIS range)	NO2VIS-SMALL	411.0 – 445.0 nm
NO <sub>2</sub> (UV range)	NO2UV	338.0 – 370.0 nm
O <sub>4</sub> (VIS range)	O4VIS	425.0 – 490.0 nm
O <sub>4</sub> (UV range)	O4UV	338.0 – 370.0 nm
HCHO	HCHO	336.5 – 359.0 nm (daily noon reference) 324.5 – 359.0 nm (sequential reference)
HONO	HONO	335.0 – 373.0 nm
CHOCHO	CHOCHO	436.0 – 468.0 nm
O <sub>3</sub> (Chappuis bands)	O3VIS	450.0 – 540.0 nm
O <sub>3</sub> (Huggins bands)	O3UV	320.0 – 340.0 nm
BrO	BRO	346.0 – 359.0 nm

For instruments performing direct-sun measurements, all spectral windows defined in Table 6 can also be applied in direct-sun mode, but using a fixed reference spectrum that will be selected in the beginning of the campaign.

In addition to these settings, we propose 4 additional windows with different settings for direct sun only. **These settings are optional and not required for participation to the semi-blind intercomparison.**

Three of them use the Chance-spectrum as a reference, since it would probably be very interesting to see how different instruments behave in this case. One is a short UV O<sub>3</sub>/SO<sub>2</sub> fitting window, which for pandora instruments gives very good results for O<sub>3</sub>, O<sub>3</sub>temp and SO<sub>2</sub>.

**Table 7 :** Optional direct sun-only data products.

Data product	Abbreviation	Fitting range
NO <sub>2</sub> using external reference spectrum	NO2EXT	430.0 – 470.0 nm
H <sub>2</sub> O using external reference spectrum	H2OEXT	492.0 – 510.0 nm
O <sub>3</sub> using external reference spectrum	O3EXT	305.0 – 325.0 nm
SO <sub>2</sub> in the UV	SO2UV	306.0 – 326.4 nm

## 7.1 Absorption cross-sections

A data base of absorption cross-sections has been prepared, based on references listed in Table 8. This database is available on the KNMI SURF repository.

**Table 8:** List of absorption cross-sections used in the semi-blind intercomparison exercise. Note that all spectral data are given in air wavelengths.

<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014), with pre-shift of +0.003nm
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014), with pre-shift of +0.003nm
<b>O<sub>4</sub> (223 K)</b>	Thalman and Volkamer (2013)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022), and (for O3VIS) Thalman and Volkamer (2013)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>H<sub>2</sub>O (UV)</b>	Polyansky et al. (2016) scaled by 2.6 (Lampel et al., 2017)
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>CHOCHO (296 K)</b>	Volkamer et al. (2005)
<b>SO<sub>2</sub> (298K)</b>	Vandaele et al. (2009)

## 7.2 Solar reference

As solar reference for wavelength calibration and other corrections, we use the solar atlas compiled by Chance and Kurucz (2010) (<https://doi.org/https://doi.org/10.1016/j.jqsrt.2010.01.036>)

## 7.3 Retrieval settings in the visible range

Note: the “Fixed reference spectrum” mentioned for direct sun retrievals will be a measured direct sun spectrum around noon from one of the first clear sky days.

**Table 9:** DOAS settings for NO<sub>2</sub>VIS and O<sub>4</sub>VIS

<b>Wavelength range</b>	425.0-490.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ), orthogonalized to NO <sub>2</sub> (294 K)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>O<sub>4</sub> (223 K)</b>	Finkenzeller et al. (2022), orthogonalized to O <sub>4</sub> (293K)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009)
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Constant
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 10:** DOAS settings for NO<sub>2</sub>VIS-SMALL (alternative VIS range)

<b>Wavelength range</b>	411.0-445.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ) orthogonalized to NO <sub>2</sub> (294 K)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009)
<b>Polynomial degree</b>	Order 4 (5 coefficients)
<b>Intensity offset</b>	Constant
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 11:** DOAS settings for CHOCHO

<b>Wavelength range</b>	436.0-468.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>CHOCHO (296 K)</b>	Volkamer et al. (2005)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ), orthogonalized to NO <sub>2</sub> (220 K)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009)
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Slope (order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 12:** DOAS settings for O<sub>3</sub>VIS

<b>Wavelength range</b>	450.0-540.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014), orthogonalized to O <sub>3</sub> (223 K)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ), orthogonalized to NO <sub>2</sub> (220 K)
<b>O<sub>4</sub> (293 K)</b>	Thalman and Volkamer (2013)
<b>O<sub>4</sub> (203 K)</b>	Thalman and Volkamer (2013), orthogonalized to O <sub>4</sub> (293 K)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009)
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity off-set</b>	Slope (Order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 13:** DOAS settings for NO2EXT (direct sun only)

<b>Wavelength range</b>	430.0-470.0 nm
<b>Fraunhofer reference spectra</b>	Chance and Kurucz (2010)
<b>Cross-sections:</b>	
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Polynomial degree</b>	Order 4 (5 coefficients)
<b>Intensity offset</b>	Constant
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 14:** DOAS settings for H2OEXT (direct sun only)

<b>Wavelength range</b>	492.0-510.0 nm
<b>Fraunhofer reference spectra</b>	Chance and Kurucz (2010)
<b>Cross-sections:</b>	
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014)
<b>H<sub>2</sub>O</b>	HITRAN2012 (Rothman et al., 2013)
<b>Polynomial degree</b>	Order 2 (3 coefficients)
<b>Intensity offset</b>	None
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

## 7.4 Retrieval settings in the UV range

Notes:

- like for VIS retrievals, the “Fixed reference spectrum” mentioned for direct sun retrievals will be a measured direct sun spectrum around noon from one of the first clear sky days.
- For the slope term on the Ring effect, please use an additional cross-section obtained by multiplying the convolved differential Ring cross-section by the term  $(\lambda - \lambda_0)$ , where  $\lambda_0$  is the center wavelength of the fit interval.

**Table 15:** DOAS settings for NO2UV and O4UV

<b>Wavelength range</b>	338.0-370.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ) orthogonalized to NO <sub>2</sub> (294 K)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ) orthogonalized to O <sub>3</sub> (223 K)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Slope (order 1)

<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch
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**Table 16:** DOAS settings for HCHO (sequential reference spectrum)

<b>Wavelength range</b>	324.5-359.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: sequential reference spectrum
<b>Cross-sections:</b>	
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with $I_0$ correction (SCD of $10^{17}$ molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> ) orthogonalized to O <sub>3</sub> (223 K)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Slope (order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 17:** DOAS settings for HCHO (noon reference spectrum)

<b>Wavelength range</b>	336.5-359.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with $I_0$ correction (SCD of $10^{17}$ molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> ) and Taylor terms (Pukite et al., 2010)
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> ) orthogonalized to O <sub>3</sub> (223 K)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Slope (order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 18:** DOAS settings for HONO

<b>Wavelength range</b>	335.0-373.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>HONO (296 K)</b>	Stutz et al. (2000)
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with $I_0$ correction (SCD of $10^{17}$ molecules/cm <sup>2</sup> ) and Taylor terms (Pukite et al., 2010)
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with $I_0$ correction (SCD of $10^{17}$ molecules/cm <sup>2</sup> ) orthogonalized to NO <sub>2</sub> (294 K)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with $I_0$ correction (SCD of $10^{20}$ molecules/cm <sup>2</sup> ) orthogonalized to O <sub>3</sub> (223 K)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)

<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>H<sub>2</sub>O (UV)</b>	Polyansky et al. (2016) scaled by 2.6 (Lampel et al., 2017)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 5 (6 coefficients)
<b>Intensity offset</b>	Slope (order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 19:** DOAS settings for O3UV

<b>Wavelength range</b>	320.0-340.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ) with Taylor terms (Pukite et al., 2010)
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ). For this term, use the difference between O <sub>3</sub> (243K) and O <sub>3</sub> (223K)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 3 (4 coefficients)
<b>Intensity offset</b>	Slope (Order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 20:** DOAS settings for BrO

<b>Wavelength range</b>	346.0-359.0 nm
<b>Fraunhofer reference spectra</b>	MAX-DOAS: daily noon reference spectrum (11:35 - 11:45 UTC)
<b>Cross-sections:</b>	
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>NO<sub>2</sub> (220 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ) and Taylor terms (Pukite et al., 2010)
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ), orthogonalized to O <sub>3</sub> (223K)
<b>O<sub>4</sub> (293 K)</b>	Finkenzeller et al. (2022)
<b>Ring</b>	Normalised Ring spectrum based on Wagner et al. (2009) and slope term
<b>Polynomial degree</b>	Order 2 (3 coefficients)
<b>Intensity offset</b>	Slope (order 1)
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 21 :** DOAS settings for O3EXT (direct sun only)

<b>Wavelength range</b>	305.0-325.0 nm
<b>Fraunhofer reference spectra</b>	Chance and Kurucz (2010)
<b>Cross-sections:</b>	
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ) with Taylor terms (Pukite et al., 2010)
<b>SO<sub>2</sub> (298 K)</b>	Vandaele et al. (2009)
<b>Polynomial degree</b>	Order 3 (4 coefficients)
<b>Intensity offset</b>	None
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

**Table 22:** DOAS settings for SO<sub>2</sub>UV (direct sun only)

<b>Wavelength range</b>	306.0-326.4 nm
<b>Fraunhofer reference spectra</b>	Fixed reference spectrum
<b>Cross-sections:</b>	
<b>HONO (296 K)</b>	Stutz et al. (2000)
<b>HCHO (298 K)</b>	Meller and Moortgat (2000)
<b>NO<sub>2</sub> (294 K)</b>	Vandaele et al. (1998) with I <sub>0</sub> correction (SCD of 10 <sup>17</sup> molecules/cm <sup>2</sup> ) and Taylor terms (Pukite et al., 2010)
<b>O<sub>3</sub> (223 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> )
<b>O<sub>3</sub> (243 K)</b>	Serdyuchenko et al. (2014) with I <sub>0</sub> correction (SCD of 10 <sup>20</sup> molecules/cm <sup>2</sup> ) orthogonalized to O <sub>3</sub> (223 K)
<b>BrO (223 K)</b>	Fleischmann et al. (2004)
<b>Polynomial degree</b>	Order 4 (5 coefficients)
<b>Intensity offset</b>	Constant
<b>Shift and stretch</b>	Each measured spectrum is aligned on the reference using shift and stretch

## 8 Output file data format for static DOAS instruments

The output data file format used for the semi-blind intercomparison is an adaptation of the CINDI-2 format, which itself was based on the ascii-text format used during the MADCAT campaign (Peters et al., 2017).

The granularity is one file per day and per data product as listed in Table 6. The file header includes all necessary information on instrument and data provider, column content, and DOAS settings. A full description of both format and file naming convention is given in Appendix A. An example file is also provided.

We request that each participating group submit a test output file, for at least one data product. Please send this material to Martina Friedrich at BIRA-IASB ([martina.m.friedrich@aeronomie.be](mailto:martina.m.friedrich@aeronomie.be)) with cc to Michel van Roozendael ([michelv@aeronomie.be](mailto:michelv@aeronomie.be)) and Karin Kreher ([karin.kreher@bkscientific.eu](mailto:karin.kreher@bkscientific.eu)).

## 9 Output file data format for mobile DOAS measurements

The output data file format used for mobile DOAS instruments follows the same structure as the one defined for static measurements, with some adaptations that are described in Appendix B.

## 10 Daily workshops

For the duration of the semi-blind intercomparison, daily briefings will be organised in a dedicated cabin at around 16:00 local time (TBC). These meetings will be hybrid to allow for non-physical participation. As in previous campaigns, the aim of these daily workshops is to provide information on the status of the intercomparison and to discuss various scientific, organisational, or logistical topics. The daily meetings are coordinated by the campaign referee (Karin Kreher).

Each day in the morning, participants are requested to deliver slant column datasets retrieved from their instrument(s) for the preceding day. The data format will be checked until 11:10 and if inconsistencies are found, the data provider is informed and asked to submit a corrected version. This allows for the inclusion of these data in daily overview plots to be prepared by the campaign referee

and displayed at the daily meetings. Following the CINDI-3 semi-blind comparison protocol, measurement results are displayed in a non-nominative way. In case data cannot be submitted in time for a given day, they won't be part of the on-site comparison for that particular day, but it will be possible to include them for further processing after the end of the campaign.

Figures to be displayed at the daily meetings are under the responsibility of the campaign referee.

## 11 Semi-blind Intercomparison Data Protocol

We request that all participants read and sign the CINDI-3 Semi-blind Intercomparison Data Protocol for approval. It is annexed to this document (see Appendix C).

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# Appendix A: Description of the output file format for static DOAS measurements

## A) File name convention

The file name is constructed from the following parts, with "\_" as the delimiter. Please do not use "\_" in any of the separate fields. E.g. "BIRA\_IASB" is **NOT** acceptable as INSTITUTE, "BIRA-IASB" is fine.

INSTITUTE\_INSTRUMENTTYPE\_INSTRUMENTNUMBER\_DATAPRODUCT\_REFTYPE\_CAMPAIGNNAME\_DATE\_VERSION.asc

An example is:

BIRA\_MAXDOAS\_4\_NO2VIS\_DAILYREF\_CINDI3\_20240916\_v1.0.asc

INSTITUTE and INSTRUMENTNUMBER: use the institute acronyms and instrument numbers listed in Table 1 and Table 2.

INSTRUMENTTYPE: possible options are MAXDOAS, PANDORA and SAOZ

DATAPRODUCT: please use the abbreviations as listed in Table 5

REFTYPE: possible options are DAILYREF, SEQREF and DSREF, respectively for MAX-DOAS evaluations using daily noon reference spectra and sequential reference spectra, and direct-sun evaluations (using a fixed reference spectrum).

CAMPAIGNNAME: Please use CINDI3

DATE: use the format YYYYMMDD

VERSION: must be preceded by "v" and can contain one (not two) sub-version, i.e. "1.0" and "1" are both allowed. Version 1.11 would be considered newer than 1.9.

## B) Header

The header consists of three parts:

- 1) general file information
  - 2) retrieval information
  - 3) information on the data columns
- The *delimiter* in each of the three parts is a colon ":", the first two consist only of "key: value", ":" can be used in the value.
  - The *header identifier* (first character in each header line) is a percentage sign "%"
  - Use *utf-8 encoding* only, no special characters.

Below, each of the three parts are described in more detail:

### Part-1:

This consists of "key: value" pairs. The keys and values are not case-sensitive.

The following keys are mandatory:

- CAMPAIGNNAME
- SITE
- LATITUDE
- LONGITUDE
- ALTITUDE
- INSTITUTE
- INSTRUMENTTYPE
- INSTRUMENTNUMBER
- DATAPRODUCT
- PRODUCTDSCD
- REFTYPE
- Missing value
- Retrieval code
- Created by
- Version

Notes:

- The DATAPRODUCT matches the name in the file name.
- The PRODUCTDSCD contains the name of the DSCD of the product in the data, see the example file for details.
- Note that the fields INSTITUTE, INSTRUMENTTYPE, INSTRUMENTNUMBER, DATAPRODUCT, REFTYPE and Version are also used to create the file name.
- The version number must be preceded by "v" and can contain one (not two) sub-version, i.e. "1.0" and "1" are both allowed. It must agree with the version number in the file name.

### Part-2:

Start this with the line:

```
% Retrieval settings
```

This consists of "key: value" pairs. The keys and values are not case-sensitive.

The following keys are mandatory:

- FITTING WINDOW
- POLYNOMIAL DEGREE
- OFFSET ORDER
- REFERENCE SPECTRUM
- MOLECULE\_TEMP

The last point is a list of all the PRODUCT molecules or pseudo-absorbers that are fitted in the spectral window. "\_TEMP" refers to the temperature and is optional.

### Part-3:

Start this with the line:

```
% Data format:
```

This section consists of three fields:

col ##: short name: description with (unit) continued description

- precede the column number by "Col "
- start the column counting at 1 (i.e. not at 0)
- the number of columns listed here has to strictly match the number of data columns!
- the long name or description is not mandatory, but the unit is, and it has to be in round brackets in the third part separated by ":" e.g.

Col 01: DOY: (days since 2023-12-31 00:00 UTC)

- You can have ":" in the description/ long name or in the unit, but not in the short name.
- the short names for slant columns and slant column errors should be constructed as:

MOLECULE\_DSCD\_EXTRA

MOLECULE\_DSCD\_EXTRA\_Error

These fields are not case sensitive, "\_EXTRA" is optional, could be temperature. The PRODUCT molecule is of course mandatory.

The following fields (short names) are mandatory (other molecules fitted in the window can be added), the order is just an example. Please take note of the notes in the long names especially for the time and the angle definition. These are mandatory to use.

- DOY: Day of year 2024, start with 1.0 for January 1st, 00:00 UTC (days since 2023-12-31 00:00 UTC)
- UTC: UTC Time of day (hours)
- ACQT: Total Acquisition Time (s)
- SZA: Solar Zenith Angle (degree)
- SAA: Solar Azimuth Angle (degree) North=0, East=90
- VEA: Viewing Elevation Angle (degree)
- VAA: Viewing Azimuth Angle (degree) North=0, East=90
- MAINMOLEC\_DSCD: Differential column density of main molecule (molec/cm<sup>2</sup>)
- MAINMOLEC\_DSCD\_ERROR: Differential column density error of main molecule (molec/cm<sup>2</sup>)
- RMS: Fit RMS in OD (1)
- SHIFT: Spectrum shift (nm), against FRS reference
- OFFSET: Intensity offset normalised by the mean intensity
- INORM\_λ: Normalised Intensity counts/integration time at wavelength λ

note that you can use e.g. (1E15 molec/cm<sup>2</sup>) as a unit.

Normalized intensities (INORM) should be averaged in a 1 nm box around the center wavelength. Please report intensities at a minimum of one wavelength. This information will be used for the analysis of horizon scan data. If possible, also report normalized intensities every ten nanometers throughout your whole spectral range. E.g., if your spectrometer covers the spectral range from 300 to 460 nm, report the following fields: INORM\_310, INORM\_320, INORM\_330, INORM\_340, INORM\_350, INORM\_360, INORM\_370, INORM\_380, INORM\_390, INORM\_400, INORM\_410, INORM\_420, INORM\_430, INORM\_440, INORM\_440, INORM\_450.

### **C) Data:**

- Use either \t or spaces as delimiter. (\t + spaces is ok, but not "sometimes spaces, sometimes tab")
- Use -999 as missing data.

### **D) Example file:**

We provide an example file that strictly follows the format convention (but does not adhere to the specified measurement protocol). This contains NO<sub>2</sub> slant columns hypothetically retrieved by BIRA on 16/09/2024 in the visible range (425-490 nm). Data are analysed using a daily noon reference spectrum.

The corresponding file name is:

BIRA\_MAXDOAS\_4\_NO2VIS\_DAILYREF\_CINDI3\_20240916\_v1.0.ASC

## Appendix B: Description of the output file format for mobile DOAS measurements

The file format used for mobile DOAS measurements follows the same rules as defined for static measurement files (see Appendix A), with the adaptations defined below. This format is specifically designed for carDOAS NO<sub>2</sub> measurements, but it can easily be adapted to other molecules.

### A) File name convention

The file name is constructed as for static measurements, but does not include the field “\_REFTYPE”:

INSTITUTE\_INSTRUMENTTYPE\_INSTRUMENTNUMBER\_DATAPRODUCT\_CAMPAIGNNAME\_DATE\_VERSION.asc

An example is:

BIRA\_carDOAS\_51\_NO2\_CINDI3\_20240916\_v1.0.asc

INSTITUTE and INSTRUMENTNUMBER: use the institute acronyms and instrument numbers listed in Table 3.

Possible options for INSTRUMENTTYPE are carDOAS or bikeDOAS

### B) Header

The header consists of the three parts already defined for static measurements, however part 2 (retrieval information) is optional here:

- 1) general file information
- 2) retrieval information (optional)
- 3) information on the data columns

#### Part-1:

The following keys are mandatory:

- CAMPAIGNNAME
- INSTITUTE
- INSTRUMENTTYPE
- INSTRUMENTNUMBER
- DATAPRODUCT
- PRODUCTDSCD
- Missing value
- Retrieval code
- Created by
- Version

#### Part-3:

As for the static DOAS instruments, the format here is:

col ##: short name: description with (unit) continued description

The following fields (short names) are mandatory

- DOY: Day\_of\_year\_2024 start with 1.0 for January 1st, 00:00 UTC (days since 2023-12-31 00:00 UTC)
- UTC: UTC Time of day (hours)
- ACQT: Total Acquisition Time (s)
- SZA: Solar Zenith Angle (degree)
- SAA: Solar Azimuth Angle (degree) North=0, East=90
- VEA: Viewing Elevation Angle (degree)
- VAA: Viewing Azimuth Angle (degree) North=0, East=90
- LATITUDE: (degree) North
- LONGITUDE: (degree) East
- NO2\_DSCD\_294: NO2 differential column density (molec/cm2)
- NO2\_DSCD\_294\_ERROR: NO2 differential column density error (molec/cm2)
- RMS: Fit RMS in OD (1)
- NO2\_AMF\_STRAT: stratospheric NO2 AMF (1)
- NO2\_AMF\_TROPO: tropospheric NO2 AMF (1)
- NO2\_VCD\_STRAT: stratospheric NO2 vertical column (molec/cm2)
- NO2\_CD\_TROPO: tropospheric NO2 vertical column (molec/cm2)
- NO2\_VCD\_TROPO\_Error: tropospheric NO2 vertical column error (molec/cm2)

note that you can use e.g. (1E15 molec/cm2) as a unit.

### C) Data:

- Use either \t or spaces as delimiter. (\t + spaces is ok, but not "sometimes spaces, sometimes tab")
- Use -999 as missing data.

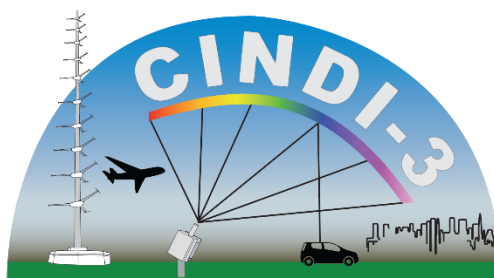
### D) Example file:

We provide a sample file that strictly adheres to the above data format. This file contains carDOAS NO<sub>2</sub> columns hypothetically measured by BIRA on 12/07/2024.

The corresponding file name is:

BIRA\_carDOAS\_51\_NO2\_CINDI3\_20240712\_v1.0.ASC

## **Appendix C: Semi-blind Intercomparison Data Protocol**



## **Third Cabauw Intercomparison of UV-VIS DOAS Instruments (CINDI-3)**

**Cabauw, The Netherlands  
21 May – 21 June 2024**

### **SEMI-BLIND INTERCOMPARISON DATA PROTOCOL**

The CINDI-3 semi-blind intercomparison exercise will be held from 21<sup>st</sup> May to 21<sup>st</sup> June 2024. The aims of this data protocol are: a) to encourage rapid dissemination of the measurement data collected during this exercise; b) to uphold the rights of the participating scientists; and c) to have all involved researchers/groups treated equitably. The rules and guidelines with respect to the production and use of measurement data are the following:

1. For their analyses, each group will apply the DOAS settings defined in the Semi-blind Intercomparison Protocol to be made available on-line. The measurement files will be formatted according to the CINDI-3 prescribed ascii text format.
2. Each group engage to follow the recommendations formulated in the Semi-blind Intercomparison Protocol, in particular to adopt the measurement sequences and to perform the required calibrations to the best of their possibilities.
3. Each group engage to submit their daily data files to the CINDI-3 web server by 10am local time at the latest. Data will be collected by the Campaign Referee and semi-blind comparison results will be presented at the daily briefings. The web server will be hosted by KNMI at an address to be communicated ahead of the campaign. KNMI will take the responsibility of the server management.
4. Each participating group engage to have at least one representative attending the daily briefings. The possibility to attend via a teleconferencing system (Skype or Webex) will be offered. Daily briefings will address the discussion of fresh semi-blind comparison results.

Upon relevance they will also cover relevant science or logistical topics in relation with the overall campaign organisation.

5. After completion of the formal intercomparison exercise, all scientists involved in CINDI-3 will have equal and complete access to all semi-blind intercomparison measurement data.
6. Data submitted to the CINDI-3 web server are and remain the exclusive property of the respective group.
7. Data will not be distributed outside the CINDI-3 consortium without prior permission of the corresponding instrument PI(s). The CINDI-3 consortium is defined as being all scientists/groups participating to the campaign.
8. Persons interested in using measurement data from others in scientific papers or presentations should offer the data owner(s) participation and co-authorship. If the data owner(s) refrain(s) from co-authorship, a second option is to mention the data owner(s) in the acknowledgements.
9. Each group funded by ESA for its participation to the semi-blind intercomparison engage submitting its measurement data to the ESA Validation Data Center (EVDC) hosted at NILU within 6 months after the end of the semi-blind intercomparison exercise, i.e. by 31 December 2024. They should also sign the EVDC/NILU data Protocol. The other participants are encouraged to submit their data according to the same protocol.
10. Each group funded by ESA for its participation to the semi-blind intercomparison, agrees to submit level-1 data files for further processing by the FRM4DOAS Centralised Data Processing system, using the common standardised data format defined on the FRM4DOAS web site (<https://frm4doas.aeronomie.be/index.php/frm4doas-guidelines>).
11. The ownership of data submitted to EVDC remains with the instrument PI.
12. EVDC will provide ECMWF meteorological fields (analysis and forecast) for the campaign area and period. Participants to the campaign are asked to not distribute these data outside the CINDI-3 consortium, neither to make commercial use of them.

The undersigned agrees to the conditions of this data protocol.

Signature : .....

Date : .....

Name : .....

Position (PI, Post-doc, student...) : .....

Address : .....

.....

.....

E-mail : .....

Please return to:

Royal Belgium Institute for Space Aeronomy (BIRA-IASB)

3, Avenue Circulaire

B-1180 Brussels

Belgium

Attn: Dr. Michel Van Roozendael ([michel.vanroozendael@aeronomie.be](mailto:michel.vanroozendael@aeronomie.be))