BIO MED 2024

LES JOURNÉES POUR L'AVENIR DE LA BIOLOGIE MÉDICALE

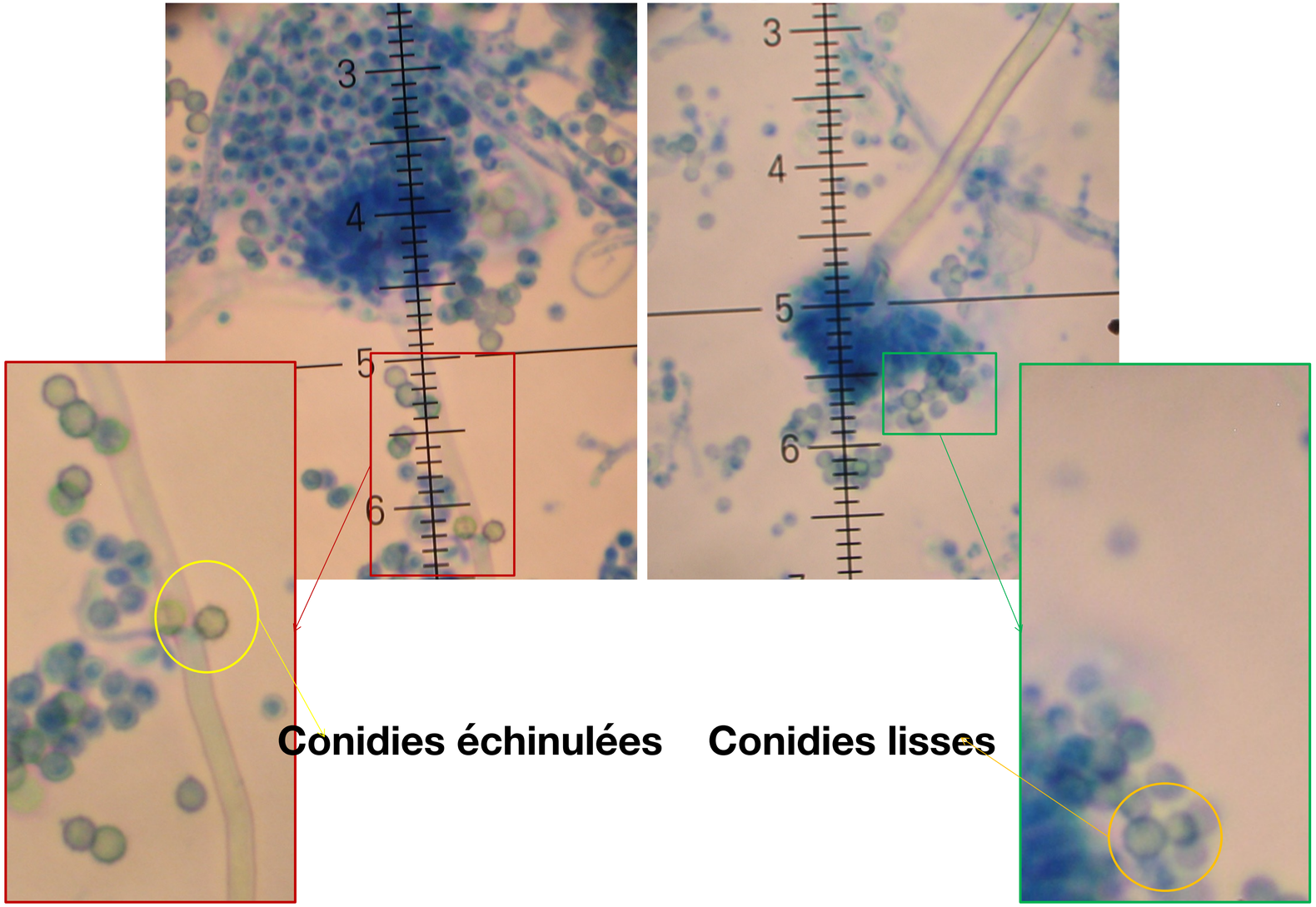
JEUDI 23 & VENDREDI 24 MAI 2024

La spectrométrie de masse : l'avenir de la mycologie ?

Professeur Renaud Piarroux
Assistance Publique-Hôpitaux de Paris
Sorbonne Université

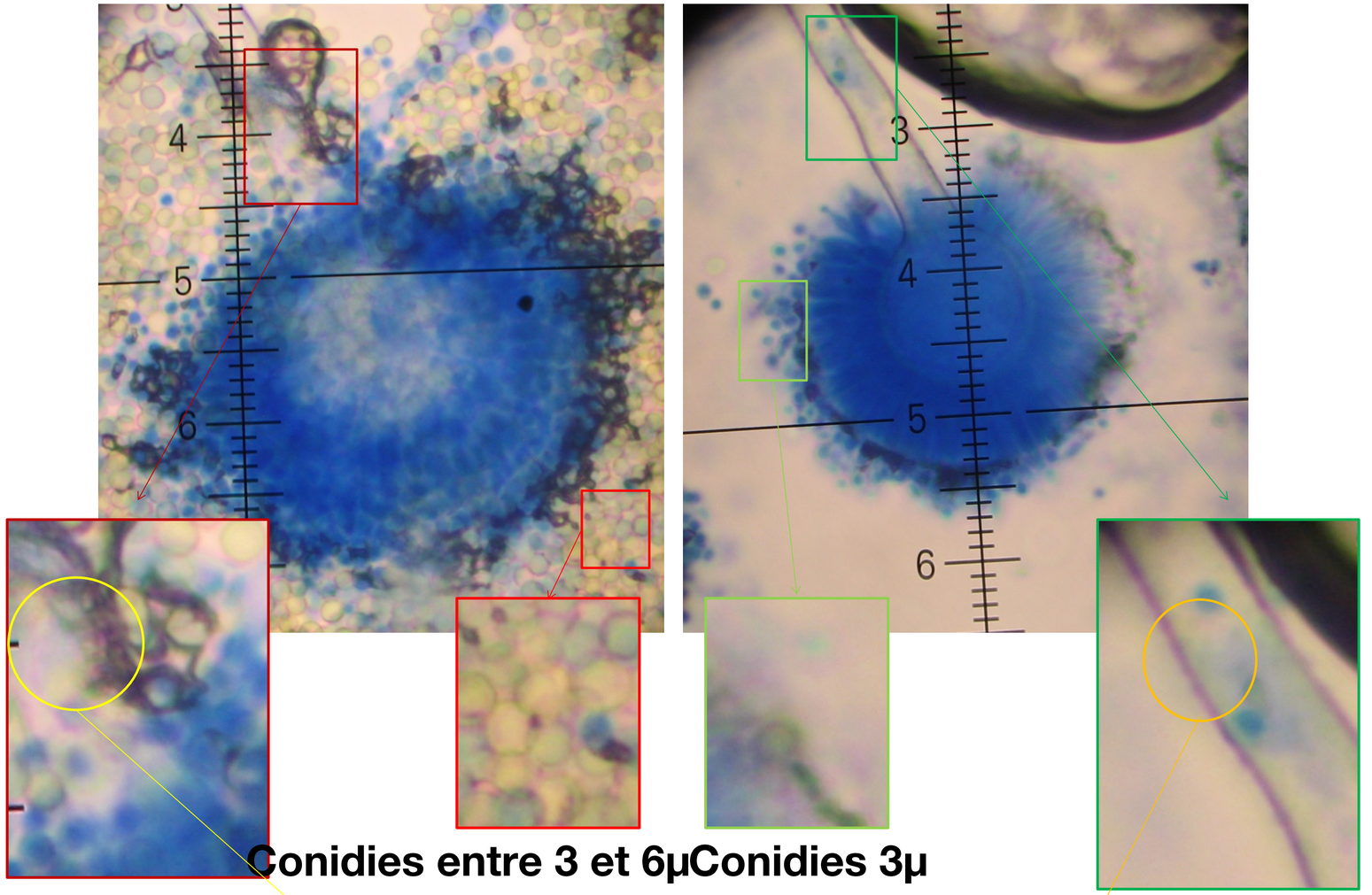
Pourquoi la spectrométrie de masse ?

Aspergillus sydowii *Aspergillus versicolor*



Conidies échinulées **Conidies lisses**

Aspergillus flavus ***Aspergillus ochraceus***

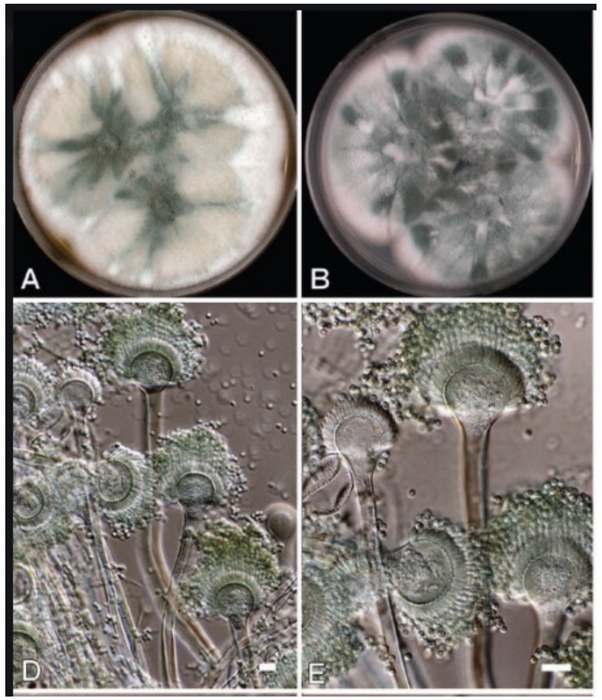


Conidies entre 3 et 6µ **Conidies 3µ**

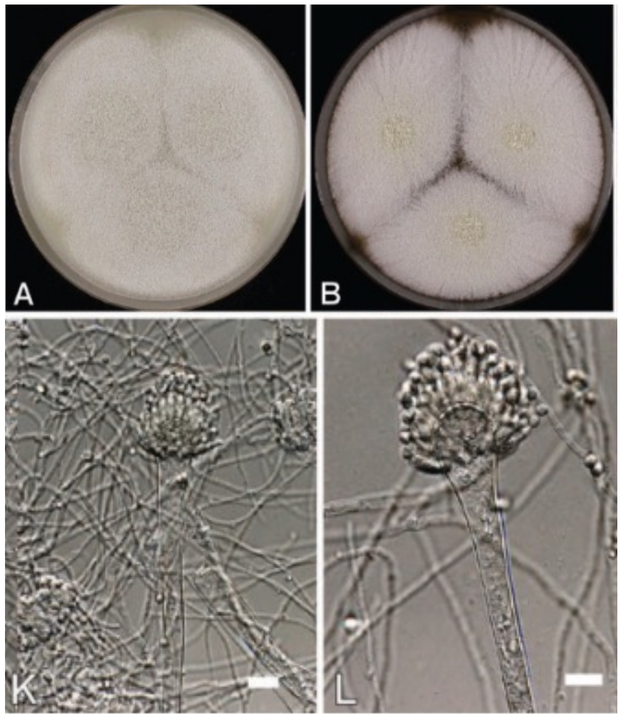
Conidiophore finement échinulé **Conidiophore très échinulé**

Problème des espèces cryptiques

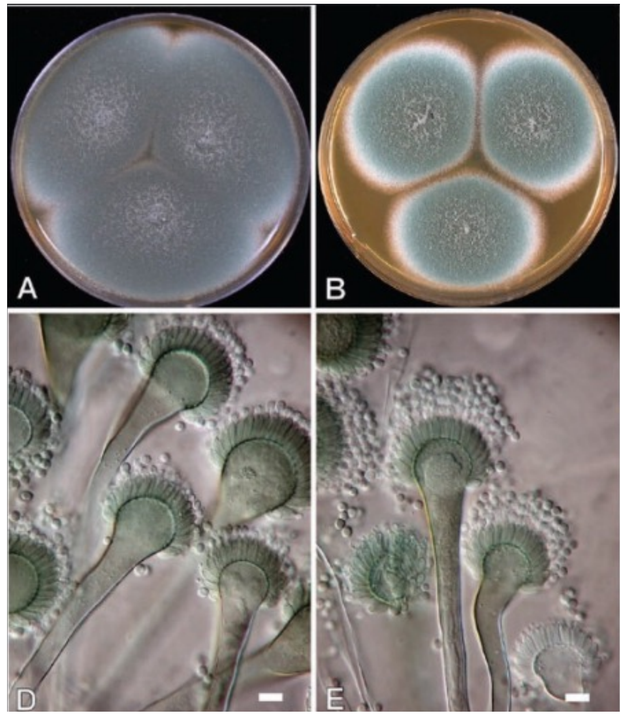
***A. lentulus*: CMI élevée aux azolés + Amphotéricine B**



***A. thermomutatus*: CMI élevée aux azolés**



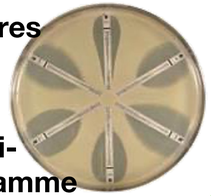
***A. fumigatus*: sensible**



Polyphasic taxonomy of *Aspergillus* section *Fumigati* and its teleomorph *Neosartorya*
R.A.Samson[1] S.Hong[2] S.W.Peterson[3] J.C.Frisvad[4] J.Varga[15]
Studies in Mycology, Volume 59, 2007, Pages 147-203

Un problème de temps…

48 heures



Anti-
fongigramme

Culture fongique

Échantillon

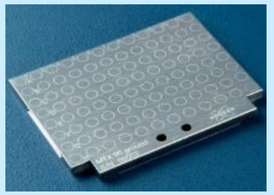
Correction du traitement

Patient

Pré-traitement

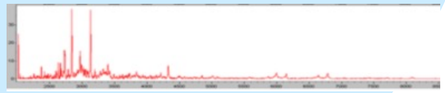
Extraction protéique

Dépôt



3-5 jours

30 minutes



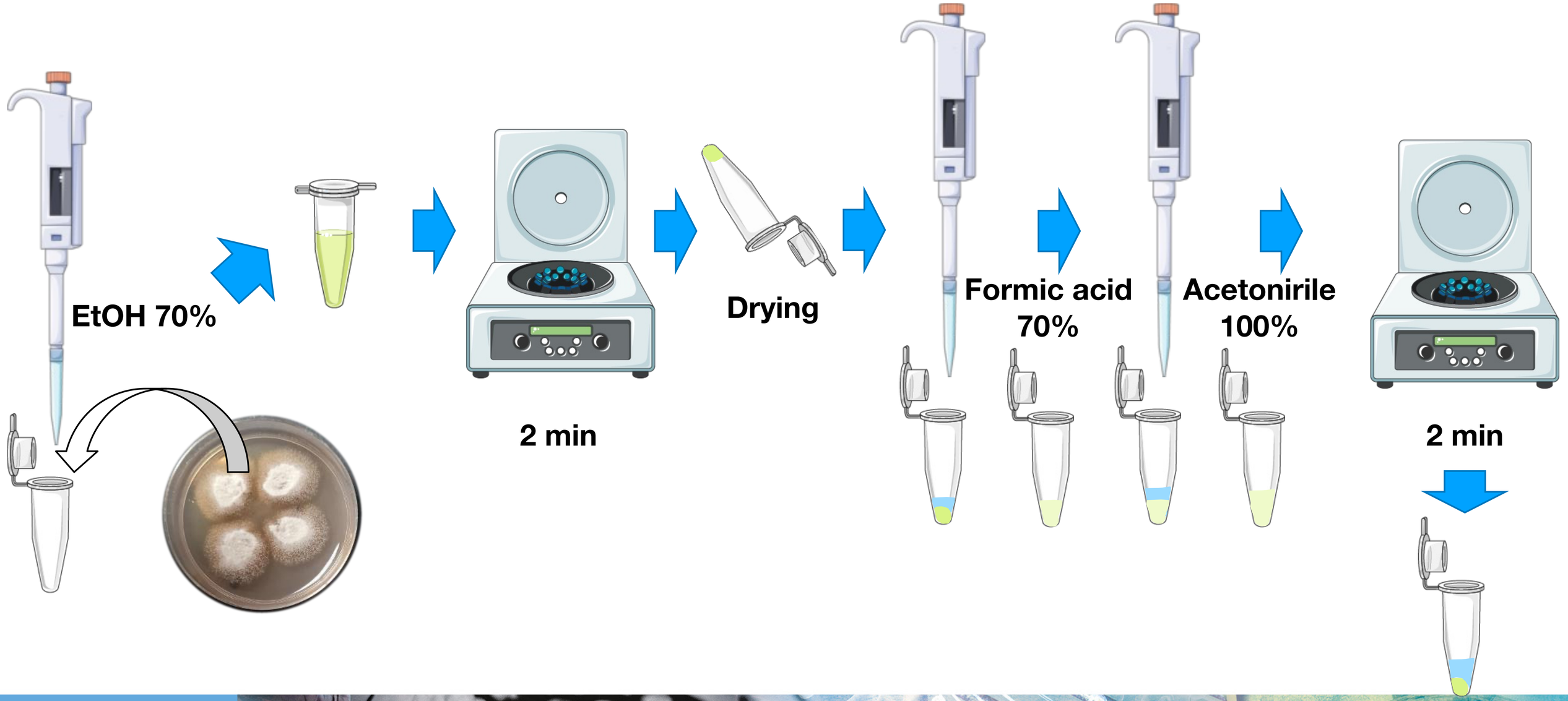
Acquisition

Matched Pattern	Score Value
Fusarium annulatum CBS258.54-CAC-1	2.13
Fusarium annulatum CBS258.54-CAC-3	1.985
Fusarium annulatum CBS258.54-CAC-2	1.934
Fusarium annulatum CBS258.54-CAC-4	1.874
Fusarium oxysporum ST62CAC-3	1.82
Fusarium oxysporum ST62CAC-1	1.803
Fusarium oxysporum ST62CAC-2	1.7
Fusarium polyphialidicum CBS463.91-CAC-1	1.659

Comparaison à la base de références

Identification

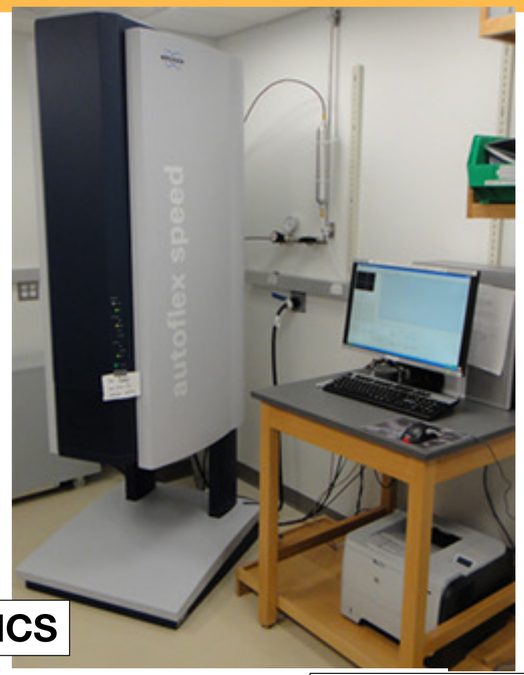
Extraction fongique



Comment ça marche ?

BRUKER

BRUKER DALTONICS



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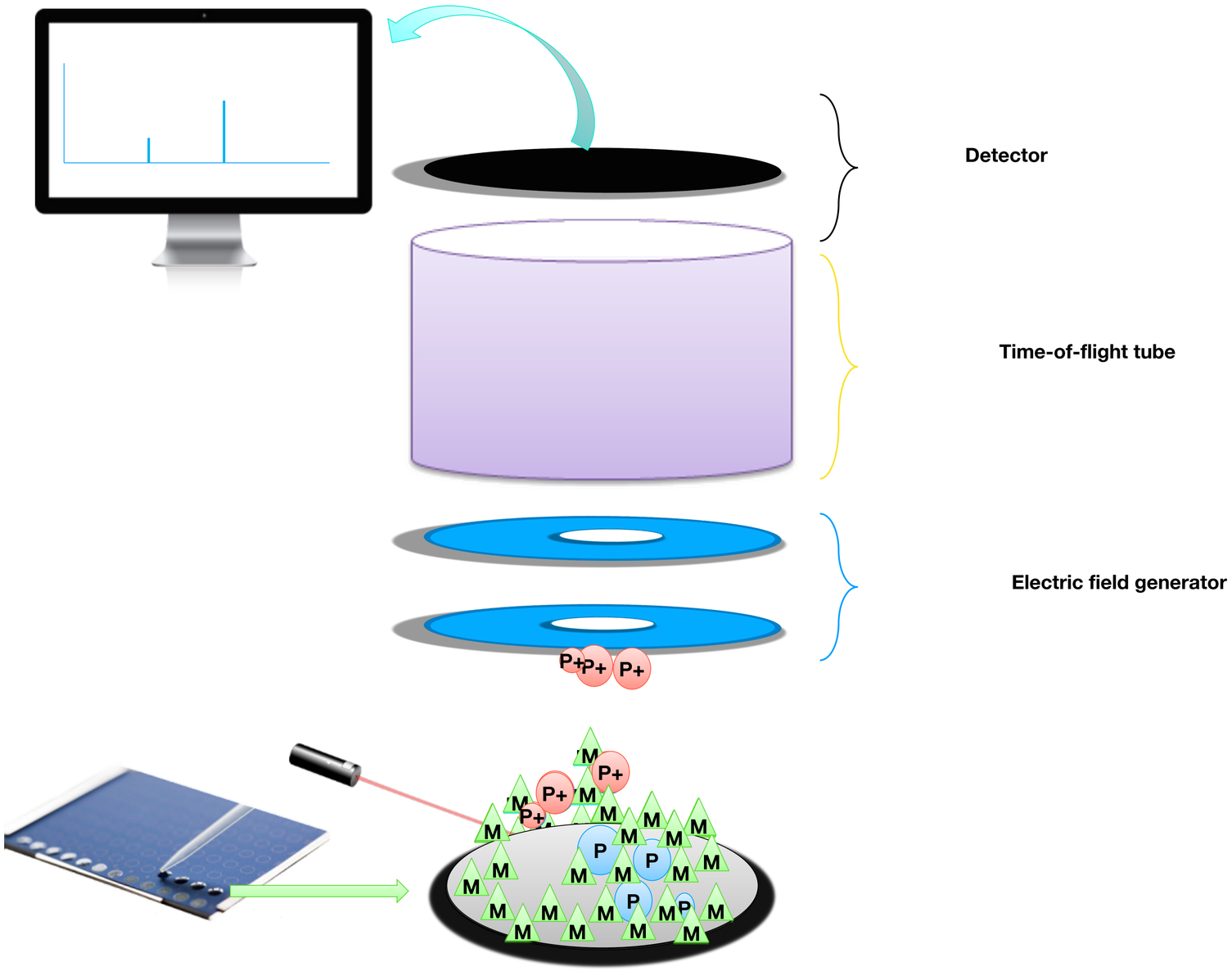
BIOMERIEUX

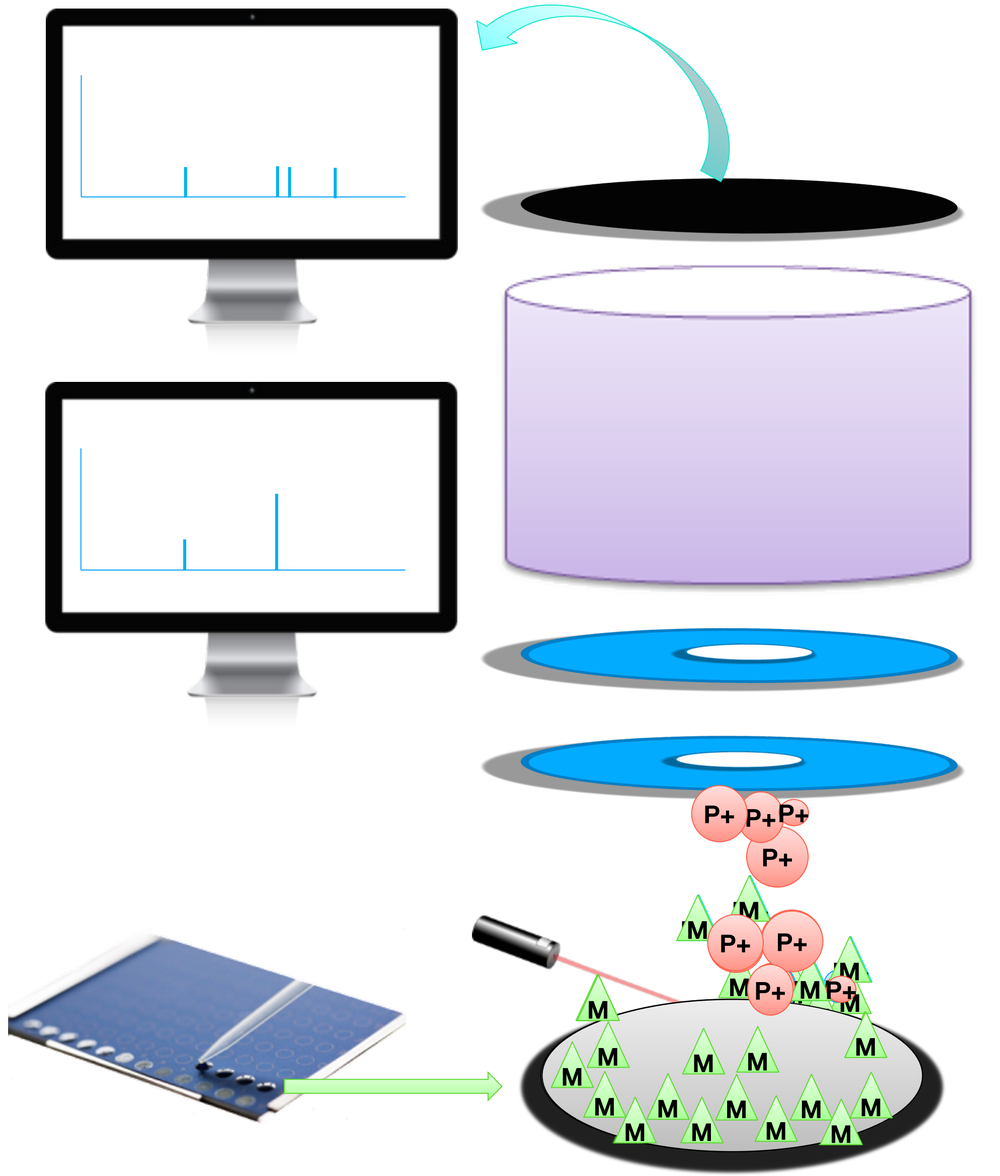
SHIMADZU

ANDROMAS

SHIMADZU

Scientific Analysis Instrument


Detector
Time-of-flight tube
Electric field generator
P+
M
P



Detector

Time-of-flight tube

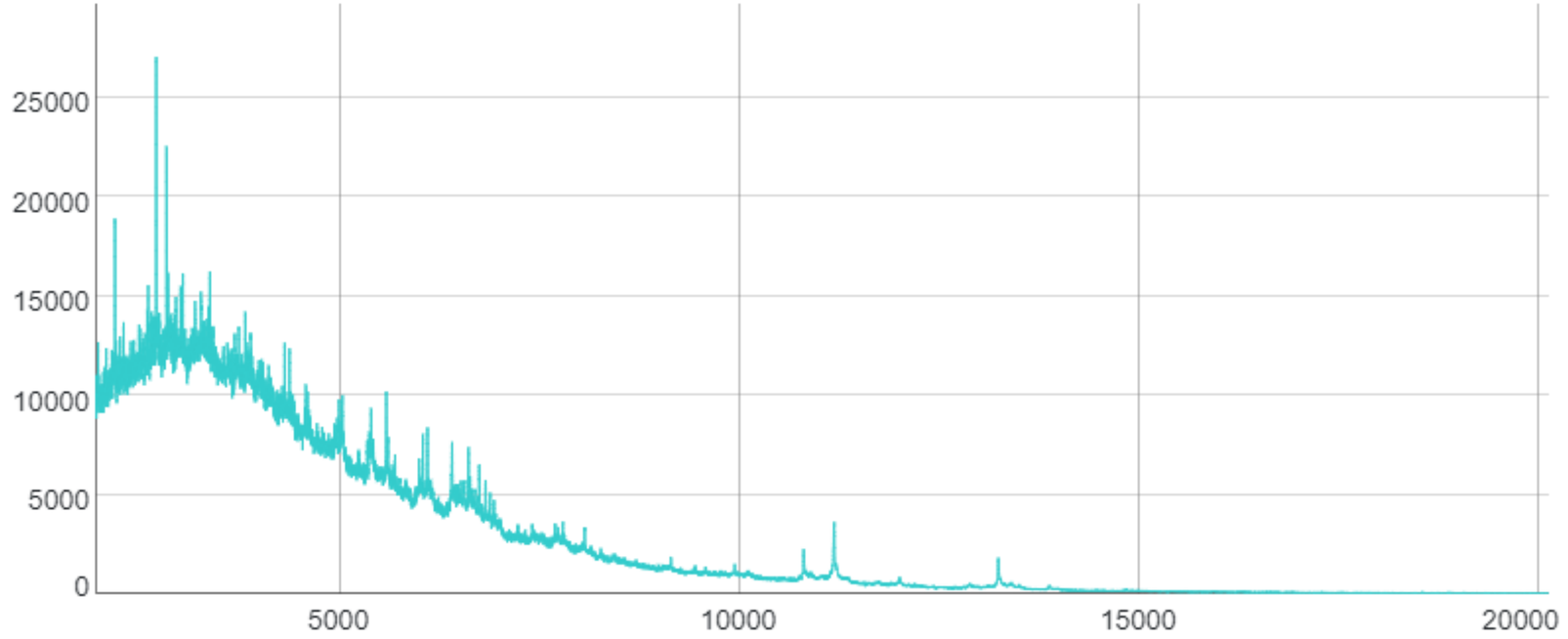
Electric field generator

Score calculation against every reference

Best identification result

Nom : 10bf9baa-c685-42e2-b550-d74ab911be37_A01

Chemin complet : petiteroutinePitie/10bf9baa-c685-42e2-b550-d74ab911be37/0_A1/1/1SLin/acqus



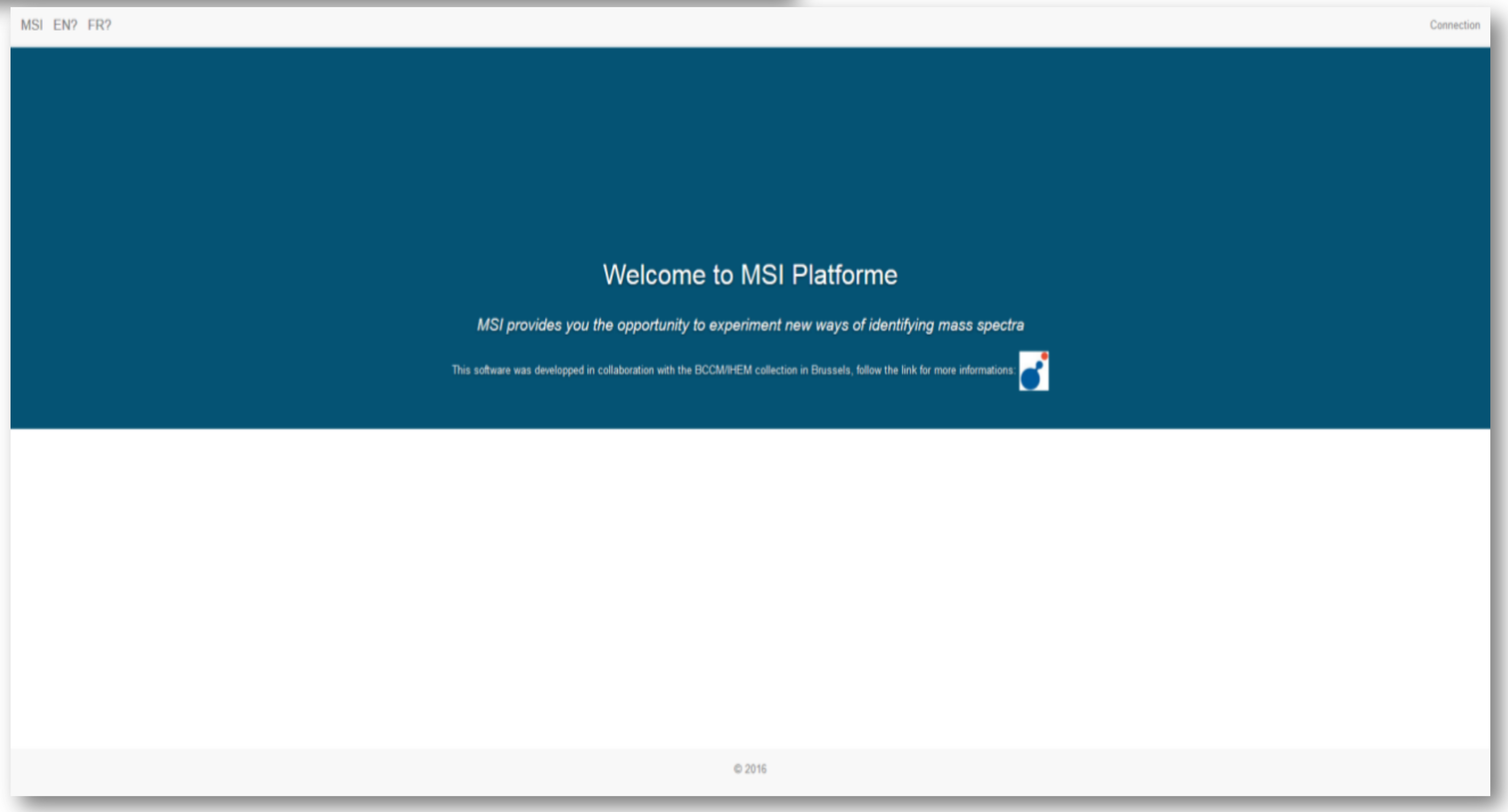
Pourquoi une application en ligne ?

AMERICAN SOCIETY FOR MICROBIOLOGY | Journal of Clinical Microbiology®

MYCOLOGY

Validation of a New Web Application for Identification of Fungi by Use of Matrix-Assisted Laser Desorption Ionization–Time of Flight Mass Spectrometry

A. C. Normand,[a] P. Becker,[b] F. Gabriel,[c] C. Cassagne,[a] I. Accoceberry,[c] M. Gari-Toussaint,[d] L. Hasseine,[d] D. De Geyter,[e] D. Pierard,[e] I. Surmont,[f] F. Djenad,[a] J. L. Donnadieu,[g] M. Piarroux,[h] S. Ranque,[a] M. Hendrickx,[b] R. Piarroux[a]



J Clin Microbiol. 2017 Sep;55(9):2661-2670. doi: 10.1128/JCM.00263-17. Epub 2017 Jun 21.

Validation of a New Web Application for Identification of Fungi by Use of Matrix-Assisted Laser Desorption Ionization-Time of Flight Mass Spectrometry

A C Normand [1], P Becker [2], F Gabriel [3], C Cassagne [4], I Accoceberry [3], M Gari-Toussaint [5], L Hasseine [5], D De Geyter [6], D Pierard [6], I Surmont [7], F Djenad [4], J L Donnadieu [8], M Piarroux [9], S Ranque [4], M Hendrickx [2], R Piarroux [4]

Affiliations + expand

PMID: 28637907 PMCID: PMC5648703 DOI: 10.1128/JCM.00263-17

Abstract

Matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry has emerged as a reliable technique to identify molds involved in human diseases, including dermatophytes, provided that exhaustive reference databases are available. This study assessed an online identification application based on original algorithms and an extensive in-house reference database comprising 11,851 spectra (938 fungal species and 246 fungal genera). Validation criteria were established using an initial panel of 422 molds, including dermatophytes, previously identified via DNA sequencing (126 species). The application was further assessed using a separate panel of 501 cultured clinical isolates (88 mold taxa including dermatophytes) derived from five hospital laboratories. A total of 438 (87.35%) isolates were correctly identified at the species level, while 26 (5.22%) were assigned to the correct genus but the wrong species and 37 (7.43%) were not identified, since the defined threshold of 20 was not reached. The use of the Bruker Daltonics database included in the MALDI Biotyper software resulted in a much higher rate of unidentified isolates (39.76 and 74.30% using the score thresholds 1.7 and 2.0, respectively). Moreover, the identification delay of the online application remained compatible with real-time online queries (0.15 s per spectrum), and the application was faster than identifications using the MALDI Biotyper software. This is the first study to assess an online identification system based on MALDI-TOF spectrum analysis. We have successfully applied this approach to identify molds, including dermatophytes, for which diversity is insufficiently represented in commercial databases. This free-access application is available to medical mycologists to improve fungal identification.

Keywords: MALDI-TOF mass spectrometry; dermatophytes; filamentous fungi; fungi; mass spectrometry; online identification.

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TABLE 3

Panel 2 identification results obtained with the five identification systems

Result for panel 2 sequenced strains[a]	No. (%) of strains identified				
	IHEM/MRS-MSI (threshold = 20)	IHEM/MRS-MBT (threshold = 1.7)	IHEM/MRS-MBT (threshold = 2.0)	Bruker-MBT (threshold = 1.7)	Bruker-MBT (threshold = 2.0)
Correct at the species level	435 (87.35)	411 (82.53)	312 (62.65)	259 (52.01)	119 (23.9)
Correct at the genus level	26 (5.22)	34 (6.83)	12 (2.41)	41 (8.23)	9 (1.81)
False at the genus level	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
Identification criteria not met	37 (7.43)	53 (10.64)	174 (34.94)	198 (39.76)	370 (74.3)

Open in a separate window

[a]For each database/software combination, the number (%) of strains is specified. Correct, concordant with the molecular identification at either the species or the genus level. False, discordant with the molecular identification at the genus level. Identification criteria not met, score below the defined threshold.

Passage de MSI-1 à MSI-2

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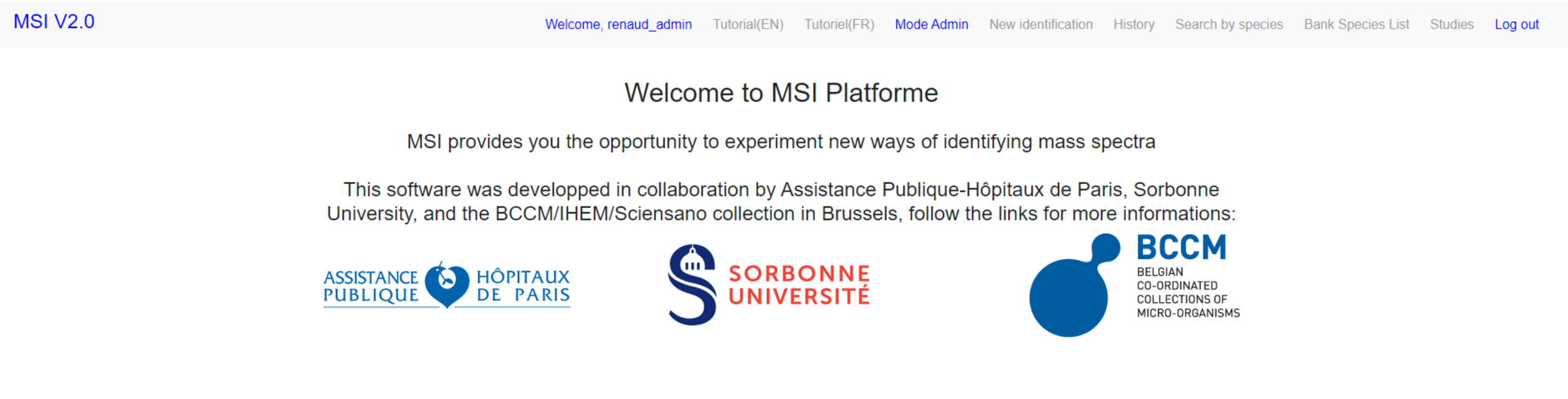

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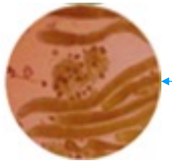
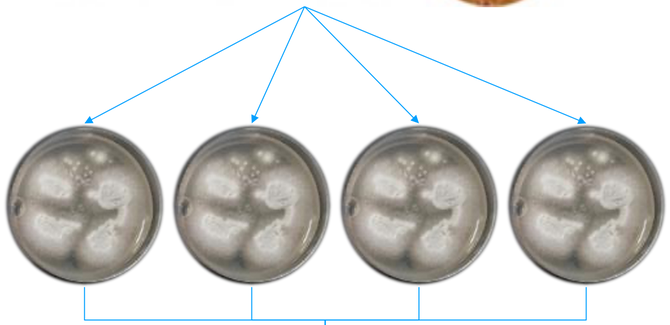




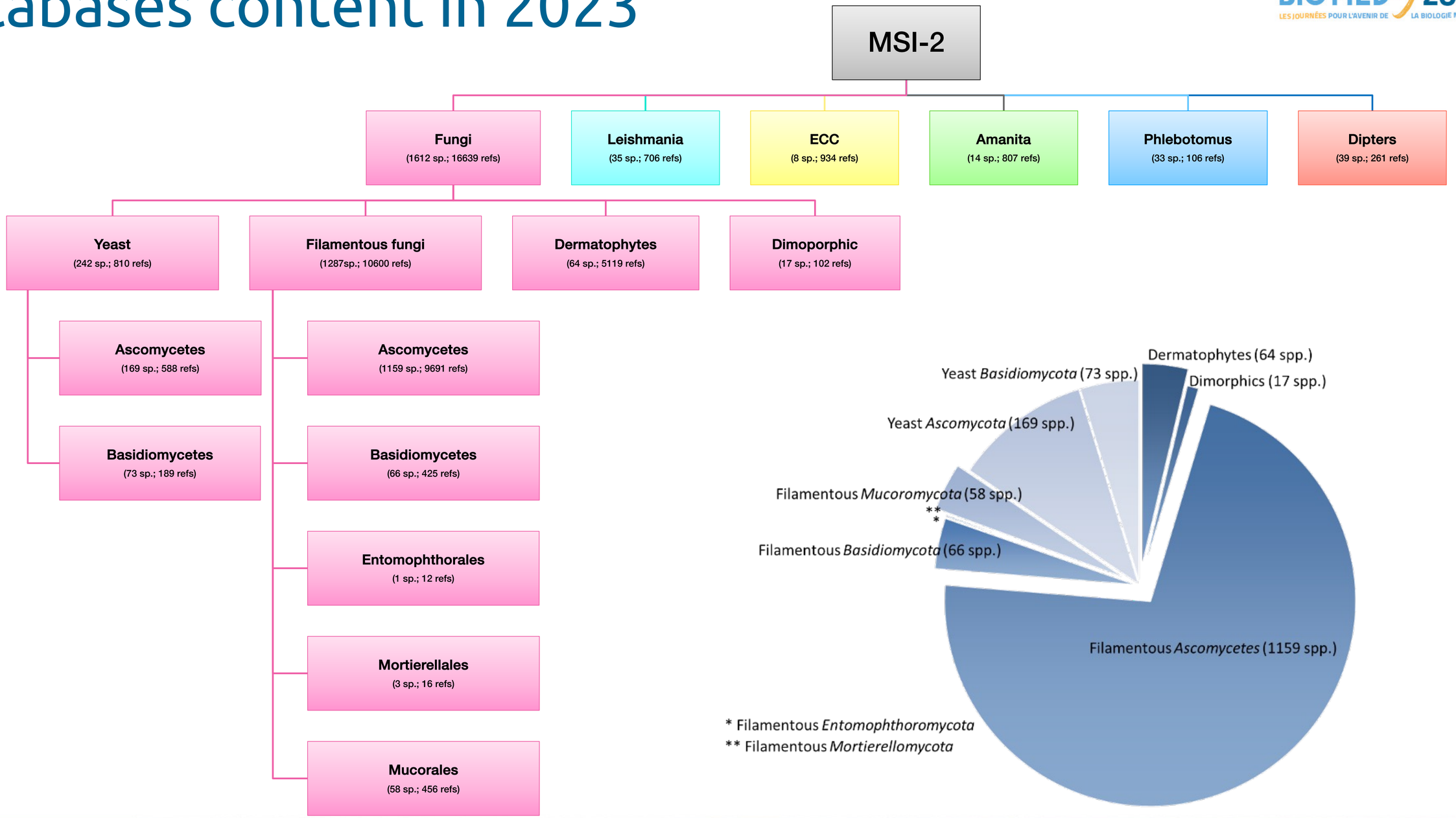
Failure

Success

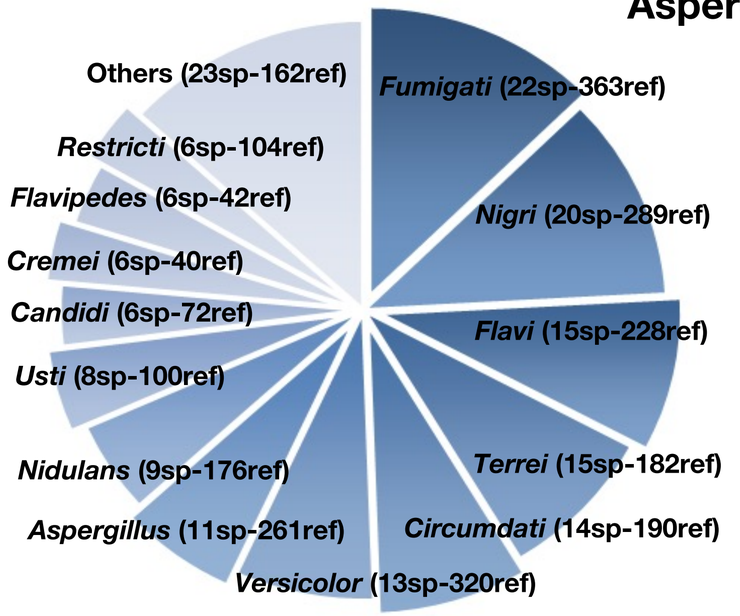
Daily routine

Reference database

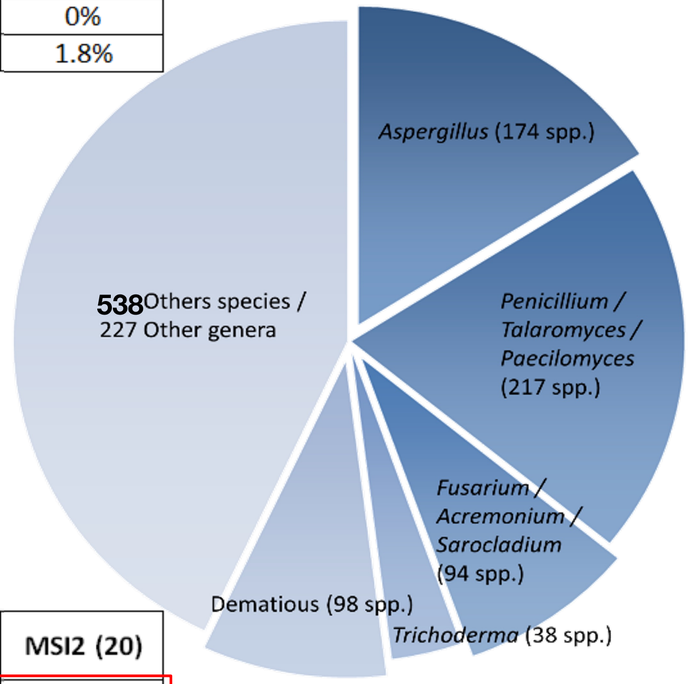
Databases content in 2023



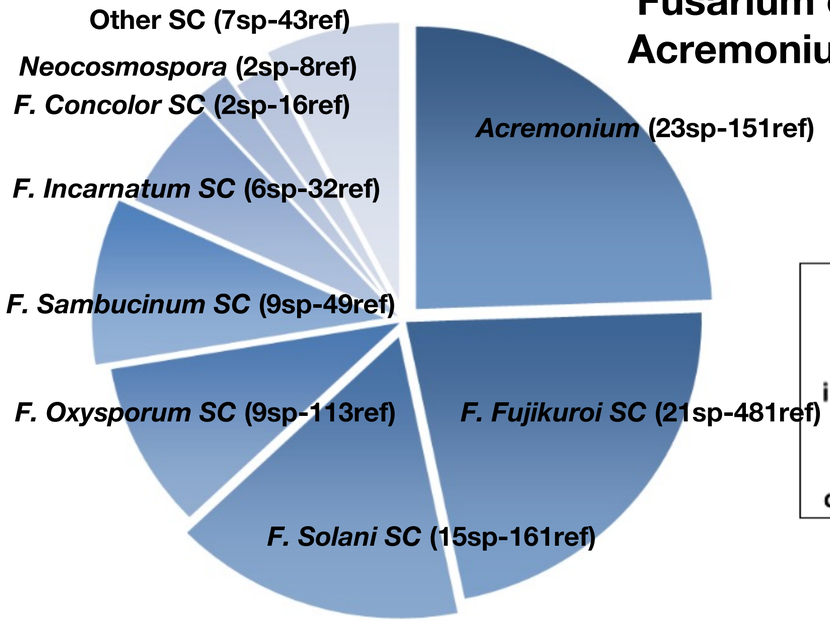
Aspergillus



B	Confidence level of the identification	Bruker (2,0)	MSI2 (20)
(n=273 isolates; 39 species in 10 complexes)	Correct at the species level	27.1%	89.7%
	Correct at the complex level	18.3	8.4
	Correct at the genus level	0	0
	Incorrect at the genus level	0%	0%
	Under the defined identification threshold	54.6%	1.8%

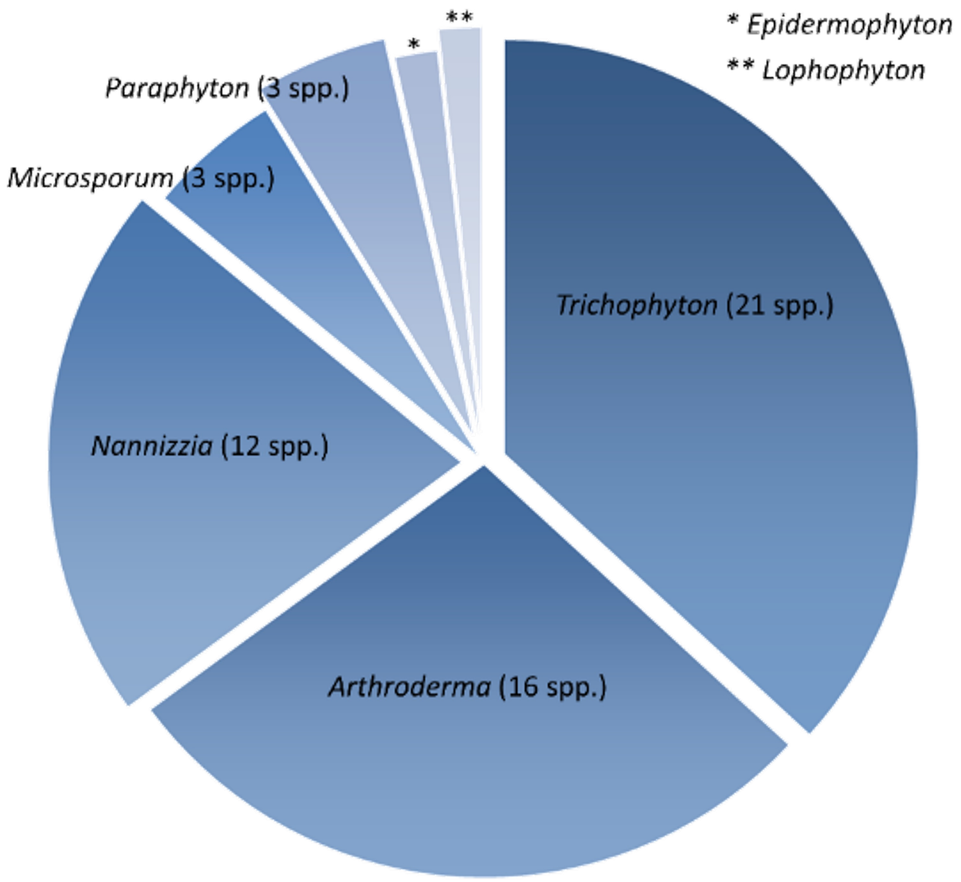


Fusarium et Acremonium



C	Confidence level of the identification	Bruker (2,0)	MSI2 (20)
(n=223 isolates; 38 species in 8 complexes)	Correct at the species level	11.2%	77.6%
	Correct at the complex level	16.6	21.5
	Correct at the genus level	0	0.4
	Incorrect at the genus level	0%	0%
	Under the defined identification threshold	72.2%	0.4%

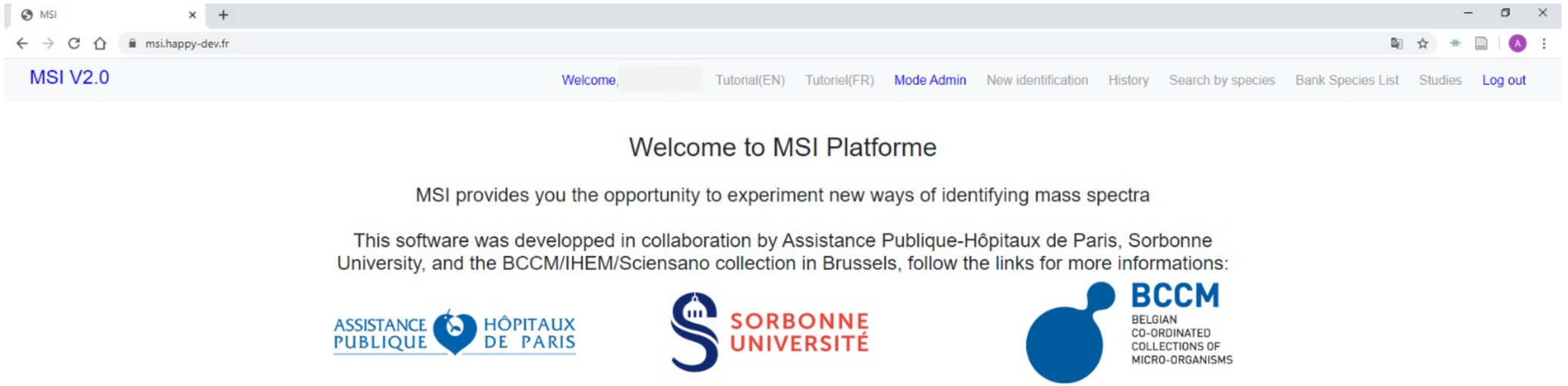
Dermatophytes



DERMATOPHYTES	MSI-1	MSI-2
E. floccosum (n=120)	56,7	**100**
M. audouinii (n=360)	57,2	**96,9**
M. canis (n=236)	86,0	**99,6**
N. fulva (n=65)	75,4	**100**
N. gypsea (n=198)	100	100
N. persicolor (n=76)	97,4	97,4
T. benhamiae (n=100)	81,0	**97,0**
T. equinum (n=258)	28,0	**89,3**
T. erinacei (n=258)	96,9	**100**
T. interdigitale (n=439)	63,6	**81,8**
T. kuryangei (n=96)	62,5	**77,1**
T. mentagrophytes (n=352)	71,6	**88,1**
T. rubrum (n=454)	84,1	**91,6**
T. soudanense (n=348)	2,6	**94,3**
T. tonsurans (n=442)	60,2	**91,2**
T. verrucosum (n=48)	0,0	**50,0**
T. violaceum (n=92)	19,6	**80,4**

MSI-2 au quotidien

MSI-2 (https://msi.happy-dev.fr)



Microflex

Vitek MS

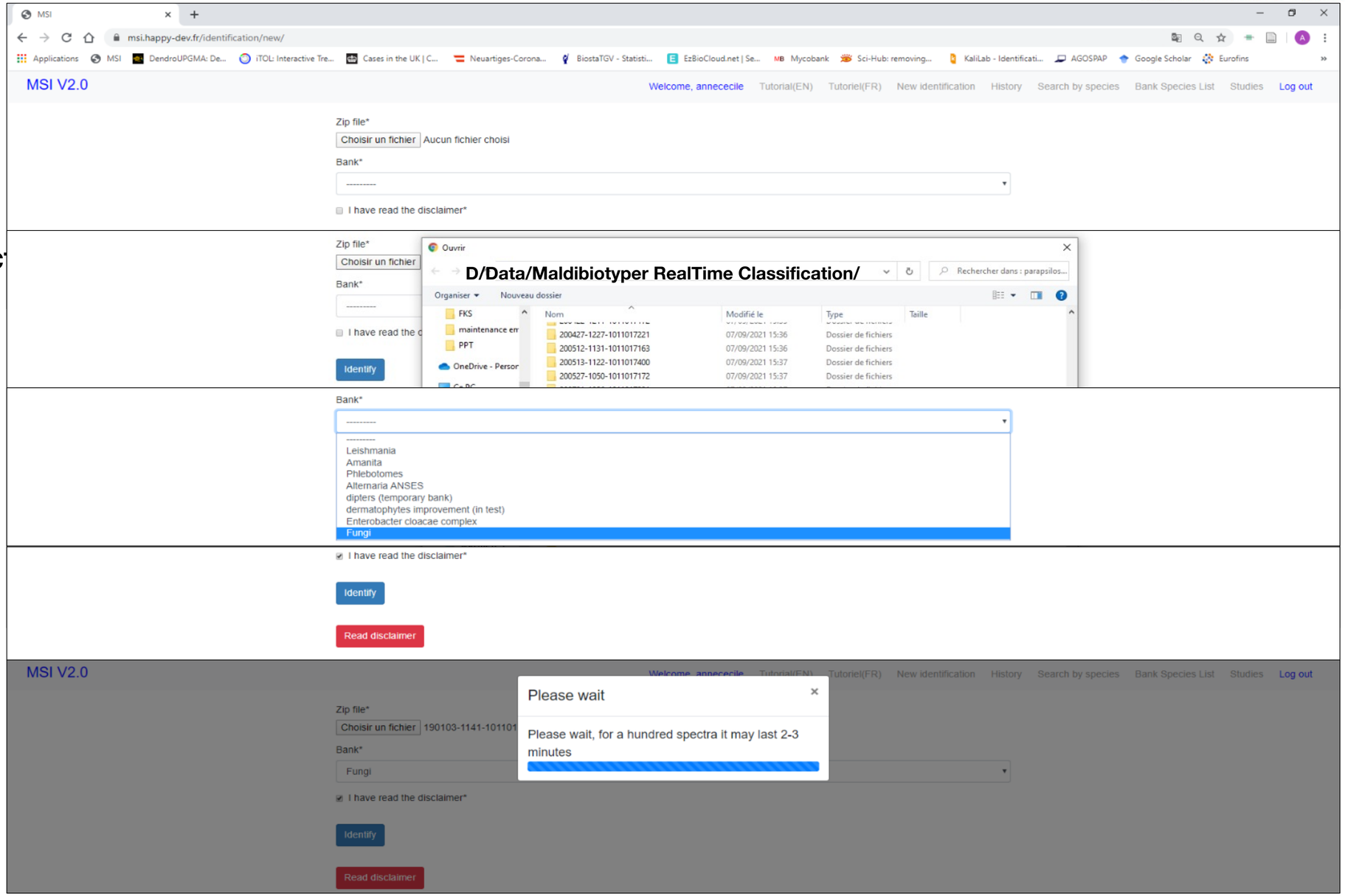
1/ Welcome page

2/ Loading of the projec

3/ Reference database selection

4/ Disclaimer

5/ Identification



MSI-2 et identification en ligne des agents

Look for past and standardized nomenclature on Myco Bank website : Here

For molds and fungi, you can have taxonomic information about a genus/species name here.

Enter only one word (enter "fumigatus" for "Aspergillus fumigatus").
You can enter partial names ("cand" will return data for "Aspergillus candidus" as well as for "Candida albicans" and other Candida species).

Write name here Search Find

Project results

Export results*

*If you have an excel error message, you can accept the file.

Spot name	Plot	Indice	Score 1 (%)	First Identified Species	Score 2 (%)	Second Identified Species	Score 3 (%)	Third Identified Species	Compare	Details
10bf9baa-c685-42e2-b550-d74ab911be37_A01	Plot	A	37.6	**Aspergillus sydowii**	28.9	**Aspergillus jensenii**	26.77	**Aspergillus puulaauensis**	Compare	Details
2a6a4929-4706-48a8-b8eb-8023115d9049_A04	Plot	A	27.53	**Aspergillus hiratsukae**	12.28	Cephalotrichum microsporum	0	Not identified	Compare	Details
2a0cab0b-027f-4fad-aad4-dd5d729184e2_A05	Plot	A	32.52	**Aspergillus hiratsukae**	17.22	Aspergillus quadricinctus	16.69	Aspergillus cf.aureolus	Compare	Details
22b53a4d-39ee-4879-b957-71f5c08d6757_A07	Plot	C	0	Not identified	0	Not identified	0	Not identified	Compare	Details
28bfae79-de61-4a55-af81-6bbb4c82d2fd_A08	Plot	C	0	Not identified	0	Not identified	0	Not identified	Compare	Details
2d9cf9a0-a848-4d2c-942f-95af0fe4e273_A11	Plot	A	52.13	**Aspergillus montevidensis**	25.45	**Aspergillus intermedius**	25.36	**Aspergillus chevalieri**	Compare	Details
69ae1724-7c9b-4cb8-b609-aaf92f8f8063_B06	Plot	B	26.64	**Aspergillus lentulus**	25.54	**Aspergillus fumigatiaffinis**	22.21	**Aspergillus fischeri**	Compare	Details
4c36dab8-8c0b-4f5c-a345-b0a703d610c9_B12	Plot	C	16.5	Aspergillus micronesiensis	14.17	Aspergillus niveus	13.22	Aspergillus terreus	Compare	Details

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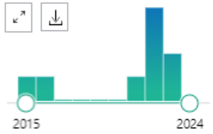

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- Clinical Trial
- Meta-Analysis
- Randomized Controlled Trial
- Review
- Systematic Review

PUBLICATION DATE

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- 5 years
- 10 years
- Custom Range

ARTICLE LANGUAGE

- French

Additional filters

1 Cite Share

MALDI-TOF **Mass Spectrometry** Online Identification of Trichophyton indotineae Using the **MSI-2** Application.

Normand AC, Moreno-Sabater A, Jabet A, Hamane S, Cremer G, Foulet F, Blaize M, Dellière S, Bonnal C, Imbert S, Brun S, Packeu A, Bretagne S, Piarroux R.

J Fungi (Basel). 2022 Oct 19;8(10):1103. doi: 10.3390/jof8101103.

PMID: 36294668 Free PMC article.

Trichophyton indotineae is an emerging pathogen which recently spread from India to Europe and that is more prone than other species of the Trichophyton mentagrophytes complex to show resistance to terbinafine, resulting in the necessity of rapid identification. Here, we improved ...

2 Cite Share

Performance of the **MSI-2** Database for Fungal Identification by **Matrix-Assisted Laser Desorption Ionization**-Time of Flight **Mass Spectrometry** from Cleanroom Environments.

Trivitt GE, Lau AF.

J Clin Microbiol. 2023 Mar 23;61(3):e0135322. doi: 10.1128/jcm.01353-22. Epub 2023 Feb 28.

PMID: 36853008 Free PMC article.

Accurate mold identification by **matrix-assisted laser desorption ionization**-time of flight **mass spectrometry** (**MALDI**-TOF MS) is dependent on robust organism representation in available databases. ...Here, we performed a retro ...

3 Cite Share

Identification of Molds with **Matrix-Assisted Laser Desorption Ionization**-Time of Flight **Mass Spectrometry**: Performance of the Newly Developed **MSI-2** Application in Comparison with the Bruker Filamentous Fungi Database and MSI-1.

Normand AC, Blaize M, Imbert S, Packeu A, Becker P, Fekkar A, Stubbe D, Piarroux R.

J Clin Microbiol. 2021 Sep 20;59(10):e0129921. doi: 10.1128/JCM.01299-21. Epub 2021 Jul 28.

PMID: 34319807 Free PMC article.

Matrix-assisted laser desorption ionization-time of flight **mass spectrometry** (**MALDI**-TOF MS) represents a promising tool for the rapid and efficient identification of molds, but improvements are still necessary to achieve sat ...

Item in Clipboard

4 Cite Share

Investigations upon the Improvement of Dermatophyte Identification Using an Online **Mass Spectrometry** Application.

Jabet A, Normand AC, Moreno-Sabater A, Guillot J, Risco-Castillo V, Brun S, Demar M, Blaizot R, Nabet C, Packeu A, Piarroux R.

J Fungi (Basel). 2022 Jan 11;8(1):73. doi: 10.3390/jof8010073.

PMID: 35050013 Free PMC article.

Online **MALDI**-TOF **mass spectrometry** applications, such as **MSI-2**, have been shown to help identify dermatophytes, but recurrent errors are still observed between phylogenetically close species. ...Nevertheless, residual confusion between close spe ...

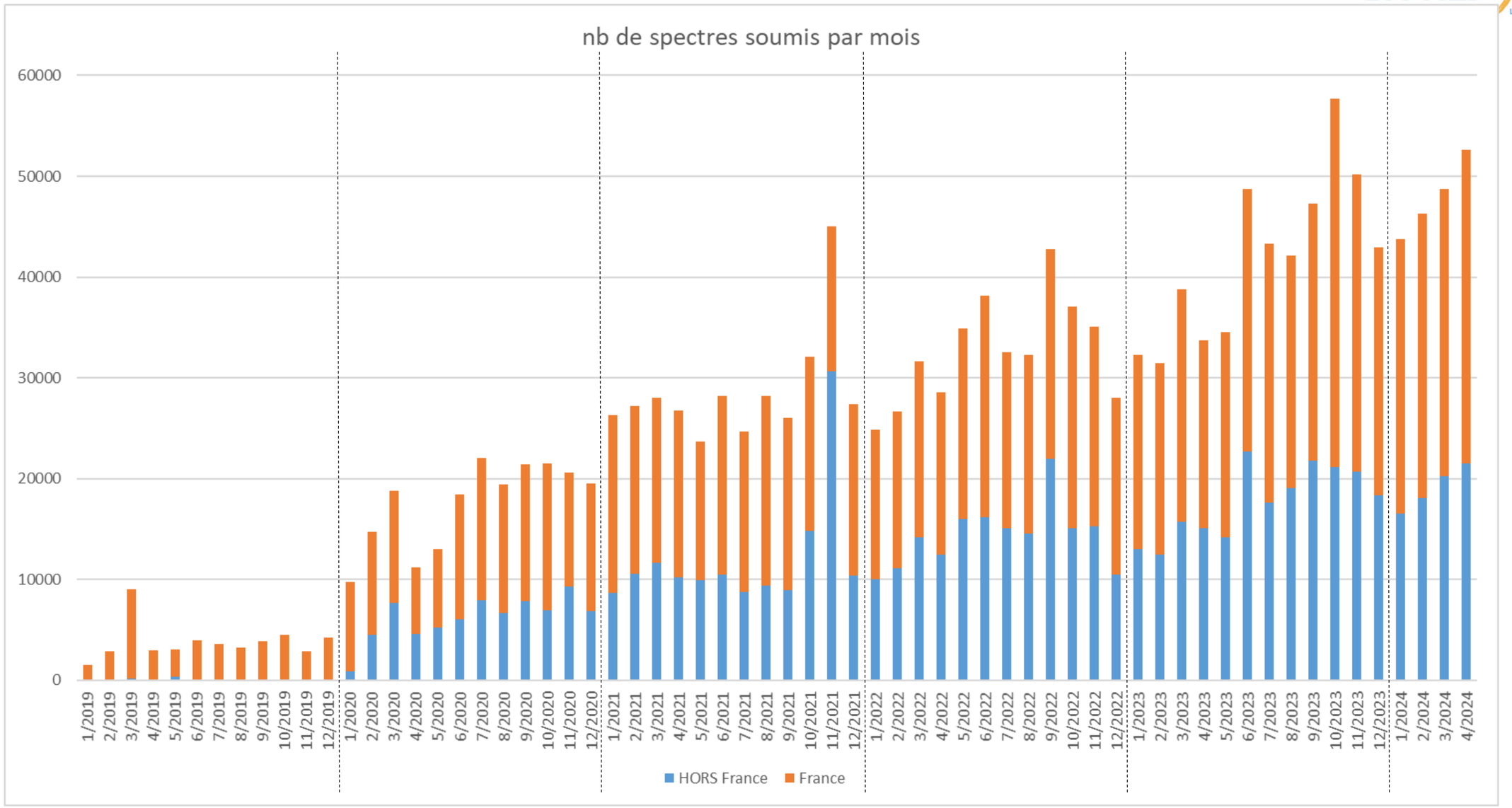
Journal Article Journal Article Jou

TABLE 3

Identification performances of the different MALDI-TOF MS identification databases

Organisms	Confidence level of the identification	% identification (95% CI[a]) with:			
		Bruker (2.0)	Bruker (1.7)	MSI-1 (20)	MSI-2 (20)
All isolates (n = 633 isolates; 124 species)	Correct at the species level	21.8 (18.64–25.22)	38.07 (34.27–41.98)	63.19 (59.3–66.96)	83.25 (80.11–86.08)
	Correct at the complex level[b]	14.22 (11.59–17.18)	25.12 (21.78–28.69)	30.17 (26.62–33.91)	12.95 (10.44–15.82)
	Correct at the genus level[c]	0.32 (0.04–1.14)	1.74 (0.87–3.09)	3.95 (2.57–5.78)	0.16 (0–0.88)
	Incorrect at the genus level[c]	0 (0–0)	0.32 (0.04–1.14)	0.16 (0–0.88)	0 (0–0)
	Under the defined identification threshold	63.67 (59.78–67.42)	34.76 (31.05–38.61)	2.53 (1.45–4.07)	3.63 (2.32–5.4)
Aspergillus spp. (n = 273 isolates; 39 species in 10 complexes)	Correct at the species level	27.11 (21.92–32.79)	46.89 (40.85–53)	69.23 (63.39–74.65)	89.74 (85.52–93.08)
	Correct at the complex level[b]	18.32 (13.91–23.42)	24.54 (19.56–30.09)	30.04 (24.66–35.85)	8.42 (5.42–12.37)

Une communauté d’utilisateurs


nb de spectres soumis par mois
60000
50000
40000
30000
20000
10000
0
1/2019
2/2019
3/2019
4/2019
5/2019
6/2019
7/2019
8/2019
9/2019
10/2019
11/2019
12/2019
1/2020
2/2020
3/2020
4/2020
5/2020
6/2020
7/2020
8/2020
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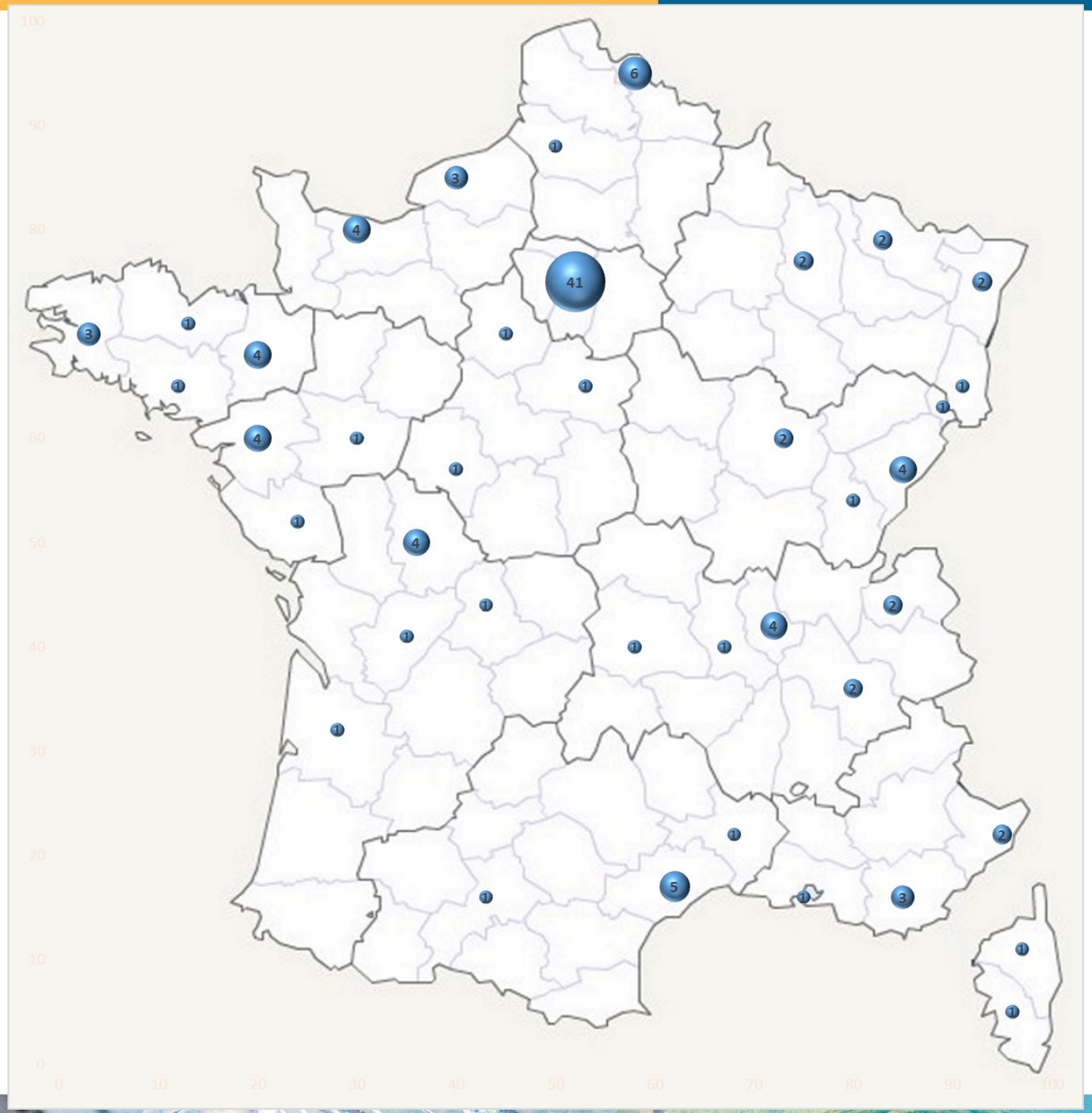
7/2023
8/2023
9/2023
10/2023
11/2023
12/2023
1/2024
2/2024
3/2024
4/2024
HORS France
France

France =
120 utilisateurs = 1 008 694 spectres soumis



Europe hors France =
177 utilisateurs = 465 394 spectres soumis

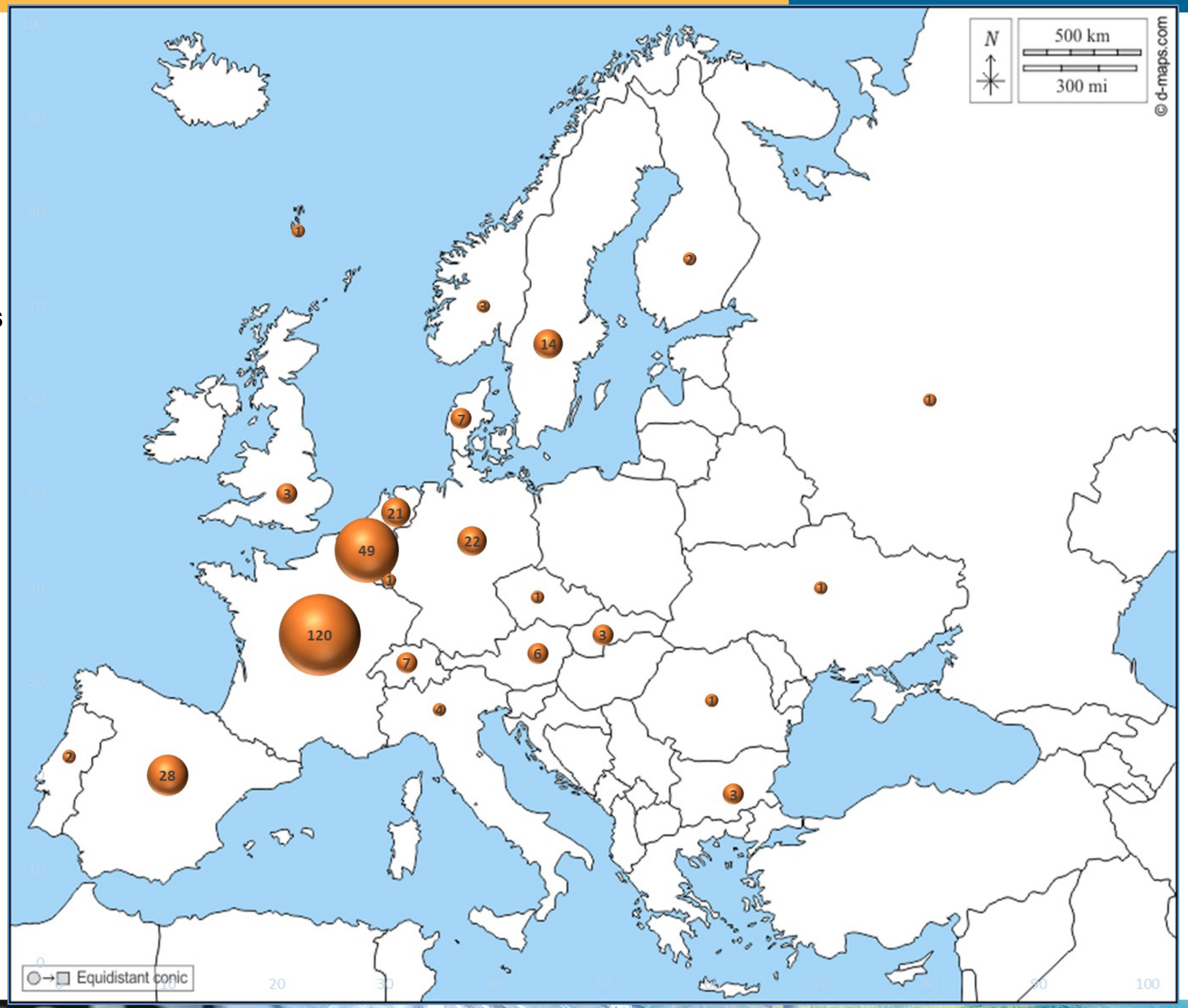
France =
120 utilisateurs = 1 008 694 spectres soumis

Belgique =
49 utilisateurs = 121 874 spectres soumis

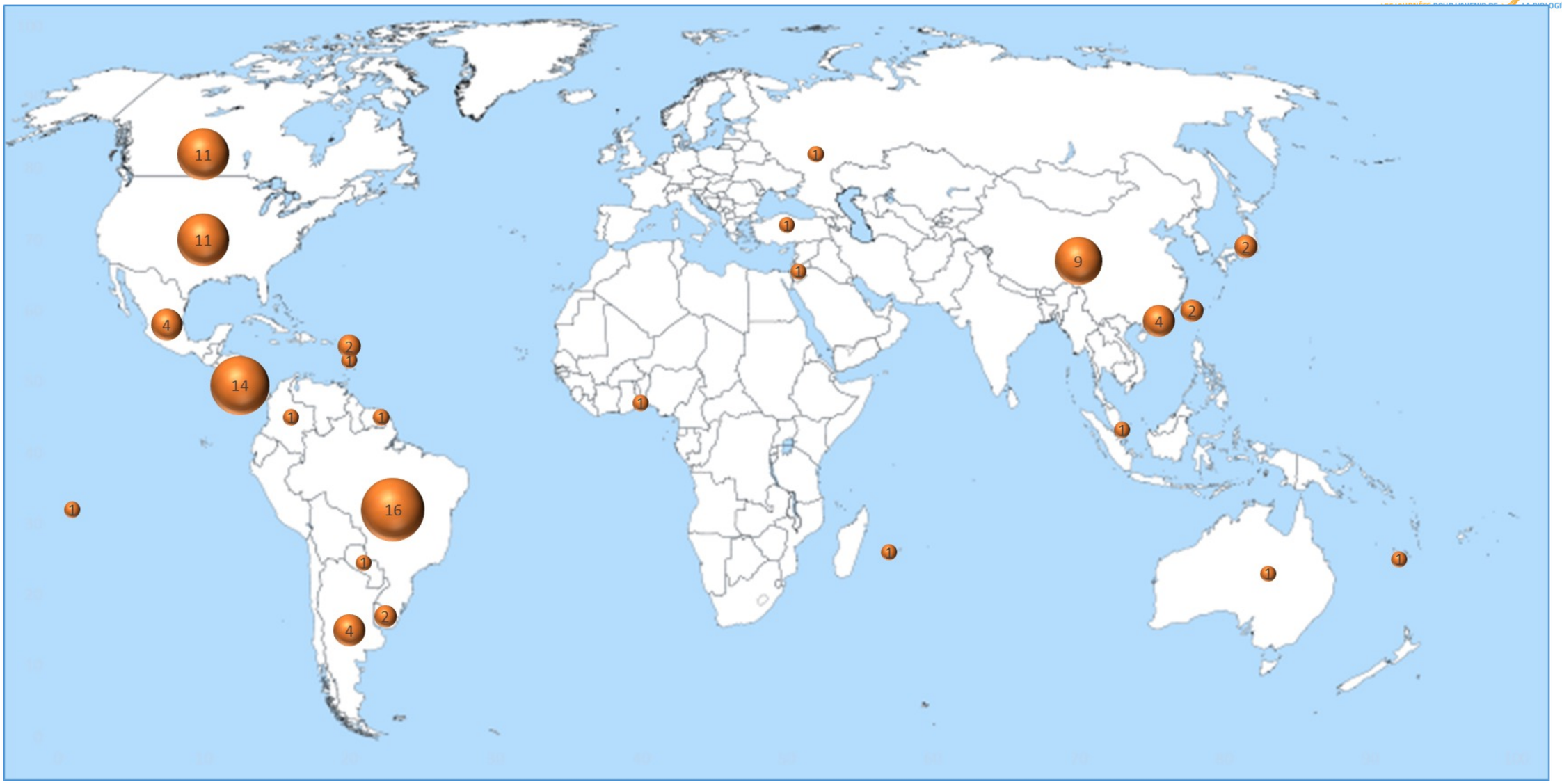
Pays Bas =
21 utilisateurs = 56 024 spectres soumis

Allemagne =
22 utilisateurs = 22 807 spectres soumis

Suisse =
7 utilisateurs = 122 137 spectres soumis



Monde hors Europe = 96 utilisateurs = 233 063 spectres soumis



Mai 2024

Access to a larger number of cases

BIO MED 2024
LES JOURNÉES POUR L'AVENIR DE LA BIOLOGIE MÉDICALE

Medical Mycology, 2019, 0, 1–11
doi:10.1093/mmy/myz098
Advance Access Publication Date: 0 2019
Original Article

Original Article

Optimization of MALDI-ToF mass spectrometry for yeast identification: a multicenter study

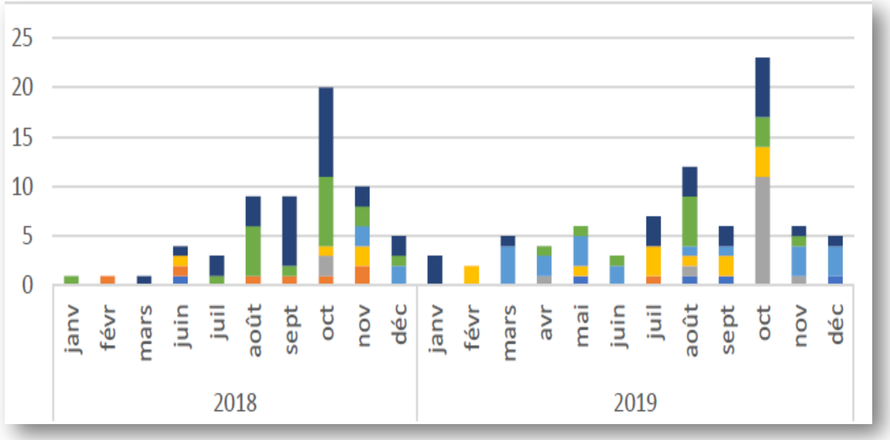
Anne-Cécile Normand[1,*], Frédéric Gabriel[2], Arnaud Riat[3], Carole Cassagne[4], Nathalie Bourgeois[5], Antoine Huguenin[6,7], Pamela Chauvin[8], Deborah De Geyter[9], Michiel Bexkens[10], Elisa Rubio[11], Marijke Hendrickx[12], Stéphane Ranque[3] and Renaud Piarroux[1,13]

Journal of *Fungi*
MDPI

Article

Clinical Origin and Species Distribution of *Fusarium* spp. Isolates Identified by Molecular Sequencing and Mass Spectrometry: A European Multicenter Hospital Prospective Study

Anne-Cécile Normand [1,*], Sébastien Imbert [1,2,3], Sophie Brun [2], Abdullah M. S. Al-Hatmi [3,4], Erja Chryssanthou [5], Sophie Cassaing [6], Christine Schuttler [7], Lilia Hasseine [8], Caroline Mahinc [9], Damien Costa [10], Christine Bonnal [11], Stéphane Ranque [12], Marc Sautour [13], Elisa Rubio [14], Laurence Delhaes [15], Arnaud Riat [16], Boualem Sendid [17], Lise Kristensen [18], Marcel Brandenberger [19], Juliette Guitard [20], Ann Packeu [21], Renaud Piarroux [1,22] and Arnaud Fekkar [1,23]



Saisonnalité des cladosporium

Medical Mycology, 2019, 0, 1–7
doi: 10.1093/mmy/myz004
Advance Access Publication Date: 0 2019
Original Article

Original Article

Multi-centric evaluation of the online MSI platform for the identification of cryptic and rare species of *Aspergillus* by MALDI-TOF

Sébastien Imbert[1,2,3,*], Anne Cécile Normand[1], Frédéric Gabriel[4], Sophie Cassaing[5], Christine Bonnal[6], Damien Costa[7], Laurence Lachaud[8], Lilia Hasseine[9], Lise Kristensen[10], Christine Schuttler[11], Hélène Raberin[12], Sophie Brun[13], Marijke Hendrickx[14], Dirk Stubbe[14], Renaud Piarroux[1,3,15] and Arnaud Fekkar[1,2,3]

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SUSCEPTIBILITY

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Multicentric Analysis of the Species Distribution and Antifungal Susceptibility of Cryptic Isolates from *Aspergillus* Section *Fumigati*

S. Imbert,[a,b] A. C. Normand,[a] S. Cassaing,[c] F. Gabriel,[d] L. Kristensen,[e] C. Bonnal,[f] L. Lachaud,[g] D. Costa,[h] J. Guitard,[i] L. Hasseine,[j] M. Palous,[a] M. Piarroux,[a,k] M. Hendrickx,[l] R. Piarroux,[a,k] A. Fekkar[a,b]

Received: 10 April 2021 | Revised: 25 June 2021 | Accepted: 25 June 2021
DOI: 10.1111/myc.13348

ORIGINAL ARTICLE

mycoses | WILEY

Invasive aspergillosis due to *Aspergillus* cryptic species: A prospective multicentre study

Sebastien Imbert[1,2] | Sophie Cassaing[3] | Christine Bonnal[4] | Anne-Cecile Normand[1] | Frederic Gabriel[5] | Damien Costa[6] | Marion Blaize[1,2] | Laurence Lachaud[7] | Lilia Hasseine[8] | Lise Kristensen[9] | Juliette Guitard[10] | Christine Schuttler[11] | Helene Raberin[12] | Sophie Brun[13] | Marijke Hendrickx[14] | Renaud Piarroux[1,15] | Arnaud Fekkar[1,2]

Vers une surveillance épidémiologique basée sur l’utilisation de MSI-2

CNR des Mycoses et Antifongiques
Laboratoire Associé « INuSuAI »
Site La Pitié-Salpêtrière

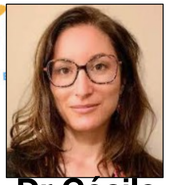
Responsable : Arnaud Fekkar
Contact : arnaud.fekkar@aphp.fr

Dr Arnaud Fekkar

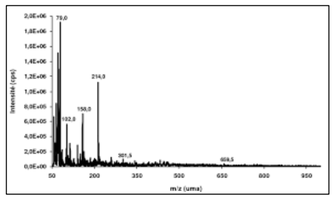
Pr Renaud Piarroux

Anne-Cécile Normand

Dr Marion Blaize


Dr Cécile Nabet

Identification Numérique



Spectre de masse MALDI-TOF

Identification rapide et performante

Surveillance épidémiologique

- **Identification des levures et des filamenteux**
- **Collecte de données**

→Analyses locales / nationales

→Evolution spatio-temporelle (influences régionales, saisonnalité…)

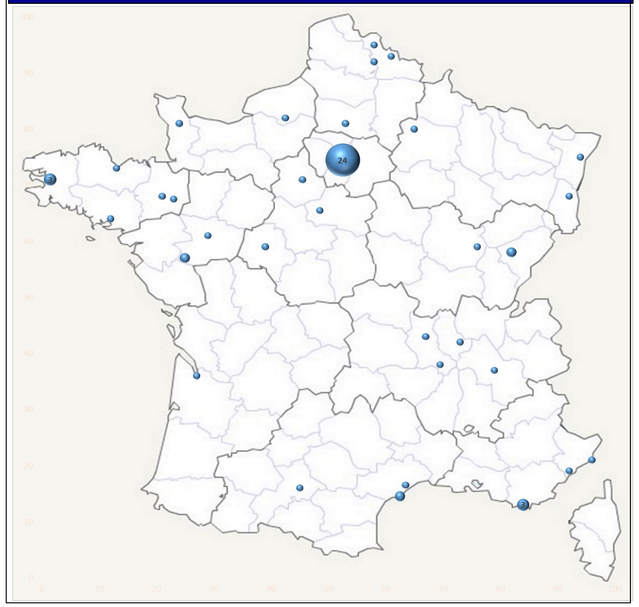
Alerte

Surveillance
CNR-IFI
Utilisateurs
SPF

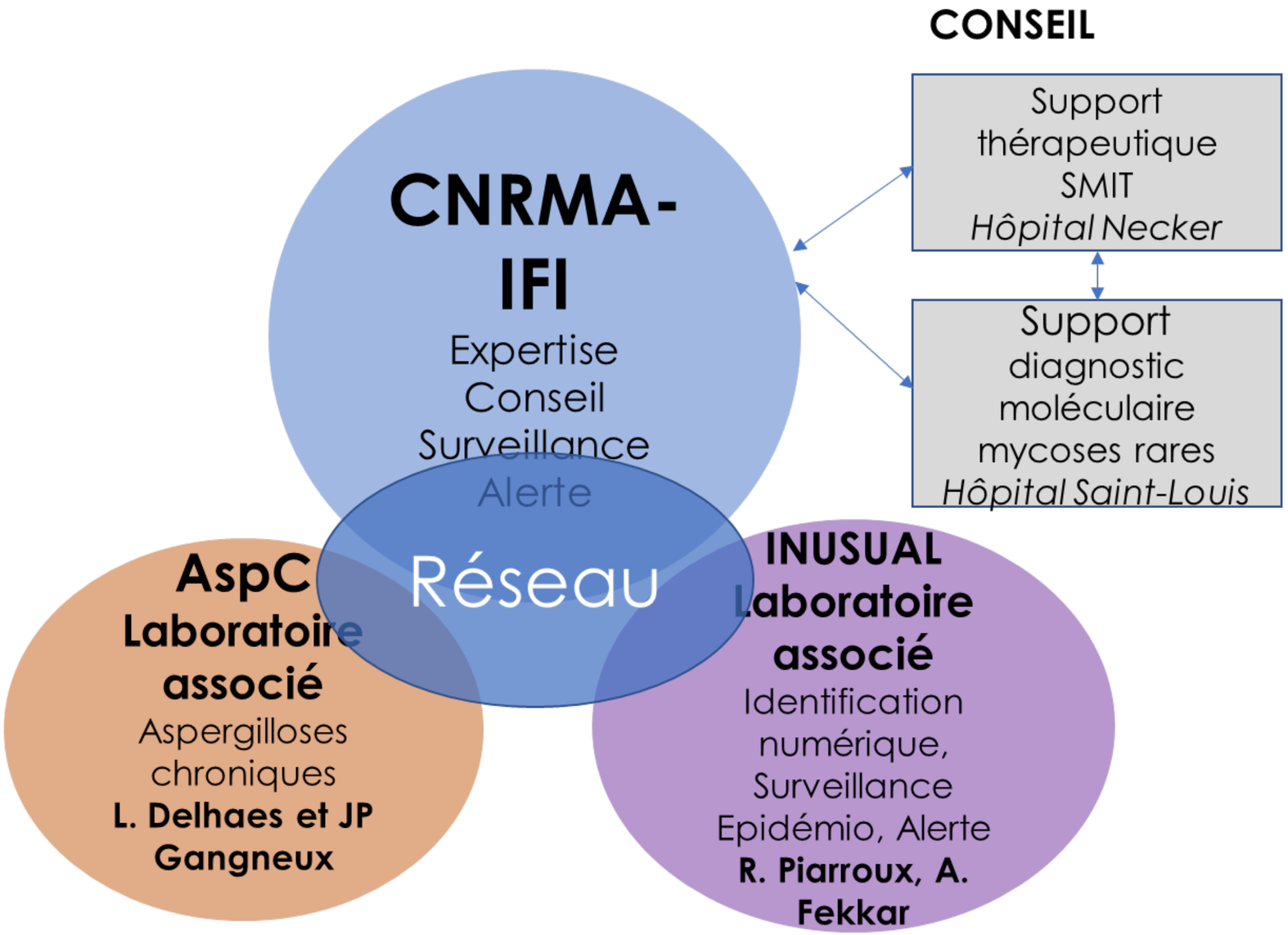
→ **Alerte épidémiologique** → **Mise en place de mesures / outils de suivi**

Réseau des utilisateurs de MSI

> 70 centres en France (métropole et Outre-mer)
> 40 000 spectres /mois



Projet CNRMA - SPF



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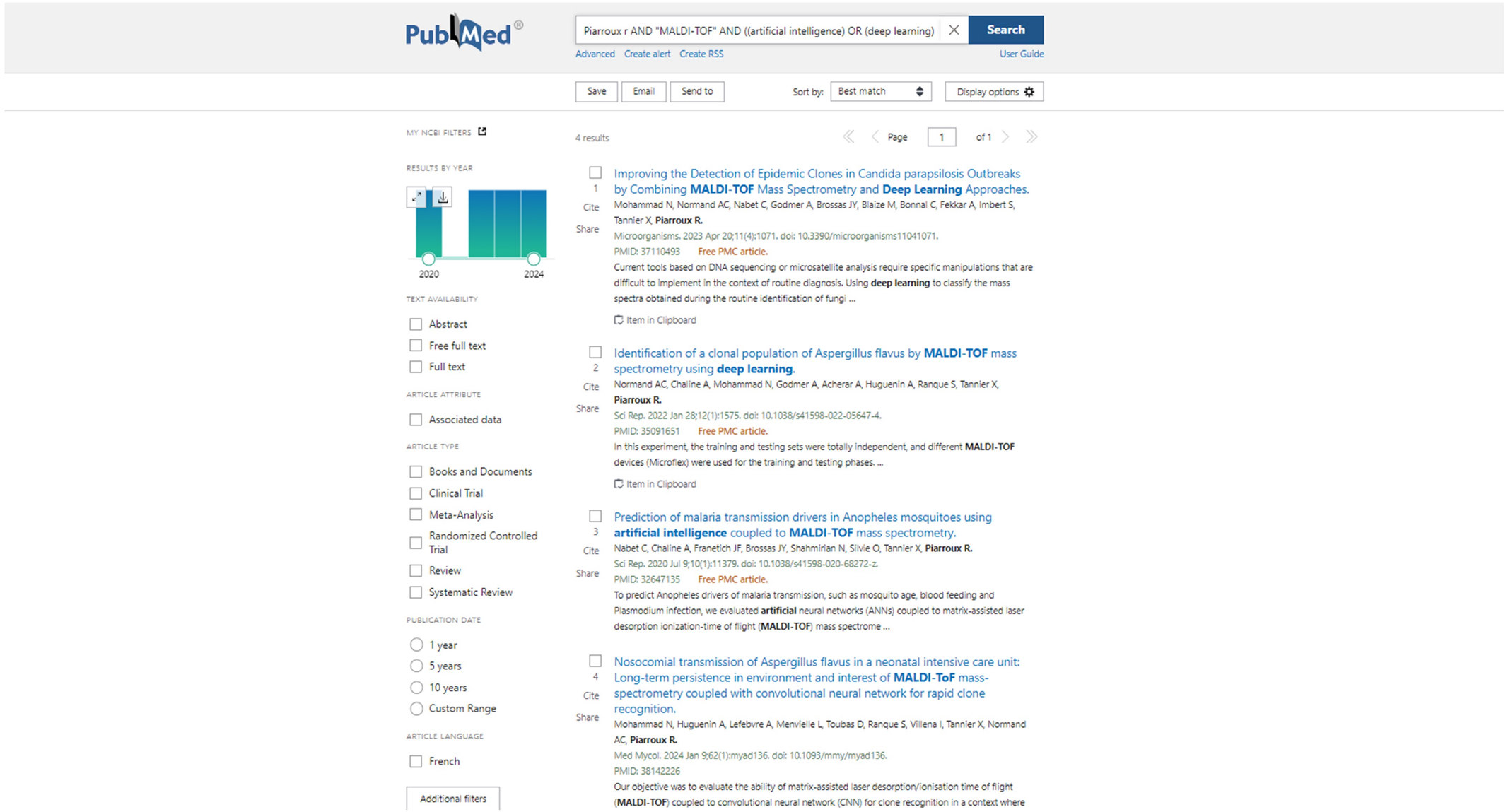
Spectrométrie de masse en ligne et IA

IA et Maldi-ToF



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Piarroux r AND "MALDI-TOF" AND ((artificial intelligence) OR (deep learning)

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1 Cite Share

Improving the Detection of Epidemic Clones in Candida parapsilosis Outbreaks by Combining **MALDI-TOF** Mass Spectrometry and **Deep Learning** Approaches.

Mohammad N, Normand AC, Nabet C, Godmer A, Brossas JY, Blaize M, Bonnal C, Fekkar A, Imbert S, Tannier X, **Piarroux R.**

Microorganisms. 2023 Apr 20;11(4):1071. doi: 10.3390/microorganisms11041071.

PMID: 37110493 Free PMC article.

Current tools based on DNA sequencing or microsatellite analysis require specific manipulations that are difficult to implement in the context of routine diagnosis. Using **deep learning** to classify the mass spectra obtained during the routine identification of fungi ...

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2 Cite Share

Identification of a clonal population of Aspergillus flavus by **MALDI-TOF** mass spectrometry using **deep learning**.

Normand AC, Chaline A, Mohammad N, Godmer A, Acherar A, Huguenin A, Ranque S, Tannier X, **Piarroux R.**

Sci Rep. 2022 Jan 28;12(1):1575. doi: 10.1038/s41598-022-05647-4.

PMID: 35091651 Free PMC article.

In this experiment, the training and testing sets were totally independent, and different **MALDI-TOF** devices (Microflex) were used for the training and testing phases. ...

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3 Cite Share

Prediction of malaria transmission drivers in Anopheles mosquitoes using **artificial intelligence** coupled to **MALDI-TOF** mass spectrometry.

Nabet C, Chaline A, Franetich JF, Brossas JY, Shahmirian N, Silvie O, Tannier X, **Piarroux R.**

Sci Rep. 2020 Jul 9;10(1):11379. doi: 10.1038/s41598-020-68272-z.

PMID: 32647135 Free PMC article.

To predict Anopheles drivers of malaria transmission, such as mosquito age, blood feeding and Plasmodium infection, we evaluated **artificial** neural networks (ANNs) coupled to matrix-assisted laser desorption ionization-time of flight (**MALDI-TOF**) mass spectrome ...

4 Cite Share

Nosocomial transmission of Aspergillus flavus in a neonatal intensive care unit: Long-term persistence in environment and interest of **MALDI-ToF** mass-spectrometry coupled with convolutional neural network for rapid clone recognition.

Mohammad N, Huguenin A, Lefebvre A, Menvielle L, Toubas D, Ranque S, Villena I, Tannier X, Normand AC, **Piarroux R.**

Med Mycol. 2024 Jan 9;62(1):myad136. doi: 10.1093/mmy/myad136.

PMID: 38142226

Our objective was to evaluate the ability of matrix-assisted laser desorption/ionisation time of flight (**MALDI-TOF**) coupled to convolutional neural network (CNN) for clone recognition in a context where

A la recherche de clones dans une épidémie

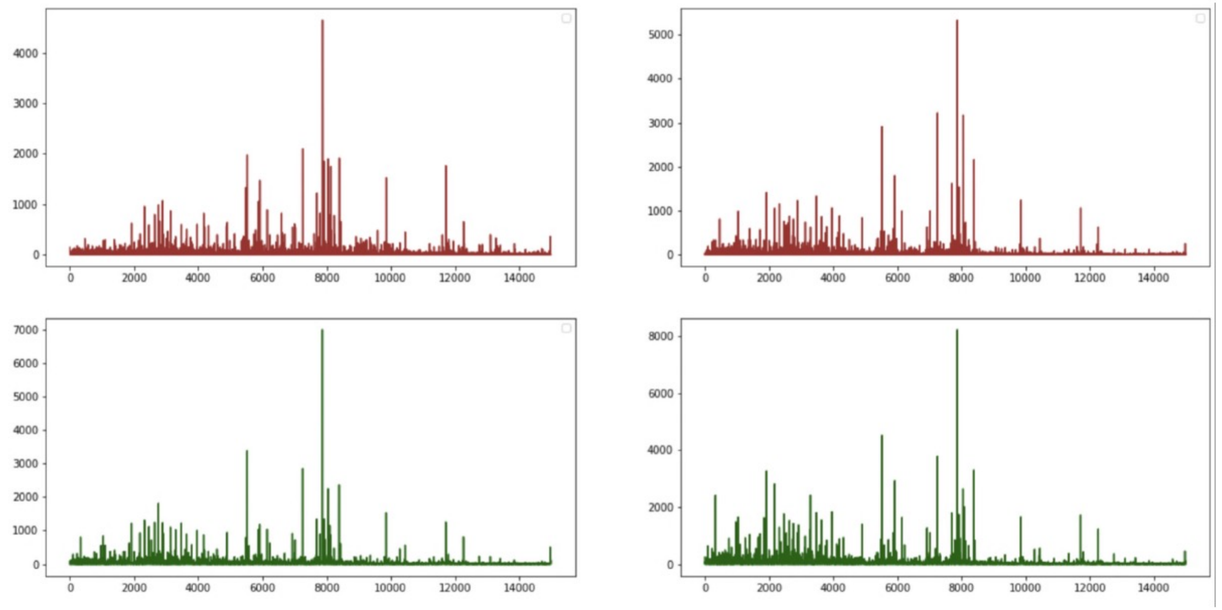


FIGURE 3.1 – **Visualisation de quatre spectres pré-traités de Clones et de Non-Clones de Candida parapsilosis.** Le rouge et le vert correspondent respectivement aux spectres des isolats appartenant ou non à l'ensemble clonal. Les isolats ont été cultivés dans les mêmes conditions et les spectres ont été acquis dans la même machine.

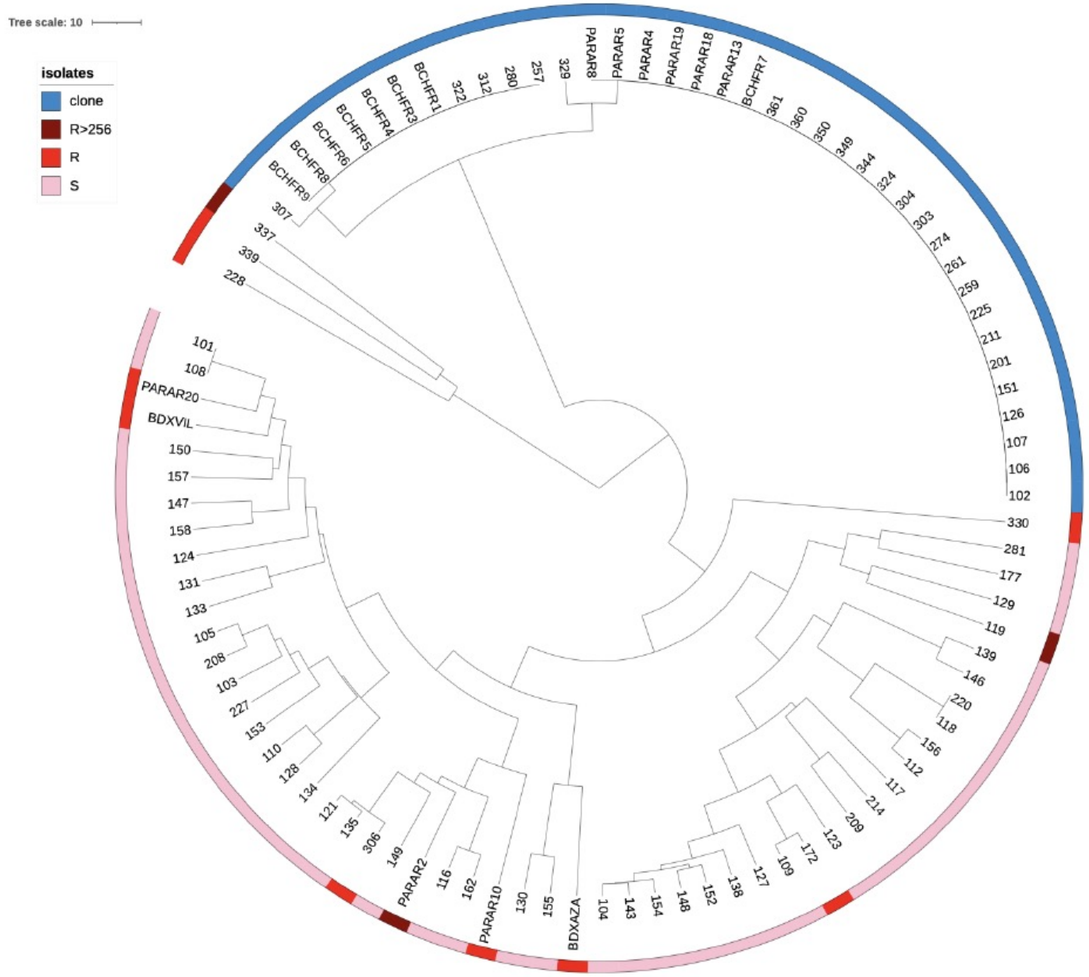


FIGURE 3.5 – **Dendrogramme des 96 isolats de *Candida parapsilosis* sélectionnés pour cette étude et typés par une approche microsatellite.**

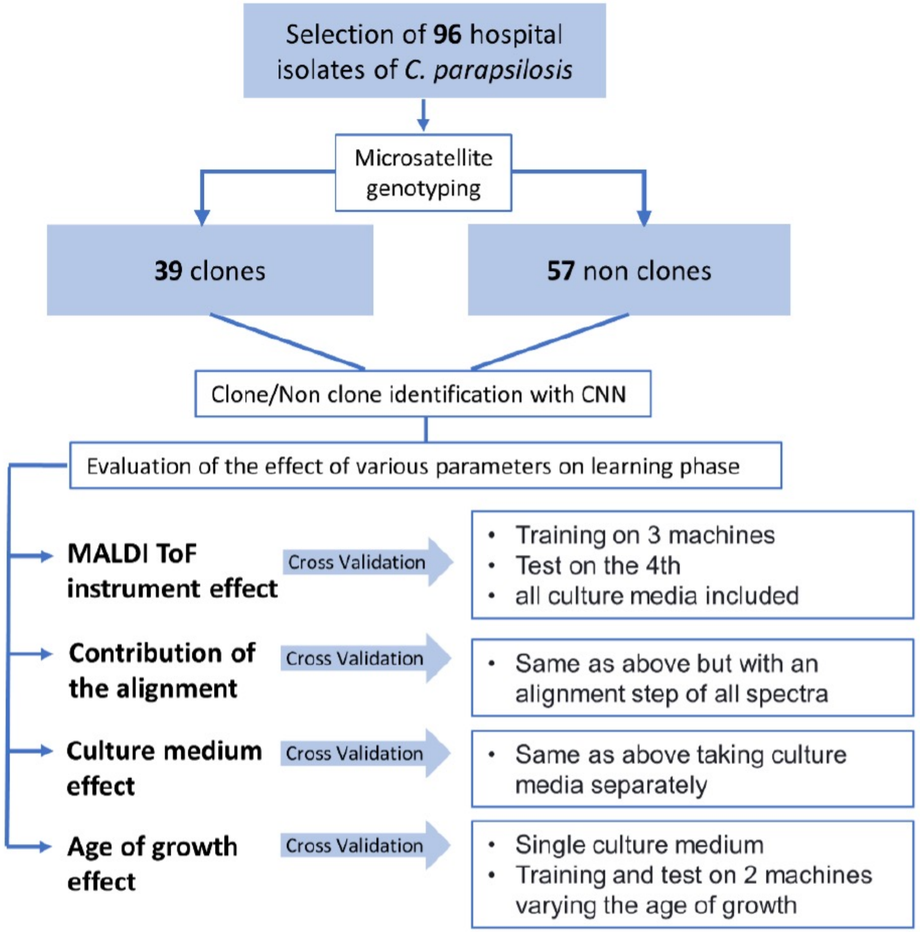


FIGURE 3.4 – **Organigramme de la conception de l'étude.**

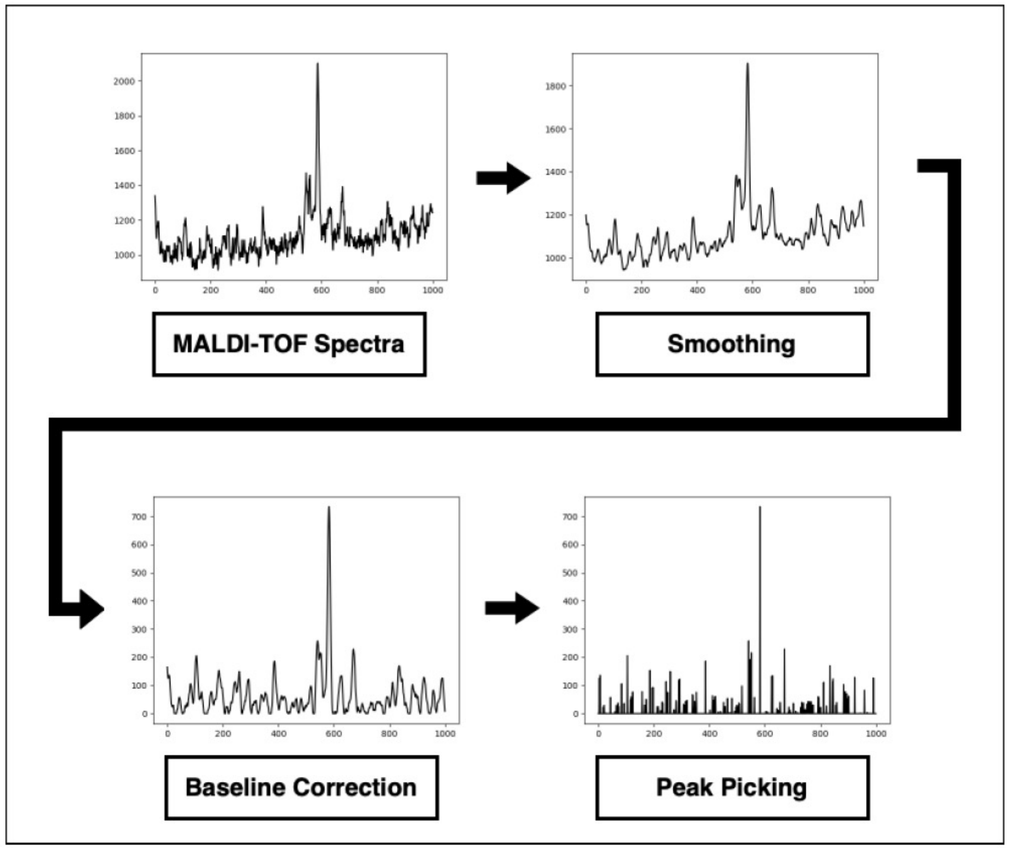


FIGURE 3.2 – **Prétraitement étape par étape des spectres, du spectre brut aux spectres traités, avant leur utilisation dans la phase d'apprentissage automatique.**

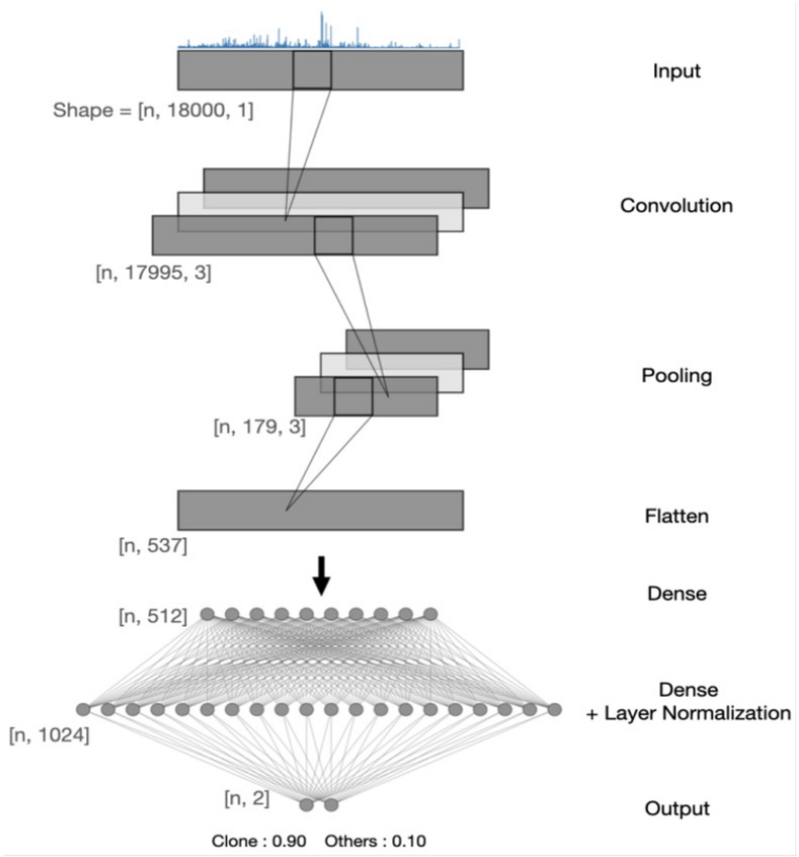


FIGURE 3.3 – **Architecture du modèle CNN créé et entraîné avec un ensemble de données.**
La forme de la couche de sortie a été ajoutée avec une taille de lot n fixée à 1 pour simplifier l'illustration.

	Accuracy	Score F1	Rappel	Spécificité
Machine Testée ; Performances Sans Alignement				
MYCO-PSL	0.89	0.87	0.90	0.86
	[0.87,0.92]	[0.84,0.90]	[0.86,0.94]	[0.83,0.90]
BACT-PSL	0.70	0.44	0.30	0.95
	[0.66,0.73]	[0.37,0.51]	[0.24,0.37]	[0.93,0.97]
SAINT-ANTOINE	0.83	0.74	0.65	0.90
	[0.80,0.86]	[0.71,0.80]	[0.59,0.71]	[0.87,0.93]
BICHAT	0.68	0.42	0.29	0.88
	[0.65,0.72]	[0.36,0.50]	[0.24,0.35]	[0.84,0.91]
Machine Testée ; Performances Avec Alignement				
MYCO-PSL	0.91	0.89	0.92	0.88
	[0.88,0.93]	[0.86,0.92]	[0.88,0.95]	[0.84,0.91]
BACT-PSL	0.81	0.74	0.64	0.92
	[0.78,0.85]	[0.68,0.78]	[0.57,0.70]	[0.89,0.95]
SAINT-ANTOINE	0.91	0.89	0.92	0.87
	[0.89,0.93]	[0.86,0.92]	[0.88,0.95]	[0.83,0.90]
BICHAT	0.84	0.79	0.75	0.87
	[0.81,0.87]	[0.75,0.83]	[0.68,0.80]	[0.84,0.91]

TABLEAU 3.1 – **Impact de la machine et de l'alignement avec MSIWarp.** Performance de l'identification des isolats appartenant à l'ensemble des clones par le modèle CNN (validation croisée sur 5 plis). Moyenne des ensembles d'entraînement de 1355 spectres obtenus sur trois machines et moyenne des ensembles de test de 113 spectres obtenus sur la quatrième machine.

	Accuracy	Score F1	Rappel	Spécificité
Machine Testée Avec Alignement ; Performances sur Chromagar				
MYCO-PSL	0.91	0.89	0.88	0.83
	[0.86,0.94]	[0.83,0.94]	[0.80,0.95]	[0.75,0.90]
BACT-PSL	0.77	0.62	0.47	0.96
	[0.71,0.83]	[0.55,0.75]	[0.37,0.59]	[0.92,0.99]
SAINT-ANTOINE	0.88	0.84	0.80	0.90
	[0.83,0.92]	[0.78,0.90]	[0.71,0.88]	[0.84,0.95]
BICHAT	0.81	0.72	0.61	0.96
	[0.75,0.86]	[0.64,0.82]	[0.50,0.71]	[0.91,0.99]
Machine Testée Avec Alignement ; Performances sur Sabouraud-CG				
MYCO-PSL	0.88	0.86	0.84	0.89
	[0.84,0.93]	[0.80,0.92]	[0.75,0.91]	[0.83,0.94]
BACT-PSL	0.93	0.92	0.95	0.88
	[0.89,0.96]	[0.87,0.96]	[0.89,0.99]	[0.82,0.94]
SAINT-ANTOINE	0.89	0.89	0.95	0.84
	[0.84,0.93]	[0.83,0.93]	[0.89,0.99]	[0.76,0.90]
BICHAT	0.89	0.88	0.89	0.92
	[0.85,0.94]	[0.82,0.92]	[0.81,0.95]	[0.87,0.97]
Machine Testée Avec Alignement ; Performances sur gélose Sang				
MYCO-PSL	0.92	0.89	0.87	0.95
	[0.88,0.96]	[0.86,0.96]	[0.79,0.94]	[0.90,0.98]
BACT-PSL	0.86	0.81	0.73	0.97
	[0.81,0.90]	[0.74,0.88]	[0.63,0.83]	[0.94,1.00]
SAINT-ANTOINE	0.93	0.92	0.96	0.87
	[0.89,0.96]	[0.87,0.96]	[0.91,1.00]	[0.81,0.93]
BICHAT	0.96	0.95	0.93	0.87
	[0.94,0.99]	[0.91,0.99]	[0.87,0.99]	[0.81,0.93]

TABLEAU 3.2 – **Impact du milieu de culture par machine.** Performance de l'identification des isolats appartenant à l'ensemble des clones par le modèle CNN (validation croisée sur 5 plis).

Vers un projet européen ?

Projet MaldiBank : architecture générale

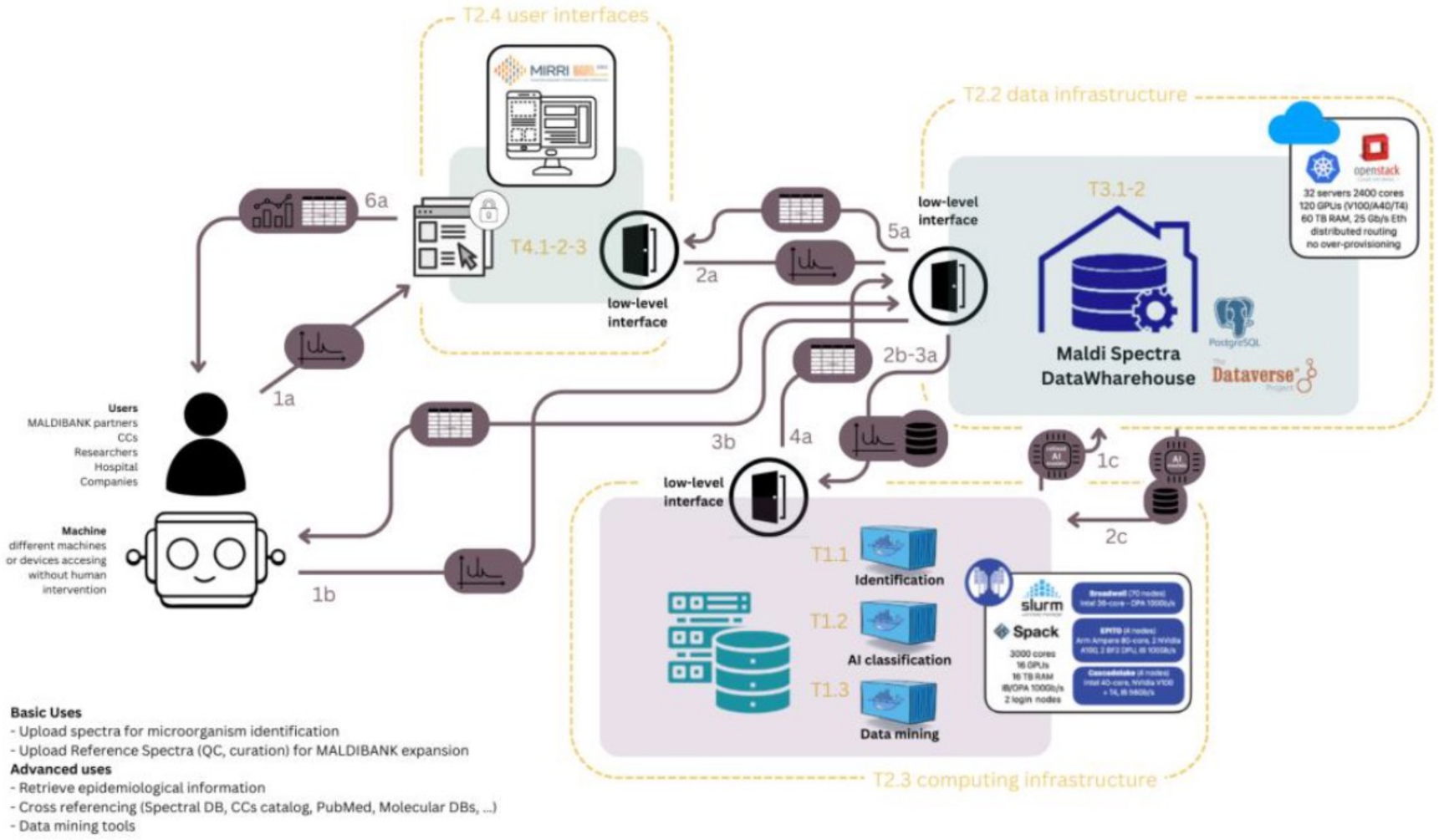


Figure 2: MALDIBANK Infrastructure interface for implemented services

Projet MaldiBank : collaboration entre les équipes

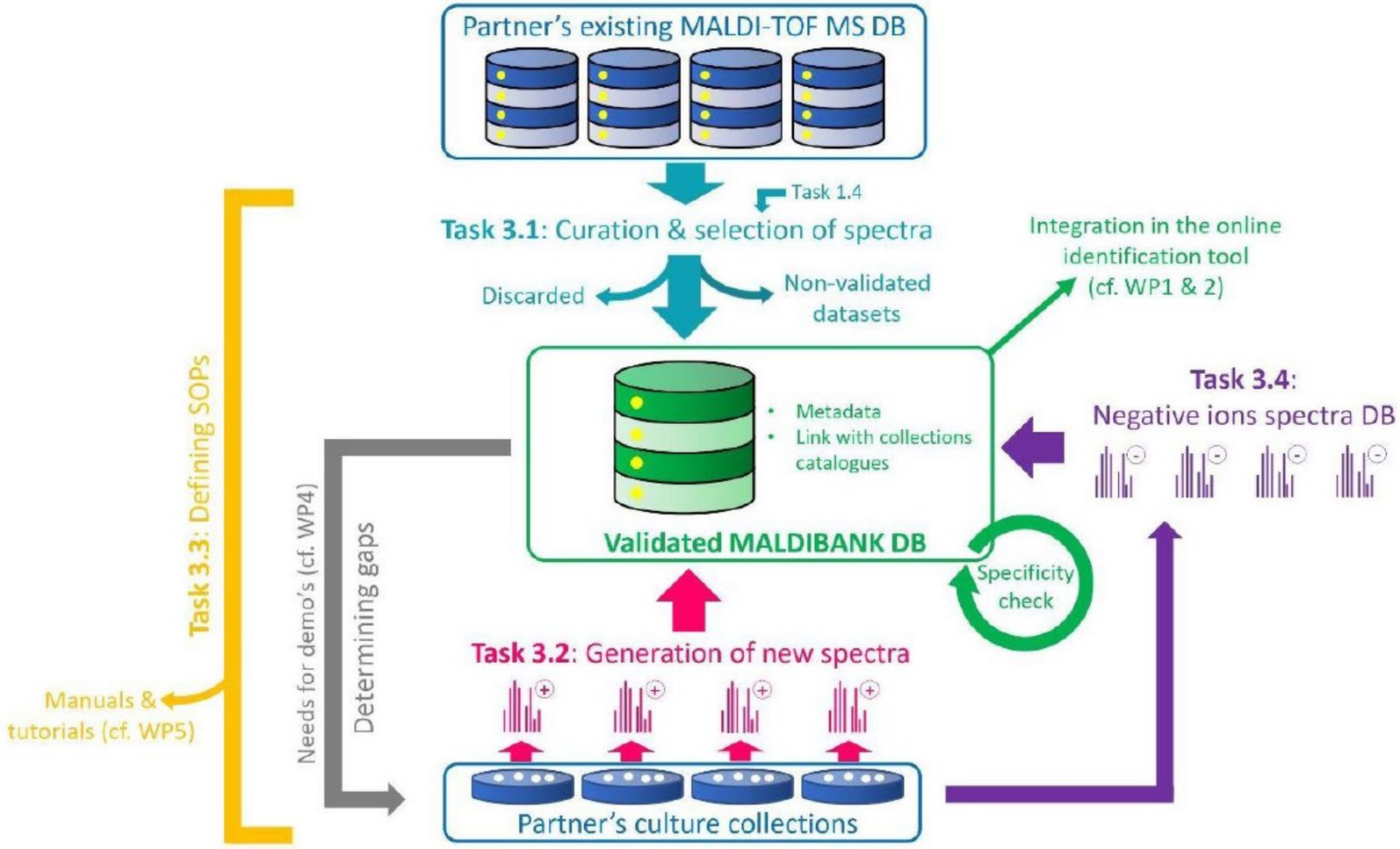
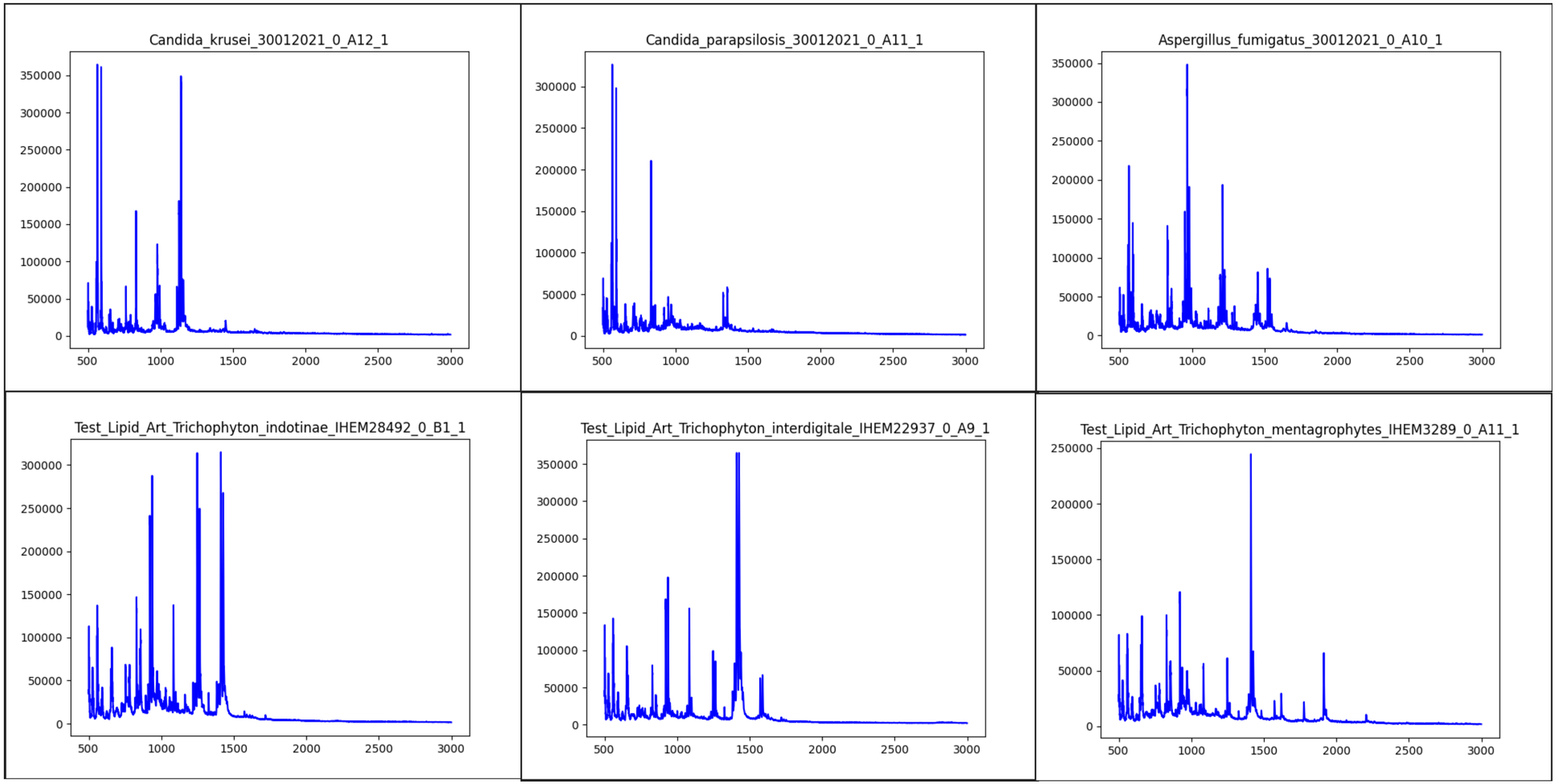


Figure 3: Workflow for the creation of the MALDIBANK datasets

Spectres en mode ions négatifs



Conclusion

La spectrométrie de masse : l’avenir de la mycologie ?

- Pour beaucoup c’est déjà le présent
- Offre de belles perspectives d’avenir
  - Capacité à affiner le diagnostic d’espèce
  - Possibilité de travailler en ligne
  - Développement IA possibles
  - Mise en commun des savoirs