



# Productions scientifiques de BIBS en 2021

INRAE Unité BIA  
Plate-forme BIBS  
Centre Pays-de-la-Loire  
La Géraudière  
44316 NANTES CEDEX 03

## Liste des productions scientifiques de la plate-forme BIBS en 2021

### 1- Articles dans des journaux à comité de lecture

- Barron, C., Devaux, M.F., Foucat, L., Falourd, X., Looten, R., Joseph-Aime, M., Durand, S., Bonnin, E., Lapiere, C., Saulnier, L., Rouau, X., Guillon, F., Enzymatic degradation of maize shoots: monitoring of chemical and physical changes reveals different saccharification behaviors. *Biotechnol Biofuels* 2021, 14, 1. <https://doi.org/10.1186/s13068-020-01854-1>
- Benkoulouche, M.; Ben Imeddourene, A.; Barel, L.-A.; Lefebvre, D.; Fanuel, M.; Rogniaux, H.; Ropartz, D.; Barbe, S.; Guieysse, D.; Mulard, L. A.; Remaud-Siméon, M.; Moulis, C.; André, I. Computer-Aided Engineering of a Branching Sucrase for the Glucodiversification of a Tetrasaccharide Precursor of S. Flexneri Antigenic Oligosaccharides. *Sci Rep* 2021, 11 (1), 20294. <https://doi.org/10.1038/s41598-021-99384-9>.
- Berger, M.; Devaux, M.F.; Legland, D.; Barron, C.; Delord, B.; Guillon, F., Darkfield and fluorescence macrovision of a series of large images to assess anatomical and chemical tissue variability in whole cross-sections of maize stems. *Frontiers in Plant Science*, 2021, 12, <https://doi.org/10.3389/fpls.2021.792981>.
- Buergy, A., Rolland-Sabaté, A., Leca, A., Falourd, X., Foucat, L., Renard, C. M., Pectin degradation accounts for apple tissue fragmentation during thermomechanical-mediated puree production. *Food Hydrocolloids*, 2021, 120, 106885. <https://doi.org/10.1016/j.foodhyd.2021.106885>
- Chateigner-Boutin, A. L., Alvarado, C., Devaux, M. F., Durand, S., Foucat, L., Geairon, A., Grélard, F., Jamme, F., Rogniaux, H., Saulnier, L., Guillon, F., The endosperm cavity of wheat grains contains a highly hydrated gel of arabinoxylan. *Plant Science*, 2021, 306, 110845. <https://doi.org/10.1016/j.plantsci.2021.110845>
- Chen, M., Falourd, X., Lahaye, M., Sequential natural deep eutectic solvent pretreatments of apple pomace: A novel way to promote water extraction of pectin and to tailor its main structural domains. *Carbohydrate Polymers*, 2021, 266, 118113. <https://doi.org/10.1016/j.carbpol.2021.118113>
- El Mecherfi, K.-E.; Lupi, R.; Cherkaoui, M.; Albuquerque, M. A. C.; Todorov, S. D.; Tranquet, O.; Klingebiel, C.; Rogniaux, H.; Denery-Papini, S.; Onno, B.; de Melo Franco, B. D. G.; Larre, C. Fermentation of Gluten by Lactococcus Lactis LLGKC18 Reduces Its Antigenicity and Allergenicity. *Probiotics Antimicrob. Proteins* 2021. <https://doi.org/10.1007/s12602-021-09808-1>.
- Favreau, B.; Yeni, O.; Ollivier, S.; Boustie, J.; Dévéhat, F. L.; Guégan, J.-P.; Fanuel, M.; Rogniaux, H.; Brédy, R.; Compagnon, I.; Ropartz, D.; Legentil, L.; Ferrières, V. Synthesis of an Exhaustive Library of Naturally Occurring Galp-Manp and Galp-Manp Disaccharides. Toward Fingerprinting According to Ring Size by Advanced Mass Spectrometry-Based IM-MS and IRMPD. *The Journal of Organic Chemistry* 2021, 86, 6390–6405. <https://doi.org/10.1021/acs.joc.1c00250>.
- Grélard, F.; Legland, D.; Fanuel, M.; Arnaud, B.; Foucat, L.; Rogniaux, H. Esmraldi: efficient methods for the fusion of mass spectrometry and magnetic resonance images. *BMC Bioinformatics* 2021, 22(1), 56. <https://doi.org/10.1186/s12859-020-03954-z>.
- Lahaye, M., Tabi, W., Le Bot, L., Delaire, M., Orsel, M., Campoy, J.A., Quero Garcia, J., Le Gall, S. Comparison of cell wall chemical evolution during the development of quality contrasted fruits from two members of the Rosaceae family: apple and sweet cherry. *Plant Physiol.*, 2021, 168, 96-104. [doi.org/10.1016/j.plaphy.2021.10.002](https://doi.org/10.1016/j.plaphy.2021.10.002)
- Laue, C. Stevens, Y., van Erp, M., Papazova, E., Soeth, E., Pannenbeckers, A., Stolte, E., Böhm, R., Le Gall, S., Falourd, X., Ballance, S., Knutsen, S.H., Pinheiro, I., Possemiers, S., Ryan, P.M., Ross, R.P., Stanton, C., Wells, J.M., van der Werf, S., Mes, J.J., Schrezenmeier, J. Adjuvant Effect of Orally Applied Preparations Containing Non-Digestible Polysaccharides on Influenza Vaccination in the Healthy Elderly: A Double-Blind, Randomised, Controlled Pilot Trial. *Nutrients* 2021, 13, 2683. <https://doi.org/10.3390/nu13082683>

12. Le Gall, S., Sole-Jamault, V., Nars-Chasseray, M., Le Goff, A., Le Bot, L., Guinet, T., Renaud, C., Gervais, J., Bansard, S., Ohleyer, L., Jeandroz, S. Data on agronomic traits, biochemical composition of lipids, proteins and polysaccharides and rheological measurement in a brown mustard seed collection. *Data In Brief*. 2021. <https://doi.org/10.1016/j.dib.2021.107417>
13. Leroy, A., Falourd, X., Foucat, L., Méchin, V., Guillon, F., Paës, G., Evaluating polymer interplay after hot water pretreatment to investigate maize stem internode recalcitrance. *Biotechnol Biofuels* 2021, 14, 164. <https://doi.org/10.1186/s13068-021-02015-8>
14. Li, F., Foucat, L., Bonnin, E., Effect of solid loading on the behaviour of pectin-degrading enzymes. *Biotechnology for Biofuels*, 2021, 14(1), 1-12. <https://doi.org/10.1186/s13068-021-01957-3>
15. Lollier, V.; Fanuel, M.; Ropartz, D.; Tessier, D.; Rogniaux, H. Oligator: A Flexible Interface to Draw Oligosaccharide Structures and Generate Their Theoretical Tandem Mass Spectra. *Bioinformatics* 2021, 37 (22), 4261–4262. <https://doi.org/10.1093/bioinformatics/btab412>
16. Lysiak, A.; Fertin, G.; Jean, G.; Tessier, D. Evaluation of open search methods based on theoretical spectra comparison. *BMC Bioinformatics* 2021. <https://doi.org/10.1186/s12859-021-03963-6>.
17. Marc, M., Risani, R., Desnoes, E., Falourd, X., Pontoire, B., Rodrigues, R., Escorcio, R., Batista, A.P., Valentin, R., Gontard, N., Silva Pereira, C., Lopez, C., Leroy, E., Lourdin, D., Marion, D., Bakan, B., Bioinspired co-polyesters of hydroxy-fatty acids extracted from tomato peel agro-wastes and glycerol with tunable mechanical, thermal and barrier properties. *Industrial Crops and Products*, 2021, 170, 113718. <https://doi.org/10.1016/j.indcrop.2021.113718>
18. Mendis, P. M.; Sasiene, Z. J.; Ropartz, D.; Rogniaux, H.; Jackson, G. P. Structural Characterization of Isomeric Oligogalacturonan Mixtures Using Ultrahigh-Performance Liquid Chromatography-Charge Transfer Dissociation Mass Spectrometry. *Anal. Chem.* **2021**, 93 (5), 2838–2847. <https://doi.org/10.1021/acs.analchem.0c04142>.
19. Mendis, P. M.; Sasiene, Z. J.; Ropartz, D.; Rogniaux, H.; Jackson, G. P. Ultra-High-Performance Liquid Chromatography Charge Transfer Dissociation Mass Spectrometry (UHPLC-CTD-MS) as a Tool for Analyzing the Structural Heterogeneity in Carrageenan Oligosaccharides. *Anal. Bioanal. Chem.* **2021**. <https://doi.org/10.1007/s00216-021-03396-3>.
20. Nikolić Chenais J, Marion L, Larocque R, Jam M, Jouanneau D, Cladiere L, Le Gall S, Fanuel M, Desban N, Rogniaux H, Ropartz D, Ficko-Blean E, Michel G. Systematic comparison of eight methods for preparation of high purity sulfated fucans extracted from the brown alga *Pelvetia canaliculata*. *Int J Biol Macromol.* 2021 Dec 27;S0141-8130(21)02752-5. <https://doi:10.1016/j.ijbiomac.2021.12.122>
21. Ollivier, S.; Tarquis, L.; Fanuel, M.; Li, A.; Durand, J.; Laville, E.; Potocki-Veronese, G.; Ropartz, D.; Rogniaux, H. Anomeric Retention of Carbohydrates in Multistage Cyclic Ion Mobility (IMSn): De Novo Structural Elucidation of Enzymatically Produced Mannosides. *Analytical Chemistry* 2021, 93 (15), 6254–6261. <https://doi.org/10.1021/acs.analchem.1c00673>.
22. Ollivier, S., Fanuel, M., Rogniaux, H., Ropartz, D. Molecular Networking of High-Resolution Tandem Ion Mobility Spectra: A Structurally Relevant Way of Organizing Data in Glycomics? *Analytical Chemistry* 2021, 93 (31), 10871-10878. <https://doi.org/10.1021/acs.analchem.1c01244>
23. Orm, R. B., Jury, V., Falourd, X., Boillereaux, L., Guihard, L., Le Bail, A., Impacts of the baking heating rate on the water mobility, starch microstructure and mechanical properties of degassed crumb during staling. *Journal of Cereal Science*, 2021, 100, 103228. <https://doi.org/10.1016/j.jcs.2021.103228>
24. Prasanna, M.; Podsiadla-Bialoskorska, M.; Mielecki, D.; Ruffier, N.; Fateh, A.; Lambert, A.; Fanuel, M.; Camberlein, E.; Szolajska, E.; Grandjean, C. On the Use of Adenovirus Dodecahedron as a Carrier for Glycoconjugate Vaccines. *Glycoconjugate J.* **2021**, 38 (4), 437–446. <https://doi.org/10.1007/s10719-021-09999-3>.
25. Sasiene, Z. J.; Mendis, P. M.; Ropartz, D.; Rogniaux, H.; Jackson, G. P. The Influence of Na/H Exchange on the Charge Transfer Dissociation (CTD) Spectra of Mannuronic Acid Oligomers. *Int. J. Mass Spectrom.* **2021**, 468, 116634. <https://doi.org/10.1016/j.ijms.2021.116634>.
26. Sasiene, Z. J.; Ropartz, D.; Rogniaux, H.; Jackson, G. P. Charge Transfer Dissociation of a Branched Glycan with Alkali and Alkaline Earth Metal Adducts. *J. Mass Spectrom.* **2021**, 56 (7), e4774. <https://doi.org/10.1002/jms.4774>.
27. Sichert, A.; Le Gall, S.; Klau, L. J.; Laillet, B.; Rogniaux, H.; Aachmann, F. L.; Hehemann, J.-H. Ion-Exchange Purification and Structural Characterization of Five Sulfated Fucoidans from Brown Algae. *Glycobiology* **2021**, 31 (4), 352–357. <https://doi.org/10.1093/glycob/cwaa064>.

28. Voisin, H., Falourd, X., Rivard, C., Capron, I., Versatile nanocellulose-anatase TiO<sub>2</sub> hybrid nanoparticles in Pickering emulsions for the photocatalytic degradation of organic and aqueous dyes. *JCIS Open*, 2021, 100014. <https://doi.org/10.1016/j.jciso.2021.100014>
29. Renard, D., Davantès, A., D'Orlando, A., Cahier, K., Molinari, M., Nigen, M., Chalier, P. & Sanchez, C., Adsorption of arabinogalactan-proteins from Acacia gums (senegal and seyal) and its molecular fractions onto latex particles. *Food Hydrocolloids*, 2021, 107360. <https://doi.org/10.1016/j.foodhyd.2021.107360>
30. Sakai, K., Citerne, S., Antelme, S., Le Bris, P., Daniel, S., Boudier, A., D'Orlando, A., Cartwright, A., Tellier, D., Pateyron, S., Delannoy, E., Laudencia-Chingcuanco, D., Mouille, G, Palauqui, J.C., Vogel, J., Sibout, R. (2021). BdERECTA controls vasculature patterning and phloem-xylem organization in *Brachypodium distachyon*. *BMC Plant Biology*, 2021, 21(1). <https://doi.org/10.1186/s12870-021-02970-2>
31. Delvart, A., Moreau, C., D'Orlando, A., Falourd, X., & Cathala, B. (2022). Dextran-based polyelectrolyte multilayers: Effect of charge density on film build-up and morphology. *Colloids and Surfaces B: Biointerfaces*, 2022, 210, 112258. <https://doi.org/10.1016/j.colsurfb.2021.112258>

## 2- Ouvrages et chapitres d'ouvrages

1. Boudry, G., Charton E., Le Huërou-Luron, I., Ferret-Bernard, S., Le Gall, S., EVEN, S., Blat, S. The relationship between breast milk components and the infant gut microbiota. *Frontiers in Nutrition*. 2021. <https://doi.org/10.3389/fnut.2021.629740>
2. Rousseaux A., Brosseau C., Le Gall S., Piloquet H., Barbarot S., Bodinier M. Human Milk Oligosaccharides: Their Effects on the Host and Their Potential as Therapeutic Agents. *Frontiers in Immunology*. 2021. DOI=10.3389/fimmu.2021.68091
3. Fertin G., David M., Rogniaux H., Tessier D. Mass spectra interpretation and the interest of specFit for identifying uncommon modifications. *Computation Intelligence Methods for Bioinformatics*. 2021. DOI=10.1007/978-3-030-63061-4. Springer.
4. Bardeau, JF., Humbert Bernard, D'Orlando, A., Louarn, G., Chapitre 7, Spectroscopies vibrationnelles. Théorie, aspects pratiques et applications, Editions des archives contemporaines, France, ISBN : 9782813002556, 322p., <https://doi.org/10.17184/eac.9782813002556>

## 3- Communications dans des colloques nationaux ou internationaux

### 3.1 Communications orales invitées

1. Ropartz, D. 2021. Experience and Perspective on the Cyclic IMS for Characterization of Oligo-/Polysaccharides Webinar Series: The innovation and Impact of IMS-MS, Webinar: 2020/02/17
2. Ropartz, D. 2021. Cyclic IMS: Structural characterization of carbohydrates and enzymes. Boston Glycobiology Discussion Group. Webinar. 2021/03/17
3. Fanuel, M. (2021) Imagerie en 3D du grain de blé : quand la spectrométrie de masse rencontre l'IRM. Animation scientifique SFSM-FPS-RFMF (Forum Labo). Paris (FR): 2021/10/05
4. Legland, D. (2021) Quantification morphologique pour l'imagerie des bio-ressources. GDR Morphéa, Nancy (FR) : 2021/10/04-05.

### 3.2 Communications orales dans des congrès nationaux ou internationaux

1. Lissarrague, A. Impact of industrial extraction processes on the enzymatic degradability and structures of carrageenans. Journée des jeunes chercheurs, Station Biologique. Roscoff (FR) : 2021/02/17
2. Nesi, N., Solé, V. & Le Gall, S. SEEDQUAL : caractérisation de la diversité génétique de la composition de la graine et du tourteau de colza pour des usages en alimentation animale. E-Carrefours Colza : 2021/01/21
3. Ollivier, S. ; Fanuel, M. ; Ropartz, D. ; Rogniaux, H. Molecular networking of tandem ion mobility data and its implications for glycomics. Journées Françaises de Spectrométrie de Masse 2021 (online): 2021/06/14-24.
4. Le, T.D.Q. ; Legland, D. ; Paré, L.; Chateigner-Boutin, A.-L.; Girousse, C. Analysis of the growth of wheat grains using improved 3D morphological filtering. 13th European Conference on Stereology and Image Analysis (ECSIA) (online): 2021/06/28-30.

5. [Grélard, F.](#); [Legland, D.](#); [Fanuel, M.](#); [Foucat, L.](#); [Rogniaux, H.](#) (2021) Fusion of Three-Dimensional Mass Spectrometry and Magnetic Resonance Images. OurCon 2021 (online): 2021/10/12-13
6. [Ollivier, S.](#) ; [Fanuel, M.](#) ; [Ropartz, D.](#); [Rogniaux, H.](#) New prospects for the structural characterization of oligosaccharides : an overview of novel analytical methods relying in cyclic ion mobility mass spectrometry. 7th International Polysaccharide conference (EPNOE), Nantes (FR): 2021/10/11-15.
7. [Legland, D.](#) (2021) Morphométrie et croissance du grain de blé par recalage d'images 3D de tomographie. Colloque Graines, Lyon (FR) : 2021/10/25-27.
8. [Lysiak, A.](#); [Fertin, G.](#); [Jean G.](#); [Tessier D.](#) (2021) SpecGlob : a new dynamic programming algorithm to interpret mass spectra. SeqBim (2021), Lyon (FR): 2021/11/25-26
9. [Falourd, X.](#), [Leroy, A.](#), [Méchin, Guillon, F.](#), [Paës, G.](#), [Foucat, L.](#) How solid-state and low-field NMR can contribute to the supramolecular organization elucidation of the lignocellulosic biomass during deconstruction? Euromar 2021 (online): 2021/07/05-08.
10. [Falourd, X.](#), [Lahaye, M.](#), [Rondeau-Mouro, C.](#) Assessment of cellulose structure diversity and interactions by ssNMR. 7th International Polysaccharide conference (EPNOE), Nantes (FR): 2021/10/11-15.
11. [Falourd, X.](#), [Lahaye, M.](#), [Rondeau-Mouro, C.](#) CRIDAM : Assessment of cellulose structure diversity and interactions by ssNMR. Réunion d'automne RMN-GBP, Orsay (FR): 2021/11/19.
12. [A. Leroy, X. Falourd, L. Foucat, F. Guillon, G. Paës.](#) Multiscale analysis of the influence of hot water pretreatment: consequences on lignocellulosic biomass recalcitrance 29th European Biomass Conference & Exhibition (visioconférence) 26-29 avril 2021 – Marseille – France
13. [De Oliveira, L.](#), [Langella, O.](#), [Balliau, T.](#), [Tessier, D.](#), [Blein-Nicolas, M.](#), [Zivy, M.](#) SpecOMS, an open modification search approach challenging high-throughput single amino acid variations identification. INPPO (International Plant Proteomics Organisation), 2021, virtual meeting. 2021/03/09-11
14. [Le Bourgot C.](#), [Richer Y.](#), [Le Gall S.](#), [Lollier V.](#), [Blat S.](#), [Le Huërou-Luron I.](#) La supplémentation en prébiotiques de l'alimentation maternelle influence la composition de son lait et est associée à des modifications de la composition et de l'activité fermentaire du microbiote de la descendance. 5eme congrès de la SF-DOHAD, Jouy-en-Josas, FR, 17-19/11/2021.
15. [Lissarrague, A.](#) Structural elucidation of a wide diversity of carrageenans by RP-IP-LC hyphenated to He-CTD MS/MS. RCJSM, online : 2021/03/30
5. [Cherkaoui, M.](#) DeepProt Project - Algorithmic approaches to decipher modifications of food proteins. Journée jeunes chercheurs BIA : 03/06/2021
6. [Cherkaoui, M.](#) (2021). A structural analysis of heated ovalbumin by crosslink proteomics. Animation scientifique de l'axe Analyses Structurales et Métabolomique de BioGenOuest. Webinar: 2021/12/09
7. [Ollivier, S.](#) (2021) Aperçu de nouvelles méthodes analytiques basées sur la spectrométrie de masse à mobilité ionique cyclique : nouvelles perspectives pour la caractérisation structurale des oligosaccharides. Animation scientifique de l'axe Analyses Structurales et Métabolomique de BioGenOuest. Webinar: 2021/12/09
16. [D'Orlando, A.](#), [Grélard, F.](#), [Reynoud, N.](#), [Bakan, B.](#), [Fanuel, M.](#), [Novales, B.](#), [Guillon, F.](#), [Devaux, MF.](#), [Jamme, F.](#), [Foucart, L.](#), [Rogniaux, H.](#), [Legland, D.](#), Imagerie Corrélative sur la plateforme BIBS. JST2021 du réseau des microscopistes INRAE (RµI), 2021/11/24-26, présentation flash
- 17.

### 3.3 Communications par affiche

1. [Chateigner-Boutin, A.-L.](#), [Alvarado, C.](#), [Devaux, M.-F.](#), [Durand, S.](#), [Foucat, L.](#), [Geairon, A.](#), [Grélard, F.](#), [Jamme, F.](#), [Rogniaux, H.](#), [Saulnier, L.](#), [Guillon, F.](#) The endosperm cavity of wheat grains contains a highly hydrated gel of arabinoxylan. PCWB2021 (Plant Cell Wall Biology), **2021**, virtual meeting, Japan (JP): 2021/06/27-2021/07/01
2. [Berger, M.](#), [Devaux, M.-F.](#), [Legland, D.](#), [Barron, C.](#), [Delord, B.](#), [Guillon, F.](#) Using darkfield and fluorescence macrovision on large images to assess anatomical and chemical variability of tissues in whole cross sections of maize stems. PCWB2021 (Plant Cell Wall Biology), **2021**, virtual meeting, Japan (JP): 2021/06/27-2021/07/01
3. [Lissarrague, A.](#) ; [Jam, M.](#); [Mangiante, G.](#); [Fanuel, M.](#); [Boulenguer, P.](#); [Ropartz, D.](#); [Hervé, C.](#); [Rogniaux, H.](#) (2021) Towards a better understanding of the structure-function relationship in carrageenans using breakthrough mass spectrometry techniques. 7th International Polysaccharide conference (EPNOE), Nantes (FR): 2021/10/11-15

4. Falourd, X., Lollier, V., Lahaye, M., Rondeau-Mouro, C. Reducing acquisition and processing duration in solid-state NMR : a critical point for wider use. 7th International Polysaccharide conference (EPNOE), Nantes (FR): 2021/10/11-15.
5. A. Leroy, X. Falourd, L. Foucat, V. Méchin, F. Guillon, G. Paës. Beyond the content, the lignin conformation has a critical impact on the cellulose accessibility. 7th International Conference on Plant Cell Wall Biology 2021 (visioconférence) 27 juin – 1er juillet 2021
6. Lysiak, A., Fertin, G., Jean, G., Tessier, D. Detection of multiple modifications in mass spectra without any a priori. 69th ASMS Conference, Philadelphia (USA) (visioconférence): 2021/10/31-2021/11/04
7. Cherkaoui, M., Larre, C., Brossard C., Tessier D., Rogniaux H., Dijk W. (2021). A structural analysis of heated ovalbumin by crosslink proteomics. HUPO Reconnect 2021. Webinar : 2021/11/15 → 2021/11/19
8. D'Orlando, A., Grélard, F., Reynoud, N., Bakan, B., Fanuel, M., Novales, B., Guillon, F., Devaux, MF., Jamme, F., Foucart, L., Rogniaux, H., Legland, D., Imagerie Corrélative sur la plateforme BIBS. JST2021 du reseau des microscopistes INRAE (RµI), 2021/11/24-26

#### 4- Enseignements (cours, ateliers, etc.)

1. Master I parcours A3M (Université de Nantes). Cours et TP en imagerie par spectrométrie de masse. Durée 3h. Rogniaux, H., Fanuel, M. 2021/01/21
2. Master II CQPS (Université de Nantes). Cours et TP en imagerie par spectrométrie de masse et en mobilité ionique. Durée 6h. Rogniaux, H., Fanuel, M., Ollivier, S. Ropartz, D. 2021/03/10

#### 5- Mémoires de stage

1. MOUALFI, Mohamed. Rapport de stage M2 Physique Appliquée et Ingénierie Physique (Université d'Angers, 6 mois). Développement d'une bibliothèque Matlab pour le traitement des images hyperspectrales.
2. VINTER, Fanny. Rapport de stage M1 A3M (Université de Nantes, 2021, 5 mois). Développement d'une méthode de fonctionnalisation de pointes AFM pour l'étude des interactions biomoléculaires de protéines végétales et polysaccharides