Leibniz Gemeinschaft

Der Senat

12. Juli 2022

Stellungnahme zum Leibniz-Institut für Lebensmittel-Systembiologie an der Technischen Universität München, Freising (Leibniz-LSB@TUM)

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Vorbemerkung

Die Einrichtungen der Forschung und der wissenschaftlichen Infrastruktur, die sich in der Leibniz-Gemeinschaft zusammengeschlossen haben, werden von Bund und Ländern wegen ihrer überregionalen Bedeutung und eines gesamtstaatlichen wissenschaftspolitischen Interesses gemeinsam gefördert. Turnusmäßig, spätestens alle sieben Jahre, überprüfen Bund und Länder, ob die Voraussetzungen für die gemeinsame Förderung einer Leibniz-Einrichtung noch erfüllt sind.[1]

Die wesentliche Grundlage für die Überprüfung in der Gemeinsamen Wissenschaftskonferenz ist regelmäßig eine unabhängige Evaluierung durch den Senat der Leibniz-Gemeinschaft. Die Stellungnahmen des Senats bereitet der Senatsausschuss Evaluierung vor.

Für die Bewertung einer Einrichtung setzt der Ausschuss Bewertungsgruppen mit unabhängigen, fachlich einschlägigen Sachverständigen ein. Der für das Leibniz-LSB@TUM zuständigen Gruppe stand eine von der Einrichtung erstellte Evaluierungsunterlage zur Verfügung. Die wesentlichen Aussagen dieser Unterlage sind in der Darstellung (Anlage A dieser Stellungnahme) zusammengefasst.

Wegen der Corona-Pandemie musste der für den 4. und 5. Oktober 2021 vorgesehene Evaluierungsbesuch am Leibniz-LSB@TUM in Freising entfallen. Die Bewertung erfolgte im Rahmen eines Ersatzverfahrens, das der Senatsausschuss Evaluierung (SAE) in Umsetzung eines Grundsatzbeschlusses des Senats vom 31. März 2020 eingerichtet hat. Der Senat hält in diesem Grundsatzbeschluss fest, dass das Ersatzverfahren ein Notbehelf ist und ausschließlich auf Einrichtungen angewendet wird, die im Regelturnus von sieben Jahren evaluiert werden. Die Bewertungen, auf deren Grundlage der Senat Stellung nimmt, sind auf zentrale Kernfragen der Entwicklung und Perspektive einer Leibniz-Einrichtung fokussiert. Ausführliche Einschätzungen und Schlussvoten zu Teilbereichen und Planungen für „kleine strategische Sondertatbestände“ müssen regelmäßig entfallen.

Die Bewertungsgruppe erstellte den Bewertungsbericht (Anlage B). Das Leibniz-LSB@TUM nahm dazu Stellung (Anlage C). Der Senat der Leibniz-Gemeinschaft verabschiedete am 12. Juli 2022 auf dieser Grundlage die vorliegende Stellungnahme. Der Senat dankt den Mitgliedern der Bewertungsgruppe und des Senatsausschusses Evaluierung für ihre Arbeit.

1. Beurteilung und Empfehlungen

Der Senat schließt sich den Beurteilungen und Empfehlungen der Bewertungsgruppe an.

Das *Leibniz-Institut für Lebensmittel-Systembiologie* (LSB; bis 2017 *Deutsche Forschungsanstalt für Lebensmittelchemie*, DFA) erforscht, so der Satzungsauftrag, die „chemische Zusammensetzung von Lebensmitteln und ihre Bewertung unter Mitberücksichtigung der einschlägigen mikrobiologischen, ernährungsphysiologischen, toxikologischen, rechtlichen und sonstigen Fragen“. Das daraus abgeleitete Ziel ist es, molekulare Netzwerke und die Prozessierung von Lebensmitteln im Organismus zu verstehen, die die Biologie und Gesundheit

[1] Ausführungsvereinbarung zum GWK-Abkommen über die gemeinsame Förderung der Mitgliedseinrichtungen der Wissenschaftsgemeinschaft Gottfried Wilhelm Leibniz e. V.

des Menschen beeinflussen. Dabei verfolgt das Institut seit einer vor fünf Jahren in die Wege geleiteten Neuordnung den Ansatz der **„Lebensmittel-Systembiologie“** und strebt an, experimentelle mit computergestützten Verfahren sowie maschinellem Lernen zu verbinden. Dieser Ansatz ist im Bereich der Lebensmittelchemie neuartig. Im Vergleich zur Zeit der vergangenen Evaluierung wird mit den neuen, äußerst ambitionierten Zielen die wissenschaftliche Ausrichtung des Instituts inhaltlich, vor allem aber methodisch, erheblich erweitert. Zur weiteren Entfaltung dieses Ansatzes werden im Bewertungsbericht wichtige kritische Hinweise und Empfehlungen gegeben, deren Umsetzung für den künftigen Erfolg des Instituts wichtig sein wird.

Der Senat der Leibniz-Gemeinschaft hatte in seiner letzten Stellungnahme zur DFA vom Juli 2015 darauf hingewiesen, dass die historisch gewachsenen **Strukturen des Instituts** verändert werden müssen, um eine wissenschaftliche Entfaltung zu ermöglichen. Weitere kritische Hinweise des Senats führten zu einer Untersuchung der Mittelverwendung am Institut. Behörden des Sitzlandes stellten Unregelmäßigkeiten zulasten der DFA fest, die eine tiefgreifende finanzielle Neuordnung einschließlich eines Insolvenzverfahrens unumgänglich machten. Vor diesem Hintergrund stellten Ende 2015 der Verwaltungsleiter und wenig später der Direktor ihre Ämter zur Verfügung. Das Aufsichtsgremium setzte eine interimistische Leitung ein.

Im August 2017 wurde ein **Prozess der Neuordnung** begonnen. Die Mission und der Name des Instituts wurden geändert (s. o.) sowie strukturelle Anpassungen in die Wege geleitet. Ein Vizepräsident der TU München wurde Direktor des Instituts, gab die Leitung aber nach seiner Berufung zum Präsidenten der TUM zwei Jahre später wieder auf.

Seit November 2019 leitet die jetzige Direktorin das LSB sowie die Forschungssektion II „Metabolische Funktion, Chemorezeption & Biosignale”. Dieser Leitungswechsel war maßgeblich für den Beginn der näheren Ausgestaltung und Umsetzung eines neuen **Gesamtkonzepts**. Die notwendige, umfassende Reform des Instituts wird von ihr mit großem Einsatz zielgerichtet vorangetrieben und führte bereits zu ersten Erfolgen. So wurde die im Grundsatz 2017 eingeführte Gliederung in Forschungssektionen mit Arbeitsgruppen, ergänzt um Technologieplattformen (inzwischen: „Technologie-Ressorts“), weiter entfaltet. Diese neue Struktur trägt erheblich zu einer verbesserten Zusammenarbeit bei. Seit 2019 wurden fünf der heute acht Arbeitsgruppen eingerichtet bzw. durch Umstrukturierung geschaffen. Positiv hervorzuheben ist auch die Einrichtung einer W2-Professur „Computational Pharmacology“ gemeinsam mit der TUM, die vor einer Entscheidung über eine Festanstellung (W3-Professur) im Rahmen des Leibniz-Professorinnenprogramms gefördert wird. Zudem übernimmt eine zuvor im Ausland tätige Wissenschaftlerin die Leitung einer drittmittelgeförderten Leibniz-*Junior Research Group*. Seit 2021 fördert die DFG erstmals seit langer Zeit mehrjährige Forschungsprojekte am Institut.

Die Neuordnung des LSB ist bei weitem nicht abgeschlossen. Derzeit werden zwei von drei Forschungssektionen (Sektion I „Chemie Sensorischer Systeme“ und III „*In-silico*-Biologie & Maschinelles Lernen“) kommissarisch geleitet. Die Sektion III spielt eine zentrale Rolle für die zukünftige Ausrichtung des gesamten Instituts. Sie wird momentan von einem ausgewiesenen Wissenschaftler mit der für die Leitung notwendigen bioinformatischen Expertise geleitet, allerdings mit lediglich 10 % seiner Arbeitszeit, denn er ist im Hauptamt Professor an

der Universität Rostock. Für die von Leitung und Aufsichtsgremium vorgesehene Entwicklung des LSB ist es zwingend erforderlich, die **Leitungspositionen** dieser Forschungssektionen ohne Verzug international wettbewerbsfähig und im Einklang mit den Empfehlungen des Bewertungsberichts zu besetzen. Der Senat erkennt die intensiven Bemühungen der Direktorin des LSB an, diesen Prozess gemeinsam mit der TU München voranzutreiben; der aktuelle Stand ist in der Institutsstellungnahme gut dokumentiert. Das Sitzland muss die geplanten Stellenbesetzungen nun seinerseits absichern.

Die **institutionelle Förderung** für laufende Maßnahmen betrug in den Jahren 2018-2020 im Schnitt 3,76 Mio. € pro Jahr. Im Vergleich zu anderen Leibniz-Einrichtungen in den Lebenswissenschaften ist dies ein außergewöhnlich geringer Betrag. Vor diesem Hintergrund war es ein für die wissenschaftliche Wettbewerbsfähigkeit des Instituts wesentlicher Schritt, dass das zuständige Ministerium des Landes die institutionelle Bund-Länder-Förderung für die Jahre 2018-2024 nahezu verdoppelte (Ø 3,6 Mio. € pro Jahr, insgesamt 25,4 Mio. €). Diese Förderung erfüllt die Funktion einer zusätzlichen Grundausstattung.

Das zuständige Fachressort des Landes strebt eine Verstetigung im Rahmen der Bund-Länder-Förderung an. Ein erster Antrag wurde in den Jahren 2020/2021 durch den Wissenschaftsrat (WR) begutachtet, der dabei eine vom Senatsausschuss Stragische Vorhaben (SAS) vorbereitete Stellungnahme des Senats berücksichtigte. Der WR sah jedoch noch keine ausreichende Grundlage für eine dauerhafte Ausweitung der Bund-Länder-Förderung über einen *großen strategischen Sondertatbestand*, auch wenn er die begonnene Reform des Instituts positiv einschätzte.

Das zuständige Fachressort Bayerns plant nun, die Erhöhung der institutionellen Förderung zum nächstmöglichen Zeitpunkt zu beantragen. Vorgesehen ist ein Antrag als *kleiner strategischer Sondertatbestand*. Ein solcher Antrag müsste am LSB bereits in diesem Jahr vorbereitet werden. Aus Sicht des Senats ist es nicht möglich, so zügig die erforderlichen strukturellen und inhaltlichen Fortschritte zu erzielen. Die Besetzung der vakanten Sektionsleitungen sind entscheidende Voraussetzungen für die weitere Ausgestaltung und Entfaltung des Gesamtkonzepts. Insofern ist nun insbesondere das zuständige Fachressort des Sitzlandes gefordert, die **strukturellen und finanziellen Voraussetzungen** des LSB in Fortführung des 2017 eingeschlagenen Wegs weiter zu sichern. In einigen Jahren kann dann evaluiert werden, ob aus wissenschaftlicher Sicht eine Ausweitung der institutionellen Förderung durch Bund und Länder gerechtfertigt ist.

Nach der vergangenen Evaluierung 2015 traten gravierende strukturelle Probleme der damaligen DFA zutage. Der Senat begrüßt, dass das Aufsichtsgremium unter Leitung des zuständigen Fachressorts des Landes Bayern in den Jahren 2017 bis 2019 entscheidende strukturelle und personelle Weichen für eine erfolgreiche Neuausrichtung des Instituts gestellt hat. Die Verbindung von wissenschaftlichen Dienstleistungen und Forschung mit Konzentration auf die Lebensmittel-Systembiologie sind in der am LSB erbrachten Form an einer Hochschule nicht möglich. Eine Eingliederung des LSB in eine Hochschule wird daher nicht empfohlen. Der Senat sieht derzeit die Anforderungen als erfüllt an, die an eine Einrichtung von überregionaler Bedeutung und gesamtstaatlichem wissenschaftspolitischem Interesse zu stellen sind.

Die Neuordnung des LSB ist aber bei weitem noch nicht abgeschlossen. Erst in einigen Jahren wird sich erkennen lassen, ob die vom Land eingeleiteten Reformen und strukturellen Verbesserungen dauerhaft tragfähig sind. Der Senat empfiehlt daher, die nächste Überprüfung der Fördervoraussetzungen durch Bund und Länder in vier Jahren vorzusehen. Zu diesem Zeitpunkt wird auch absehbar sein, ob eine dauerhafte Ausweitung der institutionellen Bund-Länder-Förderung gerechtfertigt ist.

2. Zur Stellungnahme des LSB

Der Senat begrüßt, dass die Leitung des LSB beabsichtigt, die Empfehlungen und Hinweise aus dem Bewertungsbericht bei ihrer weiteren Arbeit zu berücksichtigen.

Die Entfaltung des Gesamtkonzepts benötigt Zeit. Es wäre insofern verfrüht, bereits in diesem Jahr am Institut einen Antrag vorzubereiten, den das Land bei Bund und Ländern vorlegen möchte mit dem Ziel, den Kernhaushalt der Bund-Länder-Förderung ab 2025 fast zu verdoppeln.

3. Förderempfehlung

Der Senat der Leibniz-Gemeinschaft empfiehlt Bund und Ländern, das LSB als Einrichtung der Forschung und der wissenschaftlichen Infrastruktur auf der Grundlage der Ausführungsvereinbarung WGL weiter zu fördern.

Ferner empfiehlt er, die nächste Überprüfung der Fördervoraussetzungen in vier Jahren (2026) vorzusehen und diese Überprüfung mit einer Entscheidung über die dauerhafte Ausweitung der institutionellen Förderung zu verbinden auf der Grundlage einer Evaluierung, die sich auf beide Aspekte bezieht.

9 September 2021

Annex A: Status report

Leibniz Institute for Food Systems Biology at the Technical University of Munich, Freising (Leibniz-LSB@TUM)

Contents

1. Key data, structure and tasks

Key data

Year established:	1918
Admission to joint funding by Federal and *Länder* Governments:	1948
Admission to the Leibniz Association:	1977
Last statement by the Leibniz Senate:	2015
Legal form:	Foundation under Civil Law
Responsible department at *Länder* level:	Bavarian Ministry for Economic Affairs, Regional Development and Energy (StMWi)
Responsible department at Federal level:	Federal Ministry of Food and Agriculture (BMEL)

Total budget (2020)

3.826 k€ institutional funding

1.175 k€ revenue from project grants

0.015 k€ revenue from services

3.962 k€ revenue from Bavarian Stimulus Funds (special funding, granted 2018-2021, extension planned to 2024)

Number of staff (2021)

42 individuals in research and scientific services

26 individuals in science supporting staff

10 individuals in administration

Mission and structure

Mission according to statutes

"*The mission of the Leibniz-LSB@TUM, established by the Foundation, shall be to research the chemical composition of foods and their evaluation, taking into account the relevant microbiological, nutritional, physiological, toxicological, legal and other issues, and to promote science and research.*" (foundation charter [*Stiftungssatzung*], August 2017)

Organisation

The Leibniz-LSB@TUM (further on: LSB or Institute) is organised into three **Research Sections** (**RSs I – III**) with 2 - 3 **Research Groups** (**RGs**) each (see chapter 7 for a detailed description):

- **RS I: Sensory Systems Chemistry**

  RG Transcriptome and Proteome Profiling (**RG TransProt**, since 2020)

  RG Food Metabolome Chemistry (**RG FoodChem**, since 1995)

RG Biosystems Chemistry and Human Metabolism (**RG Metab**, since 2020)

[RG Functional Biopolymer Chemistry (until 2019)]

- **RS II: Metabolic Function, Chemoreception and Biosignals**

  RG Taste and Odor Systems Reception (**RG Reception**, since 2010/2018)

  RG Metabolic Function and Biosignals (**RG MetabFunc**, since 2020)

- **RS III**: ***In Silico* Biology and Machine Learning**

  RG Molecular Modeling (**RG MolMod**, since 2018)

  RG Network Modeling and Machine Learning (**RG NetMod**, since 2020)

  RG Integrative Food Systems Analysis (**RG FoodSys**, since 2019)

Since 2018, three **technology platforms** support the Institute's research activities in the areas of integrated IT data management (**T 1**), analytical technologies (**T 2**) and databases (**T 3**).

2. Overall concept and core results

Since the restructuring of the Institute, which started in 2017 (see chapter 3), the LSB follows the approach of Food Systems Biology and addresses questions in food science by integrating experiments with *in silico* biology and machine learning. This takes the LSB from its analytical strength, focusing on the formation of individual molecules and their chemical reactivity, towards an understanding of molecular networks and processes driving food (processing) related human biology and health.

The LSB's Food Systems Biology approach is aimed at improving the understanding of food constituents that determine (i) the sensory quality of foods and food systems, and (ii) impact body functions associated with chemoreceptors recognizing sensory-active food constituents by means of high-precision, high-density, high-throughput analytical technologies that acquire large data sets used to generate new data spaces. These data space will help predict the sensory and nutritional quality of foods by applying integrative data analysis using *in silico* models and machine learning approaches.

The LSB aims to provide the molecular understanding of the sensory perception of foods – as key determinant of the food system consisting of all processes and infrastructure involved in the dietary intake of a population – and its impact on chemoreceptor-associated human biology.

Research at the LSB is organised into three Research Sections (RS):

RS I (Sensory Systems Chemistry) analyses chemosensory relevant ingredient systems of food and their metabolisation, and develops new analytical procedures and methods of data storage.

RS II (Metabolic Function, Chemoreception & Biosignaling) examines how and via which chemoreceptors the molecular constituent systems interact with other biosystems. It also addresses the questions of how chemosensory ingredient systems mediate their effects at the molecular-biological level and what effects they possess in human biology.

RS III (*In Silico* Biology & Machine Learning) evaluates the data collected in RSs I and II using the latest bioinformatics methods. Its goal is to develop predictive models, e.g. to control the composition of molecular ingredient systems in food production or to predict their interactions and effects with or on molecular biosystems.

The Research Sections are supported by the in 2018 installed T-platforms in IT, analytical and database matter:

T 1 - Integrated Data Management helps LSB's researchers in all scientific IT matters, e.g. e-lab books.

T 2 – Analytical Technologies bundle LSB's high-performance technologies, e.g. GC/LC-ToF-MS, ICP-MS, NMR, imaging, (automated) cell-based assays.

T 3 – Databases include the Souci-Fachmann-Kraut nutrition tables, the open access database "Leibniz-LSB Odorant DB" and the open access Food Systems Biology Database.

Results

Like all Leibniz institutions that are being evaluated, the LSB was asked to select the ten most important results (in research, research infrastructure and/or transfer) since the last evaluation. Against the backdrop of the restructuring of the Institute, the LSB's information relates to the period from 2018 onwards:

Food analytics (Research Section I)

① Identification of an important odorant precursor in durian: first evidence of ethionine in plants**:** The LSB aims to not only use cutting-edge technologies, but also develop its own concepts for new, innovative, highly sensitive analytical methods. During the reporting period, researchers in RS I detected the rare amino acid ethionine in Durian fruit for the first time using a molecular sensory analysis concept developed at the LSB. – (Fischer N. S.; Steinhaus M. (2020) J. Agric. Food Chem. 68: 10397-10402. doi: 10.1021/acs.jafc.9b07065)

② Characterization of Odorants Causing Smoky Off-Flavors in Cocoa: RS I scientists have identified and characterised various odorants that cause typical off-flavours in cocoa. This allows objective assessment of the sensory quality of cocoa beans based on odorant concentrations. – (Füllemann D.; Steinhaus M. (2020) J. Agric. Food Chem. 68: 10833-10841. doi: 10.1021/acs.jafc.0c04633. Epub 2020 Sep 21)

Structure-function analyses of chemoreceptors (Research Sections II and III)

③ Copper-Mediated Thiol Potentiation and Mutagenesis-guided Modeling Suggest a Highly Conserved Copper-Binding Motif in Human OR2M3: A German-American team of scientists led by researches of RS II has shown for the first time that the odorant receptor OR2M3 responds up to fourfold more strongly to a sulphur-containing odorant from onions in the presence of copper ions. Two newly discovered copper binding sites inside the receptor have been identified to be possibly decisive for this. These results contribute to a better understanding of the fundamental relationships between the molecular structure of odorant receptors and their function – (Haag F.; Ahmed L.; Reiss K.; Block E.; Batista V.

S.; Krautwurst D. (2020) Cell. Mol. Life Sci. 77: 2157-2179. doi:10.1007/s00018-019-03279-y)

④ Reengineering the Ligand Sensitivity of the Broadly Tuned Human Bitter Taste Receptor TAS2R14: As part of an international collaborative project, researchers from RSs II and III used in vitro mutagenesis experiments coupled with functional studies and computer modelling to investigate the relationships between the molecular structure and function of the bitter receptor TAS2R14. The results are envisioned to be able to contribute to the development of novel, biological test systems for sensory-active substances that are present in foods but for which either safety data or larger amounts needed for sensory evaluations are lacking. They can also be used to develop personalised nutrition concepts. – (Nowak S.; Di Pizio A.; Levit A.; Niv M. Y.; Meyerhof W.; Behrens M. (2018) Biochim. Biophys. Acta Gen. Subj. 1862 (10): 2162-2173. doi: 10.1016/j.bbagen.2018.07.009)

⑤ *In silico* molecular study of tryptophan bitterness**:** Researchers at RS III have made further progress in the structural characterisation of the bitter receptor TAS2R4, based on preliminary studies showing that TAS2R4 responds to the essential amino acid tryptophan. Tryptophan supplements are useful in numerous medical contexts. However, its strong perceived bitterness and its impact on mechanisms regulating gastric acid secretion is disadvantageous for various food and drug formulations. Researchers at RS III performed computational modelling simulations in order to better understand the molecular interaction between tryptophan and bitter receptors. – (Di Pizio A.; Nicoli A.; (2020) Molecules 25(20): 4623-4632. doi: 10.3390/molecules25204623)

⑥ Numerous compounds orchestrate coffee's bitterness: Analyses of RS II and III in cooperation with the TUM provide novel information on the way in which the bitterness of coffee is determined by a complex interaction of multiple bitter compounds with several human bitter taste receptors. The results contribute to a better understanding of the complex effects of bitter tasting food systems. – (Lang T.; Lang R.; Di Pizio A.; Mittermeier V. K.; Schlagbauer V.; Hofmann T.; Behrens M. (2020) J. Agric. Food Chem., 68: 6692-6700. doi: 10.1021/acs.jafc.0c01373)

Sweet receptor-mediated metabolic effects (Research Section II)

⑦ Sweet taste antagonist lactisole administered in combination with sucrose, but not glucose, increases energy intake and decreases peripheral serotonin in male subjects: This intervention study provides new insights into the relationships between the sweet taste of sugar, energy intake, and hunger-satiety regulation. – (Schweiger K.; Grüneis V.; Treml J.; Galassi C.; Karl C. M.; Ley J. P.; Krammer G. E.; Lieder B.; Somoza V. (2020) Nutrients, 12(10): 3133. doi: 10.3390/nu12103133)

Data storage and analysis (Research Section I und III)

⑧ Low cost DNA data storage using photolithographic synthesis and advanced information reconstruction and error correction: As part of an international team of scientists, a researcher from RS I has been involved in finding a way to reduce the cost of DNA data storage. In this context, RS I have recently acquired DFG funding to develop an open-source, table-top instrument capable of parallel synthesis of millions of unique sequences.

– (Antkowiak P.L.; Lietard J.; Darestani M. Z.; Somoza M. M.; Stark W. J.; Heckel R.; Grass R. N. (2020) Nat. Commun. 11: 5345. doi: 10.1038/s41467-020-19148-3)

⑨ Integrated microbiota and metabolite profiles link Crohn's disease to sulphur metabolism: Scientists from RS III were significantly involved in the measurement of the extensive metabolome data generated from research into Crohn's disease and its bioinformatic analysis. They have contributed to prove that characteristic changes in the microbiome of Crohn's disease patients are associated with changes in sulphur metabolism. – (Metwaly A.; Dunkel A.; Waldschmitt N.; Raj A. C. D.; Lagkouvardos I.; Corraliza A. M.; Mayorgas A.; Martinez-Medina M.; Reiter S.; Schloter M.; Hofmann T.; Allez M.; Panes J.; Salas A.; Haller D. (2020) Nat. Commun. 11: 4322, doi: 10.1038/s41467-020-17956-1)

Curated database platforms

⑩ The Leibniz-LSB@TUM Odorant Database was initially released in 2020. It is a freely accessible online tool supporting the identification of naturally occurring odorants in food which currently contains information on 1.500 odorants from more than 640 publications. Its target user group is comprised of flavour research professionals in both the academic and private sector. – (J. Kreissl J.; V. Mall; P. Steinhaus and M. Steinhaus, Version 1.0 released in 2020) Furthermore, the LSB hosts the Souci-Fachmann-Kraut nutrition tables (SFK) and the Food Systems Biology Database.

Over the past three years, LSB researchers have published 156 articles in journals (142 peer-reviewed, 38 thereof in open access formats), 16 monographs and 16 individual contributions to edited volumes. Additionally, they acted as editors for two edited volumes.

3. Changes and planning

Development since the previous evaluation

Scientific changes

Having focused on the chemical characterization of sensory active food constituents for almost 100 years, the Institute spent the last three years transforming its research profile into Food Systems Biology. The aim of the LSB is to identify the chemosensory relevant components of food ingredient systems along the entire value chain.

The LSB's interdisciplinary research approach combines basic chemical-analytical and molecular-biological application-oriented research on highly complex systems of chemosensory active molecules that influence each other in their functions in the food itself and in their effects on human biology with computer-aided mathematical analyses and modeling of complex networks and systems at a single location.

In order to consolidate the new research program "Food Systems Biology" and to further develop it in a future-oriented manner, the four program areas that existed until 2018, were transferred into three research sections (Research Sections I–III, s. chapter 2 and 7). The aim of the new structure is to foster works on interdisciplinary scientific issues in cross-sectional cooperation.

Structural changes

In the last evaluation in July 2015, the scientific performance of the Institute, which was then still called the *German Research Institute for Food Chemistry* (*Deutsche Forschungsanstalt für Lebensmittelchemie*, DFA), was assessed positively. However, there were very critical comments on structural issues. In particular, the cooperation with the food industry, which is important for the Institute, was administered at the Institute in a way that was not transparent in the view of the Senate of the Leibniz Association. A subsequent audit revealed irregularities in the use of funds. In December 2015, investigations by the public prosecutor's office were initiated against the then director. In October 2016, insolvency proceedings had to be opened. DFA's institutional funding from the federal and state governments was suspended until February 2017. Nevertheless, the Institute's operations could always be maintained in full, as the responsible Bavarian ministry explained at that time.

In August 2017, the Foundation Council decided on the structural and scientific-strategic realignment of the Foundation, which also included the renaming of the DFA to *Leibniz Institute of Food Systems Biology at the Technical University of Munich (Leibniz-LSB@TUM)*. As the Institute explains, the range of services and the task definition of LSB were realigned in cooperation with the Scientific Advisory Board and the Board of Trustees and based on indications from the last evaluation in 2015. Since 2018, the state of Bavaria has been supporting the LSB's reorientation with additional, time-limited funding ("Bavarian Stimulus Funds"). The management and committees of the LSB are striving to make this funding permanent within the framework of institutional funding (see below).

The LSB points out that the insolvency in 2016 led to massive upheavals at the Institute. Not least against this backdrop, numerous measures were initiated to develop a lively research and competitive culture at LSB. For example, publication and third-party funding strategies have been implemented to consistently strengthen hypothesis-driven basic research, increase the number of publications in high-impact journals, and diversify the acquisition of third-party funding. These measures are complemented by the promotion of independent research groups at the LSB.

Overview of the changes in leading positions since the last evaluation in 2015:

Scientific Director

- 2016/02 Resignation of DFA Scientific Director (working with LSB since 1995)
- 2016/03 to 2017/07: Interim DFA Scientific Director
- 2017/08 to 2019/10: LSB Scientific Director, resignation after two years due to his election as President of the TUM (Technical University Munich)
- 2019/11: Starting of the activities of the Acting LSB Scientific Director

Head of Administration

- 2015/12: Resignation of the Head of Administration
- 2016/01 to 2017/08: Interim

- 2017/09 to 2021/06: New Head of Administration, since 2018/07 Member of the Steering Board
- 2021/07 to 2021/12: Interim Head of Administration and member of the Steering Board (15 h/week), post was announced at the end of August 2021

Strategic work planning for the coming years

Scientific aspects

In the coming years, the implementation of the Food Systems Biology approach will continue to be pursued. Research will deepen in deciphering the molecular mechanisms by which raw and processed foods unfold their chemoreceptor-mediated effects in the sensory as well as the nutritional and microbiological context. With these research tasks, the overarching goal of the scientific development perspective of the LSB is to help develop effective and economical solutions in the food, nutrition and health sector.

Structural aspects

Most important strategic structural elements are:

- to continue implementing Food Systems Biology at the LSB
- to continue fostering RS III
- the appointment of the heads of RS I and III (joint appointments of W3 professorships with the TUM),
- the establishment of an independent junior research group in the field of "Biophysics & Mechanoreception" (RS I),
- a further strengthening of the interactions between the RSs and the technology platforms,
- the establishment and continuation of strategically important collaborations with partners from the Leibniz Association and the regional, national and international scientific environment.

In order to realise these plans, the LSB sees a need to expand its institutional funding.

Planning for additional funds deriving from institutional funding

Since 2018, the state of Bavaria has been supporting the LSB's reorientation with additional, time-limited funding ("Bavarian Stimulus Funds"). This funding amounts at the moment to a total of 16.7 M€ for the period 2018-2021. In the years 2018-2020, 10.4 M€ of this was spent (see annex "revenues and expenses").

The aim of the LSB's management and committees, including the responsible ministries, is to secure this additional funding in the long term as part of the institutional funding provided by the federal and state governments.

Prehistory and central aspects of a first evaluation by the Council of Science and Humanities (January 2021)

The state of Bavaria initially planned to provide its additional funding only until the end

of 2021. However, an initial application for subsequent continuation by the federal government and all the Länder was rejected. The application had been evaluated by the German Council of Science and Humanities (*Wissenschaftsrat*).

In its statement of 22 January 2021, the Council noted that it was an ambitious goal of the LSB to "integrate the systems biology approach into food research". The "fundamentally convincing concept" is "unique worldwide" and has "great potential".

However, the Institute "so far only partially has the prerequisites" for implementation. In analytics, the level is high, in chemoreceptor research, the LSB enjoys international recognition, argues the Council. The areas of systems biology and bioinformatics, however, are still in their infancy. In view of the scope and framework conditions, the period from 2017 onwards is judged to be too short for the necessary transformation. The crisis threatening the existence of the Institute and the resulting frequent changes in the Institute's management since 2017 had unsettled the LSB and its employees and hindered the development of a lively research and competitive culture for a long time.

According to the Council's assessment of January 2021, successful implementation of the concept requires the following improvements in particular:

- *The LSB needs to clarify its understanding of systems biology. The unconvincing limitation to machine learning should be overcome in favour of a broader connection of molecular work with systems biology studies of molecular networks. It was recommended to seek advice from external experts on the selection of concrete topics and methods.*

  In response to this recommendation, the LSB states that the Institute now no longer exclusively investigates the composition and hedonics of foods. Rather, it contributes to developing a molecular systems biology understanding of chemosensory-relevant food ingredient systems. According to the LSB's understanding, Food Systems Biology means exploring and predicting the composition and intrinsic interactions of dynamic food ingredient systems along the entire value chain, as well as investigating their complex effects on biosystems such as the human organism or the gastrointestinal microbiota and predicting them by using bioinformatics methods.

- *The filling of the leadership positions in Research Sections I (then "Biofunctional Systems Chemistry", now "Sensory Systems Chemistry") and III ("In Silico Biology and Machine Learning") with proven scientists must be achieved.*

  According to the LSB, both positions are to be filled jointly with the TUM as W3 professorships, insofar as institutional funding is permanently extended (see Chapter 5: Senior Scientific Positions). Currently, RS I is headed by an LSB senior scientist and RS III has been headed by a W3 professor from the University of Rostock since November 2020. His involvement in the LSB is not least a response to the recommendation to integrate external expertise in the field of systems biology.

- *In the 2018 newly established Research Section 3 "In Silico Biology & Machine Learning", only 2.5 of the requested 7.0 FTEs were filled at the time of the review; by November 2020, one additional position (1.0 FTE) was filled. Accordingly, the research concept is still being developed.*

The LSB notes that Research Section III could be expanded considerably in terms of content and personnel within the framework of the currently available funds. As of 31 May 2021, 5.85 FTEs are employed in the RS (for further details on RS III, see Chapter 7).

- *The course set by the new director towards strengthening hypothesis-driven basic research and formulating appropriate third-party funding and publication strategies should be consistently continued. Interdisciplinary and international cooperation should also be expanded.*

  For the LSB's actions on these issues see chapter 4: quality management and chapter 6: cooperation.

New Planning for additional institutional funding

In light of the assessment by the Council (*Wissenschaftsrat*), those responsible for the LSB are planning a second application for the expansion of the LSB's institutional funding. The intention is to consolidate LSB's strategic and structural developments towards Food Systems Biology, initiated by the Bavarian Stimulus Funds. The application for an "extraordinary item of expenditure" (*kleiner strategischer Sondertatbestand*) is to be submitted to the Federal Government by the next possible date (1 January 2023) and could lead to an increase of the institutional funding starting on January 2025. The application can be submitted in case of a positive statement of the external evaluation. In a further and independent procedure, the application then has to compete with applications for an increase of the core budget by other Leibniz institutions.

According to the rules, the LSB application has two financial components: the required additional funds (3.995 k€/year) and an own contribution of the Institute (150 k€/year). The total amount (4.145 k€/year) is composed of

- personnel funds of 2.100 k€/year (approx. 26 FTE). – At the moment the LSB funds approx. 89 FTE, thereof 36 FTE by institutional funding (40 %), 23 FTE by the Bavarian Stimulus Funds (26 %) and 30 FTE by third-party funds (34 %).
- operating funds of 1.395 k€/year.
- investment funds of 650 k€/year. – The Bavarian Stimulus Funds enabled the fast modernization of the LSB's infrastructure, e.g. IT hardware, high-performance analytics, which now has to be consolidated by an annual investment to run the instruments.

The increased costs (approx. 1.500 k€/year without own funds) resulting from new infrastructure and personnel resources (e.g. IT concepts, digitalisation, maintenance concepts, trainings, administrative structure and processing) can then largely be covered by the increased institutional budget.

„Extraordinary item of expenditure": summary of funds planning

	2025	**2026**	**Permanently**
Own funds + additional funds = „extraordinary item of expenditure"	*3.985 k€*	*4.090 k€*	*4.145 k€*
Own funds from existing funding by institution (at least 3 % of core budget)	*130 k€*	*140 k€*	*150 k€*
Additional funds of institutional funding	*3.855 k€*	*3.950 k€*	*3.995 k€*

4. Controlling and quality management

Facilities, equipment and funding

Funding (see appendix 3)

In 2020, the LSB's institutional budget amounted to 3.8 M€. In that year, the Institute received 3.9 M€ from the "Bavarian Stimulus Funds" (s. above in chapter 3). A total of 1.1 M€ was raised in third-party funding (thereof 0.7 M€ public funds, mostly funds of the AiF [German Federation of Industrial Research Associations] and 0.4 M€ from industrial projects).

An additional 0.015 M€ were earned in 2020 from fees for the use of LSB's SFK nutritional table. In the future, the Institute aims to extend its scope of revenue into patent monetisation through licensing its intellectual and property rights.

Facilities

The LSB facilities are located in a TUM building (free of rent and serviced by the TUM facilities management) on the campus of the TUM School of Life Sciences in Freising/Weihenstephan and, since 1 June 2020, in a neighbouring building owned by the Innovation and Start-up Centre for Biotechnology (IZB), for which the rent is financed by the responsible Ministry. Current negotiations with the state of Bavaria focus on a long-term solution to provide a separate building for the LSB to be located next to the Freising/Weihenstephan TUM campus and adjacent to the existing LSB facilities.

Since the LSB started to implement its new Food Systems Biology approach in 2018, three technology platforms (T 1 – integrated data management, T 2 – analytical technologies, and T 3 - databases) were installed as core facilities in order to support the LSB scientists and their collaboration partners in IT, analytical and database matters. Furthermore, LSB is currently implementing a food grade lab in order to be able to synthesize and isolate food constituents under food-grade conditions, thereby allowing their further sensorial and dose-effect analysis in human intervention studies.

The Institute's IT strategy comprises two areas: The *Administrative IT & Services* area includes all core processes of the Institute's administration as well as the procurement, care and maintenance of the basic IT infrastructures. *Science IT*, on the other hand, focuses on the development and implementation of research data management (RDM) and follows a strategy that is meant to ensure long-term accessibility and usability of research data created at the LSB.

Organisational and operational structure

Since 2018, the Scientific Director (responsible for research agenda and strategic interaction) and the Head of Administration (responsible for administration and finances) form a Steering Board with the Scientific Director as speaker. The members of the Steering Board are appointed by the Board of Trustees.

The Institute is organized in three research sections with research groups and three T-platforms. Beside this, the Scientific Director leads a Directorate. Three years ago, an ex-

tended Management Board was implemented, consisting of the Steering Board, the leaders of the 8 research groups (including the chairs of the research sections), 3 T-platforms, elected co-workers' representatives and a representative of the LSB´s PhDs as guest. The extended Management Board meets regularly to discuss research-relevant and organisational topics. Furthermore, the chairs of the research sections and research groups discuss strategic questions in regular meetings.

Quality Management

The LSB has implemented rules for "Ensuring Good Scientific Practice", which are based on the recommendations of the DFG and the "Guidelines for Good Scientific Practice in the Leibniz Association". The Institute has an ombudsperson. In 2020, the position of an officer for genetic engineering and biodiversity was implemented to support the scientists in questions related to research involving access to genetic resources and the fair and equitable sharing of benefits arising from their utilisation to the convention on Biological Diversity (*Nagoya Protocol*) and ensure scientific work in accordance to the respective rules.

The LSB's publication strategy was initiated in December 2019 and strives for (high impact) peer-reviewed, open access publications. For this purpose, the LSB implements the "Berlin Declaration on Open Access to Scientific Knowledge" and the guidelines on Open Access of the Leibniz Association. The Institute states that the number of open access publications increased significantly within the last 3 years.

The LSB intends to make scientific data freely accessible as databases (e.g. odorant database) in the future via part of its information infrastructures. To secure the quality and reusability of research data according to the FAIR data principles (*Findability, Accessibility, Interoperability, and Reusability*) an electronic lab notebook system has been implemented in early 2020. Furthermore, the implementation of the research information system PURE is planned for the last quarter of 2021.

The LSB has developed an intellectual property rights (IP) strategy to enhance the awareness of IP generated at the LSB among the scientific employees and to provide options for its protection and exploitation in various utility models. The Institute also collaborates with Ascenion GmbH to further explore patenting and commercialisation options.

The Institute has established a system of performance-based allocation of funding (LOM) with the aim to increase the number of open access publications and set incentives for acquisition of third-party funding. Within this framework a target of 280 k€/year over an average of three years per research group (corresponding to the average amount raised by a German university professor) was agreed upon in target agreements with the group leaders.

Besides the scientific changes, the administrative structures have been changed as well since 2017, in particular with a cost centre structure installed, which is constantly being adapted to the current conditions and envisioned future structural changes. Many further arrangements and regulations were implemented to secure good governance in administrative affairs.

Quality management by advisory boards and supervisory board

The Scientific Advisory Board (SAB) advises the Board of Trustees and the Steering Board on fundamental scientific and interdisciplinary topics. The SAB meets twice a year and carries out an audit between two evaluations as it is common for Leibniz institutes. It consists of up to fifteen members, who are appointed by the Board of Trustees for a period of up to four years with one possible consecutive reappointment. Out of the LSB's SAB members, 9 % are women and 27 % are from abroad. The appointment period of six of the 11 members ends by the end of next year. In the long term, a balanced ratio of men and women in the SAB is aimed for.

The supervisory board of the LSB is the Board of Trustees (*Stiftungsrat*), which consists of a maximum of six members chaired by a representative of the state of Bavaria. The main tasks include appointment of the steering board and the SAB, the approval of the LSB's organisation and rules of procedure as well as approval the annual programme budget and the annual financial statements.

5. Human Resources

As of 31 May 2021, the Institute has 78 employees, thereof 42 in research and scientific services, 26 in scientific support (science IT, laboratory staff), and 10 in administration. Beside this, 6 PhD candidates with scholarships are supervised at the Institute. Furthermore, the LSB funds 2 student assistants.

Leading scientific and administrative positions

Since the last evaluation, there were three changes in the Institute's scientific leadership (see overview in chapter 2) in 2016, 2017 and 2019. At the time of the last evaluation by the Leibniz Senate in 2015, the position of the Scientific Director was a secondary appointment (*Nebenamt*) for a person being appointed at professor at TUM. As recommended by the Leibniz Senate this structure was changed. Today, the Scientific Director works primarily at the LSB (75%) and with a TUM affiliation (25%).

The Scientific Director chairs RS II, whereas Research Sections I and III are chaired interim. RS I is chaired by a LSB senior scientist, RS III since November 2020 by a W3 professor of the University of Rostock. The LSB's long-term goal is to achieve joint appointments with TUM for both sections. This depends on a positive decision on the application for an extended institutional funding (see chapter 3).

At the moment, the position of the Head of Administration is being refilled (s. chapter 3).

Staff with a doctoral degree

As of 31 May 2021, the LSB hosted 11 postdocs. The LSB states that it aims to provide appropriate measures and budgets for professional support and career development for every career stage.

Research groups started by early-career scientists in 2020 were provided with a two-year post-doc position since the financial situation of the LSB did not allow funding beyond the end of 2021 due to the termination of the Bavarian Stimulus funds.

Doctoral Candidates

As of 31 May 2021, 28 doctoral candidates worked at the LSB, 22 of who were employed on a contract while 6 held a scholarship. Between 2018 and 2020 a total of 20 PhD theses were completed. The time needed to complete the dissertation (including public defence) was 4.7 years on average.

Following the DFG recommendations, the PhD's salaries were increased from 50% to 65% TV-L 13 in 2020**.** The four years of contract are structured according to the Leibniz Guidelines on Career Development (i.e. 3+1). As the Institute points out, a publication-based doctoral thesis is strived for, with the final PhD exam to be passed after a total period of approx. 4.5 years.

The supervision of doctoral students at the LSB is based on the "Career Guidelines of the Leibniz Association" and the guidelines by the TUM Graduate School. LSB doctoral students are required to participate in this structured PhD programme of TUM. A central part of the quality assurance and the successful completion of a PhD thesis is the supervision agreement between the doctoral candidate and the PhD supervisor defining rights and responsibilities. In meetings with the Thesis Advisory Committee, which includes the supervisor, an external scientific mentor, and the second examiner, the progress of the thesis is evaluated. In addition, progress meetings between supervisor and doctoral student are firmly established.

Science supporting staff

Starting in fall 2021, the Institute's administration will offer vocational training for an office management assistant. In a further step, vocational training for chemical-technical assistants is planned as well.

Within the framework of a Leibniz network, the concept "colleagues train colleagues" was established, which enables employees to train at another Leibniz Institute in order to receive further knowledge in the specialist field. In addition, external specialised training is planned for the administrative staff, if possible in cooperation with other Leibniz Institutes.

Equal opportunities and work-life balance

As of 31 May 2021, the proportion of women in "Research and Scientific Services" was 43 % (18 of 42). One out of three RS chairs (33%) and 2 out of 8 group leaders (25%) are female. In total 78 % of the employees at the LSB are women and the Steering Board is made up of two women. The LSB has implemented the cascade model and its own internal regulations on gender equality. Currently, a female scientist applies for a Leibniz Junior Research Group "Mechanoreceptors".

The Institute has an equal opportunity officer since 2004 and pursues an active equality policy. The Institute points to a series of measures to improve the compatibility of work and family, e.g. part-time employment, deviations from the 5-day working week, individual parental leave agreements and a parent-and-child office.

6. Cooperation and environment

Cooperation with universities

The LSB cooperates with the Technical University of Munich (TUM) for long term collaborations in research, teaching, and outreach. The current LSB Director is jointly appointed with TUM (W3 professorship). Two additional W3 appointments as chairs of RSs I and III are planned depending on the permanent extension of the Institute's institutional funding. Further, one RG head is currently striving for a W2 application within the *Leibniz Programme for Woman Professors* with full support of the TUM. 11 LSB scientists engage in teaching and thesis supervision at different levels at the TUM.

The negotiation of a cooperation agreement between the LSB and the TUM is currently under way. This agreement aims to secure and expand the scientific and technical synergies between the LSB and different departments at the TUM as well as the *University Hospital rechts der Isar*.

The director of the LSB is also a member of the *ZIEL Institute of Food and Health at the TUM School of Life Sciences*. A collaboration with several other members has been initiated in order to apply for a DFG Collaborative Research Centre (CRC) in 2023 as a continuation of the current CRC 1371 "Microbiome Signatures".

In a national context, the LSB collaborates closely with the University of Rostock, the University Hospital of the Technical University of Dresden and the Saarland University Medical Centre. Internationally, cooperation exists with the University of Vienna, ETH Zurich, Johns Hopkins University, Rice University Texas and University of Milan.

Cooperation within the Leibniz Association

Currently, the LSB is a member of two Leibniz Research Networks (LFN): "Immune-Mediated Diseases" and "Green Nutrition - Healthy Society". Until 2021, the Institute was partner in the Leibniz Research Alliances (LFV) "Bioactive Compounds and Biotechnology" and "Sustainable Food Production and Healthy Nutrition", the former of which was recently transferred to an LFN.

The LSB also works with other Leibniz Institutes in the field of science communication. Together with the Leibniz Research Institute for Molecular Pharmacology (FMP), it has acquired funding for the development and evaluation of a "Leibniz-Wirkstoff-Nachrichten-Portal". Furthermore, the LSB cooperates with the German Institute of Human Nutrition Potsdam-Rehbrücke (DIfE), e.g. via a common SAW proposal.

Further collaborations and networks

On a national level, the LSB cooperates with the Max Rubner Institute (MRI) which facilitates the inclusion of the LSB's data from the Souci-Fachmann-Kraut Food Composition and Nutrition Tables (SFK) into the German Nutrient Database (BLS).

The LSB also states to work closely with economic and scientific partners, such as within the frameworks of the Research Association of the Food Industry (FEI) and the German Federation of Industrial Research Associations (AiF), and it is a partner in the BMEL-funded competence network "Food Profiling - solutions for food authentication" as well

as the BMBF-funded nutrition competence cluster "ENABLE - healthy food choices in all stages of life".

The Institute collaborates with industrial partners both on a national and international level, namely in the USA and Japan, and is aiming to further expand them in the future.

Internationally, research cooperation spans from the area of high-resolution spatial transcriptomics of plant tissue (with the Donald Danforth Plant Science Center in St. Louis / MO, USA) to high throughput approaches which quantitate networks of function and identity in microbial communities (with the Chemical Sciences Division of the Lawrence Livermore National Laboratory, CA, USA).

The Institute also participates actively in the *ERNEST Cost Action* with 21 European core partners investigating G-protein coupled receptors (GPCR). Lastly, the LSB cooperates with AgResearch (a Crown Research Institute based in New Zealand that focuses on pastoral and agri-food research and technology transfer) to internationally implement and foster the Food Systems Biology Approach.

Institution's status in the specialist environment

According to the institute, LSB's recently established interdisciplinary research approach "Food Systems Biology" is unique in the national and international environment. It combines the core disciplines of Food Chemistry, Natural Product Analysis, Chemoreceptor-based Research, Human Biology and Bioinformatics with high-performance technologies and integrated data management. Therefore, the LSB research programme is claimed to have little conceptual overlap with other institutes working in the area of nutrition and food research and to maximize synergies.

In the regional environment, the Institute states essential similarities and synergies with work areas of the *Chair of Food Chemistry and Molecular Sensory Science* of the TUM. In Germany, the Max Rubner Institute (MRI) and German Institute of Human Nutrition Potsdam-Rehbrücke (DIfE) are among the central research institutes working on individual areas of nutrition and food. Internationally, LSB states the *Monell Chemical Senses Center (MCSC)*, USA and the *Wageningen Food & Biobased Research Institute* at Wageningen University (NL) are two leading research institutions.

7. Subdivisions of the LSB

Research Section I "Sensory Systems Chemistry"

[20 FTE, thereof 6.7 FTE Research and scientific services, 7.1 FTE Doctoral candidates, and 6.3 FTE Service staff]

This Research Section (RS) includes three Research Groups (RGs):

- RG Transcriptome and Proteome Profiling (RG TransProt, since 2020)
- RG Food Metabolome Chemistry (RG FoodChem, since 1995)
- RG Biosystems Chemistry and Human Metabolism (RG Metab, since 2020)

The expertise of all three RGs is based on analytical techniques to detect, identify, and

quantitate specific target molecules in foods and their raw materials as well as in the human body after ingestion. These analytical techniques are applied to characterise foods, monitor changes along the food value chain, and optimise processes with the aim of providing the consumer with food of improved quality. Additionally, analytical tools are further developed and made available to the scientific community in order to promote science and research.

The target molecules of the RG TransProt are RNA and proteins. At a very early level in the food value chain, the analysis of the transcriptome and the proteome in plant tissues already allows to conclude on sensory and nutritional parameters of the foods made thereof. Moreover, the team can also apply its methodologies on the downstream end of the LSB's research space in order to study the influence of food constituents and their metabolites on human biology. The target molecules of the RG FoodChem are sensory-active compounds in foods, with a focus on odour-active compounds. The team identifies the key players contributing to the sensory quality of foods, studies the formation of key odorants, and optimises processes on the levels of agriculture, post-harvest treatment, food industry, and storage. The target molecules of the RG Metab are metabolites formed in the human body from dietary key compounds including, but not limited to, sensory-active compounds. This RG studies digestion, absorption, metabolic transformations, and excretion, and, thus, is closely linked to RS II, in which the biological functions of the namely molecules are investigated, and RS III where *in silico* models are applied to predict their impact on human biology.

The future development of RS I is envisioned to further strengthen the interactions of the RGs "TransProt", "FoodChem", and "Metab" with each other as well as with the RGs in RSs II and III. The RG "Functional Biopolymer Chemistry" moved to KIT in 2019. In the coming years, RS I will continue to identify sensory active food constituents in foods, elucidate their formation, biochemically in the raw materials including the genetic background and gene expression as well as by food processing, characterise their transformation into sensory active and sensory inactive metabolites upon digestion and absorption in the human body, and study their effects on the transcriptome and proteome in human tissues by means of high-sensitive, high-throughput technologies, such as hyper-fast GC, high-resolution LC-MS/MS and spatial transcriptome and proteome analyses.

Over the period 2018-2020, the section published on average 34 articles in peer-reviewed journals per year. Average yearly revenues from Stimulus Funds amounted to 1 M€. The section's average yearly revenue from third-party funding was 962 k€, with 734 k€ from Federal and *Länder* governments, 160 k€ from Industry and 57 k€ from the Leibniz Association. In the same period 19 section members received their doctoral degrees, and one section member obtained a habilitation.

Research Group Transcriptome & Proteome Profiling (TransProt) [2.9 FTE]

The RG TransProt was established in 2020. Transcriptomics and proteomics play important roles in food systems, underpinning at a molecular level the development of the chemical components and enzymatic reactions that determine the sensory and nutritional

properties of foods. Biotic and abiotic processes strongly influence the chemical composition of plants and derived foods, but these changes are mediated by, and reflected in the transcriptomes and proteomes of cells. At the same time, the ways humans respond to the sensory and nutritional properties of food constituents are also determined by genetic factors, making transcriptomics and proteomics important tools to understand the effect of the chemical composition of foods on human physiology. The RG combines physical, chemical and molecular biology approaches to develop high-throughput approaches to study transcriptomics and proteomics, with a particular emphasis on high-resolution spatial analysis. Their goal is to understand, at the most fundamental level, the origin, development and physiological consequences of the molecular food constituents.

Research Group Food Metabolome Chemistry (FoodChem) [12.1 FTE]

Research within this RG focuses on odour-active compounds in foods. Consumers' food and beverage selection is mainly driven by sensory aspects to which odour-active compounds make the most crucial contribution. Using state-of-the-art molecular sensory science approaches, the team identifies the key odorants in foods and beverages. Quantitation of the key odorants and their precursors along the food value chain allows them to identify the crucial parameters influencing the sensory quality. Targeted optimisation of these parameters finally results in foods and beverages with improved quality and increased eating pleasure for the consumer. Beyond these major activities, the RG works on the advancement of the analytical approaches used for key food odorant characterisation, aiming to provide the scientific community with a free database on food odorants, and they additionally employ their GC-MS expertise for untargeted volatilome analyses in projects on food authenticity.

Research Group Biosystems Chemistry & Human Metabolism (Metab) [3.7 FTE]

Overall sensory attractiveness and individual preferences strongly affect the choice of foods, as eating and drinking is a daily procedure with fundamental hedonic aspects. The new working group "Biosystems Chemistry & Human Metabolism" formed in 2020, targets the metabolic fate of dietary flavour compounds, thereby continuing the research on "Biosystems Chemistry & Metabolism" initiated by former Scientific Director [Thomas F. Hofmann] in 2017. Flavour compounds of foods comprise odour and taste active food constituents that give foods hedonic, nutritional or health related values. The RG investigates the biochemical processes during consumption, digestion and metabolism with the aim to clarify which metabolites arise, and when, for how long and to what extent they circulate in the system and, thus, can interact with extra-oral receptors. The work of the group therefore links food chemistry and sensory perception to human biology.

Research Group Functional Biopolymer Chemistry [1.9 FTE]

Until 2019, the RG studied the complex interplay between structure, functionality and bioactivity of food proteins in an interdisciplinary way. New discoveries from modern food proteomics techniques were combined with functional characterisation and analysis of the biochemical activity of food proteins to predict structure-functionality-bioactivity relationships. The research at the LSB addressed the following three key questions:

1. Why does the prevalence of food-related disorders, e.g., celiac disease, non-celiac gluten sensitivity (NCGS) or allergies, increase within the population?

2. How do different factors influence the structure, functionality and bioactivity of proteins?

3. How do changes in environmental conditions affect the protein composition of food crops?

Research Section II "Metabolic Function, Chemoreception & Biosignals"

[17 FTE, thereof 6 FTE Research and scientific services, 5.2 FTE Doctoral candidates, and 5.8 FTE Service staff]

This Research Section (RS) hosts two Research Groups (RGs):

- Taste and Odor Systems Reception (Reception, odor since 2010, taste since 2018)
- Metabolic Function & Biosignals (MetabFunc, since 2020).

The main aim of this RS is to explain the molecular mechanisms of the sensory perception of foods and their impact on chemoreceptor-associated human biology. Chemoreceptors located in the oral-nasal cavity sense taste, odour or chemesthetically active food constituents, thereby chiefly determining food choice, which has a major impact on body composition and function. Additional pathways by which chemoreceptors modulate body composition and function are linked to their expression outside the sensory tissues, which has been a focus of this field over the past two decades. Although protein structure elucidation is largely lacking and only for very few of the chemoreceptors expressed in extrasensory tissues, a specific biological function in the human body has been demonstrated, there is growing evidence for a direct impact of chemoreceptors on metabolic pathways that determine body functions. Since recent data show a close correlation between body mass index and taste perception, the research will help to understand and support a perception-driven healthy food choice by explaining the underlying molecular mechanisms. In recent years, the RS achieved the deorphanisation of odorant receptors (OR) and taste receptors (TAS). Furthermore, functional OR and taste receptor variants were characterised and associated with normosia and anosmia. The RS also succeeded in characterising of structure-function relationships and activation kinetics and identifying biological functions mediated by TAS (e.g. bitter taste sensing) and ion channels (e.g. pungent or salty taste sensing).

Over the period 2018-2020, the section published on average 9 articles in peer-reviewed journals per year. Average yearly revenues from Stimulus Funds amounted to 2.1 M€. The section's average yearly revenue from third-party funding was 269 k€, with 206 k€ from Industry and 64 k€ from Federal and *Länder* governments. In the same period one section member received a doctoral degree.

<u>Research Group Taste and Odor Systems Reception (Perception)</u> [10.5 FTE]

The RG identifies chemoreceptor activation profiles of volatile and non-volatile food constituents, metabolites, and endogenous agonists. Therefore, the group maintains large sets of chemoreceptors for screening, using well-established cellular assays and the necessary machinery for high-throughput analyses. Together with the RG MetabFunc, its work bridges the identification of chemosensory-active food constituents (RS I) with their

assignment to receptor activity patterns and physiological functions, and with data-based *in silico* analyses (RS III) to facilitate a systems-oriented work-flow. During the reporting period, the RG contributed to the understanding of the structural determinants of odorant receptors (OR) and taste receptors (TAS) involved in agonist and modulator interactions.

Research Group Metabolic Function & Biosignals (MetabFunc) [6.5 FTE]

The central goal of the RG is to explain the functional role of ectopically expressed chemoreceptors that are responsible for the sensory perception of food constituents in the oronasal cavities. Specifically, the conducted research is aimed at improving the understanding of the yet largely unknown role of chemoreceptors sensing taste (TAS), odour (OR) or chemesthetically active food constituents (TRP channels) in mechanisms controlling food intake and metabolic consequences thereof. The RG verifies the functional role of these chemoreceptors by means of *in vitro* and *ex vivo* approaches using food constituents as agonists and antagonists as well as the CRISPR-Cas9 knock down methodology. This is linked with changes in the transcriptome, metabolome and a specific biological function, which is verified in proof-of-concept human intervention studies.

Research Section III "*In Silico* Biology & Machine Learning"

[5.9 FTE, thereof 2.6 FTE Research and scientific services, 2 FTE Doctoral candidates, and 1.3 FTE Service staff]

This Research Section (RS) was established in 2018 and includes three Research Groups (RG):

- Molecular Modeling (RG MolMod, since October 2018)
- Network Modeling & Machine Learning (RG NetMod, since November 2020)
- Integrative Food Systems Analysis (RG FoodSys, since November 2019)

Research of the section focuses on the elucidation of molecular mechanisms eliciting sensory perception, the comprehensive characterisation of complex food systems and the development of molecular interaction networks and machine learning algorithms. The unifying research theme of the section seeks to understand the underlying molecular systems defining the functional properties of foods and their effects on human health and well-being. The section aims at the integrative multi-scale analysis of food composition and food-relevant effector systems to enable the prediction of functional changes accompanied by the targeted reformulation of food products. The intra-sectional interactions within the LSB are supported by expertise on the *in silico* analysis of ligand-receptor interactions, the development of data analysis workflows for untargeted metabolomics and microarray-based gene expression studies as well as the integrative analysis of multi-omics datasets by machine learning and network modelling tools.

In the future, the section plans to establish elementary tools and workflows for the emerging field of Food Systems Biology and to play a central role for the research area by building a network of interdisciplinary, international collaborations. The section is therefore seeking a deeper integration with the bioinformatics community, including de.NBI, more collaborations with bioinformaticians and modelers in other Leibniz institutes and closer connections to TUM activities in data science, machine learning and AI. As a core resource

for the prediction of functional changes in food systems and associated effector systems, the Food Systems Biology Database will provide access to structured, high-quality, interdisciplinary information. To ensure the successful long-term development of the research themes in section III, the implementation of a full professorship in food and health bioinformatics in collaboration with the TUM is intended.

Over the period 2018-2020, the section published on average 12 articles in peer-reviewed journals per year. Average yearly revenues from Stimulus Funds amounted to 305 k€. The section's average yearly revenue from third-party funding was 69 k€, with 46 k€ from Industry and 23 k€ from Federal and *Länder* governments. In the same period 0 section members received a doctoral degree.

Research Group Molecular Modeling (MolMed) [1.7 FTE]

Life is the result of the chemical activity of molecules and decoding the structures of molecules and their interactions is the key to understanding and modulating protein function and biological activities. Molecular modeling tools were developed and are in standard use to develop drugs by modulating altered protein functions. However, the use of these tools is currently broadening to several fields. This RG was established in 2018 to promote this pioneer discipline in the field of chemical senses. Using molecular docking, molecular dynamics simulations, pharmacophore modeling, quantitative structure-activity relationship (QSAR) models, machine learning and virtual screening, the MolMed group develops predictive models to be applied to search and rationally design new ligands for taste and odorant receptors.

Research Group Network Analysis and Machine Learning (NetMod) [0.1 FTE]

Like molecular and cell biology in general, food science is largely technology-driven. New technologies are generating new kinds of data, which requires new algorithms, and workflows for data analysis and mathematical modelling. An example of this is single cell technologies. Section III reflects the changes, from a focus on single molecules to networks in which they function by adopting a systems biology approach, combining classical statistics with bioinformatics and modelling of molecular interaction networks. Starting around 2016, there have also been major advances in data science, machine learning and AI. This is providing new tools to analyse experimental data but also allows us to ask new questions. To build up Section III's expertise in machine learning, the Research Group (RG) is focusing on the analysis of untargeted metabolomics and single cell data.

In food research, machine computational approaches are not yet widely established. This provides an opportunity for Section III to establish itself as a leading force in data analysis and mathematical modelling in the context of Food Systems Biology. The mathematical and computer science foundations for the methodologies used here, as well as the tools that were developed and applied, are mostly generic complementary expertise: the Molecular Modeling group, whose field is traditionally focusing on the analysis of single molecules, is now studying key molecules within the context of networks in which they function. The RG Network Modeling & Machine Learning is developing with the RG Molecular

Modeling a network approach for cells signaling in the olfactory epithelium and collaborates with the Integrative Food Systems Analysis group on machine learning approaches.

Research Group Integrative Food Systems Analysis (FoodSys) [4.1 FTE]

Research of this Research Group centers on analytical and bioinformatics approaches for comprehensive characterisation of complex food systems along the entire value chain and their effects on the human body following ingestion. The systematic aggregation of data from diverse analytical platforms establishes the basis for successful prediction of compositional changes in raw materials and throughout processing into final food products as well as of the chemoreceptor-mediated modulation of biological functions in the human body. Until today, characterisation of foods primarily occurs by the isolated analysis of preselected targets on small sample sets preventing a holistic understanding of the interactions between food components and the generalisation beyond the limited focus of individual studies. Therefore, the working group combines high-throughput tools for untargeted and large-scale targeted metabolomics with computational approaches to support the structured characterisation of food systems and the integration of complementary data provided by research groups within the LSB and outside. Based on this expertise, current research focuses on three connected key areas:

1. Development and integration of high-throughput methods into food analysis
2. Implementation of workflows for integrative analysis of data from various analytical platforms
3. Development of data structures and databases to provide the foundation for Food Systems Biology models

8. Handling of recommendations from the previous evaluation

In the last evaluation of the Institute in 2015, the following recommendations were made:

Overall concept and core results

*1) Results must be **published** in high-ranking journals that are received beyond the field of food chemistry. (Leibniz Senate 2015, German Council for Science and Humanities 2021)*

*2) **Third-party funding** for basic science projects should be acquired to a greater extent, especially from the DFG (in addition to funding from application-oriented sponsors). (Leibniz-Senate 2015, German Council for Science and Humanities 2021)*

Following her appointment in November 2019, the new Scientific Director has implemented a publication strategy, a scientific data strategy, an intellectual property rights strategy and a strategy to improve third-party funding acquisition. The LSB has introduced performance-based funding allocation (LOM; see chapter 4: quality management and chapter 3: development since the previous evaluation). Staff are encouraged and supported through further measures to engage in publishing and acquiring funds. The number of (open access) publications and the journal diversity significantly increased within the last years.

Since mid-2020, eight DFG proposals have been submitted by LSB scientists. DFG funding was recently obtained for a major basic research project (500 k€) of RS I.

Internationally, the Director and further LSB scientists are represented in three EU COST actions and one scientist participates in the *Global Consortium for Chemosensory Research*, which aims to investigate a possible link between respiratory diseases (including COVID-19) and their effects on the biological systems of odour and taste perception.

Human Resources

3) *The Leibniz Senate welcomed the starting of a structured **doctoral programme**. The LSB should hire doctoral students from outside Munich and from abroad. The time-slot between the submission of the thesis by a PhD student and the graduation is too long and must be reduced. **Promotion of young scientists with a doctoral degree** should be improved. (Leibniz Senate 2015)*

   In recent years, the LSB explains, more attention has been paid to ensuring that young scientists take advantage of the wide range of courses offered by the TUM Graduate School. Doctoral students are encouraged to present their work results at symposia. Habilitation candidates are supported by the establishment of independent junior research groups (see chapter 5: Staff with a doctoral degree, Doctoral candidates). The Institute implemented measures to shorten the total duration of the PhD to approx. 4.5 years.

4) *The Institute should take advantage of opportunities to fill higher-ranking positions in the coming years preferably with **female scientists**, as planned. Female scientists should be more strongly encouraged to pursue independent scientific careers. (Leibniz Senate 2015)*

   In 2019, a female scientist was appointed Scientific Director for the first time.

   In the same year, the head of the RG "Functional Biopolymer Chemistry" received a junior professorship with W3 tenure track option at the Karlsruhe Institute of Technology.

   Currently, the LSB and TUM are supporting a female scientist for being funded with a junior research group (applications in the *Leibniz Junior Research Group* programme). In addition, the Institute and the University support an LSB scientist's application for a tenure track professorship within the *Leibniz Programme for Women Professors* in 2020/2021 (see chapter 5: Equal opportunities).

Governance / Quality management

5) *The Institute's university partner, the Technical University of Munich, has considerably expanded the subject of food chemistry since 2007, complementing the Institute. The **structural development of the DFA** has not yet kept pace with this forward-looking policy, although the scientific prerequisites are very good. The historically grown structures of the Institute must now be changed quickly in order to enable further scientific development of the Institute. (Leibniz Senate 2015)*

   The Leibniz Senate recommended in detail:

*a) As planned at that time, the Board of Trustees must achieve a **full-time appointment to the scientific management of the Institute** within the framework of a joint appointment with the Technical University of Munich.*

After the former Scientific Director's resignation in 2016 the Director's position was established as full-time (75% at the Institute, 25% at the TUM) (see chapter 5: Leading scientific and administrative positions).

*b) The Supervisory Board must clarify whether, in addition to the scientific leadership, other positions at DFA can be filled as **professorships or junior professorships** via joint appointments with TU Munich.*

In case of an extended institutional funding, the LSB management and boards will establish two further W3 positions to lead the research sections I and III (beside the Scientific Director leading research section II). The positions shall be appointed jointly with TUM (see chapter 5: Leading scientists, chapter 6: cooperation with universities).

As mentioned above, the Institute and the TUM support the application of a LSB scientist for a tenure track professorship under the *Leibniz Programme for Women Professors* in 2020/2021 (see chapter 5: Equal opportunities) and an application for a Leibniz Junior Research Group.

*c) The supervisory board must review how **cooperation with the food industry** is to be organised in the future. At present, it is organised in a non-transparent form, mainly through the "Hans-Dieter Belitz Institute for Flour and Protein Research" (HDBI). The HDBI is headed by the acting DFA director. The necessity and function of this Institute for DFA must be critically examined.*

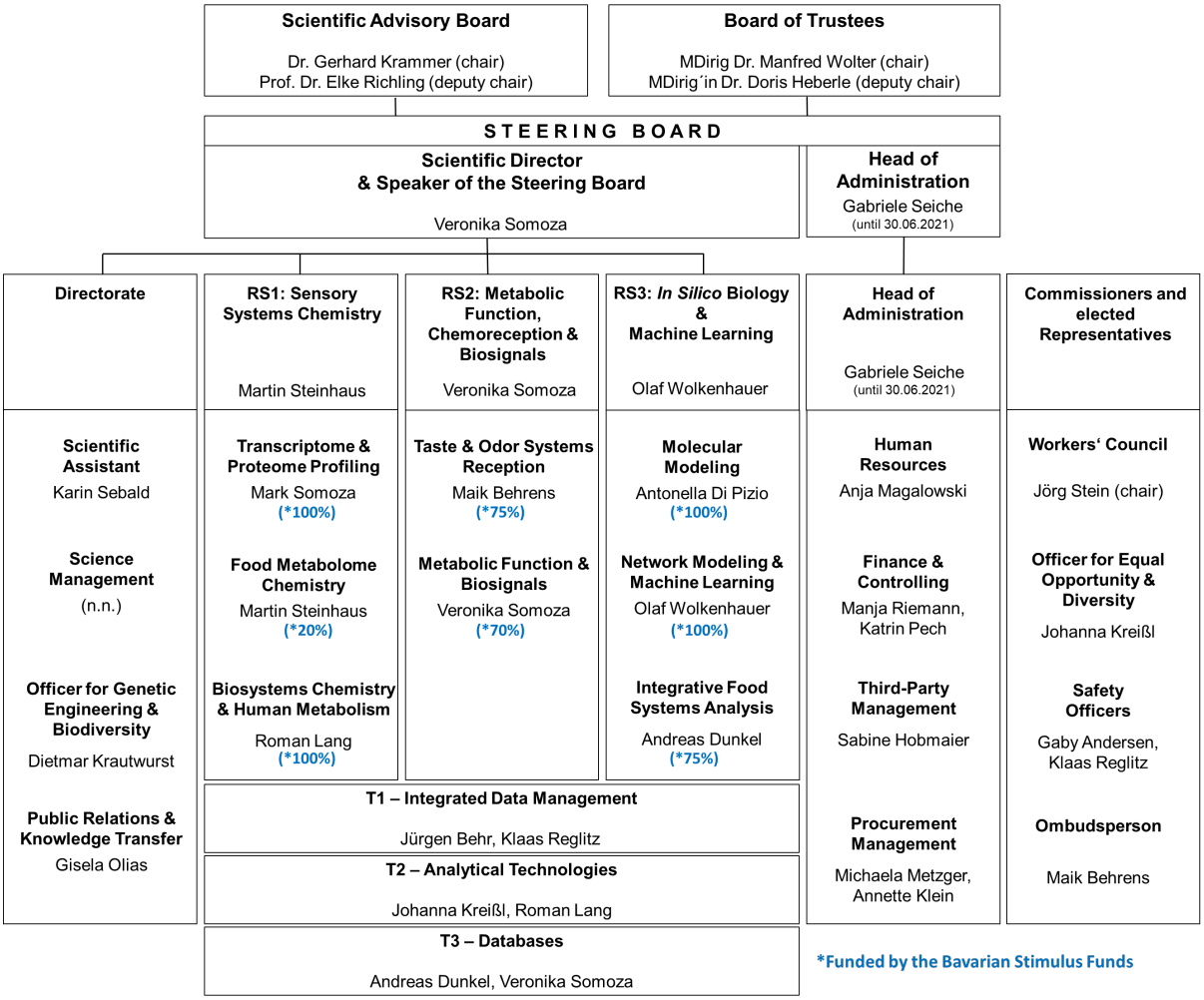
The Board of Trustees reported to the Leibniz Senate on this issue in March 2016 and May 2017 as requested. The third-party funded projects managed via the HDBI were transferred to the DFA and any connection between the HDBI and DFA was severed. In August 2017, the Foundation Council decided on the structural and scientific-strategic realignment of the DFA Foundation (see Chapter 3: Development since the last evaluation). The cooperation with the business community and the administrative processes in the Institute were restructured from the ground up (see Chapter 4: Quality Management). The LSB strives for transparent collaborations with the industry.

*d) In the Institute's statues it must be achieved that the **advisory board elects the chair from among its members**.*

This recommendation was implemented in October 2016.

Appendix 1

Organisational Chart



Appendix 2

Publications, patents, and expert reviews

	Period		
	2018	**2019**	**2020**
Total number of publications			
Monographs	9	5	2
Individual contributions to edited volumes	8	2	6
Articles in peer-reviewed journals Thereof open access articles	32 6	53 14	57 28
Articles in other journals	5	4	5
Working and discussion papers	0	1	0
Editorship of edited volumes	1	1	0

Appendix 3 Revenue and Expenditure

Revenue		2018			2019			2020 [1]		
		€k	% [2]	% [3]	€k	% [2]	% [3]	€k	% [2]	% [3]
Total revenue (sum of I., II. and III.; excluding DFG fees)		**8,887.4**			**7,924.6**			**9,495.5**		
I.	**Revenue (sum of I.1.; I.2., and I.3.)**	**5,205.0**	100		**5,107.2**	100		**4,938.4**	100	
1.	Institutional Funding	3,715.0	71		3,752.0	73		3,826.0	77	
1.1	Institutional funding by Federal and *Länder* governments according to AV-WGL	3,715.0			3,752.0			3,826.0		
2.	Revenue from project grants	1,473.9	28	100	1,341.2	26	100	1,097.4	22	100
2.1	DFG	34.0		2	0.0		0	0.0		0
2.2	Leibniz Association (competitive procedure)	111.0		8	52.0		4	9.0		1
2.3	Federal, *Länder* governments	935.9		63	837.3		62	689.6		63
2.4	EU	0.0		0	0.0		0	0.0		0
2.5	Industry	393.0		27	451.9		34	398.8		36
3.	Revenue from services	16.1	0		14.0	0		15.0	0	
3.5	Revenue from SFK	16.1			14.0			15.0		
II. [4]	**Bavarian Stimulus Funds**	**3,682.4**			**2,685.5**			**3,962.1**		
III.	**Miscellaneous revenue**	**0.0**			**131.9**			**95.0**		
IV.	**Revenue for construction projects**	**0.0**			**0.0**			**500.0**		

Expenditures		€k	€k	€k
Expenditures Institutional Budget		**5,044.4**	**5,174.0**	**5,422.7**
1.	Personnel	2,849.8	2,977.0	2,887.8
2.	Material expenses	881.3	985.0	998.0
2.1	*Proportion of these expenditures used for registering industrial property rights*	*1.0*	*2.0*	*1.0*
3.	Equipment investments	444.3	462.0	499.5
4.	Construction projects, acquisition of property	0.0	0.0	500.0
5.	Other operating expenses[4]	869.0	750.0	537.4
Expenditures Bavarian Stimulus Funds[4]		**3,682.4**	**2,685.5**	**3,962.1**
1.	Personnel	268.5	780.0	1,272.4
2.	Material expenses	136.3	112.6	327.1
3.	Equipment investments	3,277.6	1,555.0	2,159.4
4.	Construction projects, acquisition of property	0.0	0.0	0.0
5.	Other operating expenses[4]	0.0	237.9	203.2

[1] Preliminary data: yes
[2] Figures I.1., I.2. and I.3. add up to 100%. The information requested here is thus the percentage of "Institutional funding (excluding construction projects and acquisition of property) " in relation to "Revenue from project grants" and "Revenue from services".
[3] Figures I.2.1 to I.2.7 add up to 100%. The information requested here is thus the percentage of the various sources of "Revenue from project grants".
[4] Rent IZB, operating costs rooms, DFG levy, WGL contribution, legal advice, payroll accounting, tax office, publications, Corona, ancillary personnel costs etc.

Appendix 4

Staff

(Basic financing and third-party funding / proportion of women (as of: 31/05/2021)

	Full-time equivalents				Employees		Female employees		foreigners
	Personnel On Institutional Funds	Personnel on Bavarian Stimulus Funds	Total	on third-party funding	Total	on temp. contracts	Total	on temp. contracts	Total
	Number	Number	Number	%	Number	%	Number	%	Number
Research and scientific services	**15.35**	**15.90**	31.24	16.7	**42**	59.5	**18**	77.8	**6**
1st level (Scientific Director)	0.40	0.00	0.40	0.0	1	0.0	1	0.0	0
2nd level (chairs of RS)	0.20	0.04	0.24	0.0	1	0.0	0	0.0	0
3rd level (RG leaders)	2.52	2.32	4.84	13.2	6	33.3	1	100.0	2
Scientists in non-executive positions (E13, E14)	5.97	5.20	11.17	2.0	12	50.0	7	57.1	3
Doctoral candidates (E13)	6.26	8.35	14.60	29.8	22	77.3	9	100.0	1
Science supporting staff	**13.82**	**6.83**	20.65	13.1	**26**				
Press & Public Relations	0.65	0.35	1.00	0.0	1				
Laboratory (E9 to E12)	7.35	2.30	9.65	20.2	13				
Laboratory (E5 to E8)	1.50	2.50	4.00	12.5	5				
IT-Support	0.15	0.10	0.25	0.0	0				
T platforms (Core Facilities) leader	1.05	0.40	1.45	0.0	1				
T platforms (Core Facilities) non-executive	0.20	0.98	1.18	0.0	2				
T platforms (Core Facilities) supporting staff E9 -E10	2.72	0.00	2.72	9.2	3				
T Platforms (Core Facilities) supporting staff E5 -E8	0.20	0.20	0.40	0.0	1				
Science supporting staff (administration)	**7.3**	**0.0**	7.3	0.0	**10**				
Head of administration	1.0	0.0	1.0	0.0	1				
Staff positions (E9 to E12)	0.6	0.0	0.6	0.0	1				
Internal administration (financial administration, personnel, etc.) (E9 to E12)	3.3	0.0	3.3	0.0	4				
Internal administration (E5 to E8)	2.4	0.0	2.4	0.0	4				
Student assistants	**0.5**	**0.5**	1.0		**2**				
Scholarship recipients at the institution	**6.0**		6.0		**6**		**2**		**5**
Doctoral candidates (supervised)	6.0		6.0		6		2		5

11 March 2022

Annex B: Evaluation Report

Leibniz Institute for Food Systems Biology at the Technical University of Munich, Freising (Leibniz-LSB@TUM)

Contents

1. Summary and main recommendations

According to the foundation charter of August 2017, the mission of the Leibniz-LSB@TUM (LSB) "shall be to research the chemical composition of foods and their evaluation, taking into account the relevant microbiological, nutritional, physiological, toxicological, legal and other issues, and to promote science and research". The strategic aim derived from this mission is to reach an understanding of molecular networks and processes that drive food (processing)-related human biology and health. The LSB intends to follow a 'food systems biology' approach by integrating experiments with *in silico* biology and machine learning.

Since the last evaluation, these highly ambitious aims have expanded the scientific direction of the institute considerably, in terms of both content and, above all, methodology. The new direction led to the institute's name being changed to the *Leibniz Institute for Food Systems Biology*. Since it was founded in 1918 until the middle of 2017, the LSB had been called the *German Research Centre for Food Chemistry* (*Deutsche Forschungsanstalt für Lebensmittelchemie, DFA*). The modernisation efforts are welcomed.

They are a reaction to a major structural crisis that shook the LSB after the last evaluation. In July 2015, the Leibniz Association Senate pointed out that the institute's historic structures would need to change to enable further scientific development. Other criticisms by the Senate led to an investigation into the use of funds at the institute. Against this backdrop, the Head of Administration offered his resignation at the end of 2015, followed shortly afterwards by the Director, who had been in post since 1995. Irregularities were found at the institute (called the DFA at that time) that made far-reaching financial restructuring of the institute unavoidable, including insolvency proceedings. The Supervisory Board installed an interim management team. The proceedings understandably placed the employees at the DFA under a lot of pressure and led to a reduction in output.

Halfway through 2017, the direction was set for the realignment: first, the mission and name of the institute were changed and the internal structure was adjusted accordingly. The LSB is now organised into three Research Sections (RS) each of which currently has two or three Research Groups (RG). Three technology platforms work in tandem with the Research Sections. These structural changes have led to much better internal collaboration than was evident at the time of the last evaluation. At the top leadership level, a Vice President of the Technical University of Munich (TUM) was appointed Scientific Director of the LSB in August 2017. In October 2019, he became President of the university and gave up his position as Director of the LSB.

The current Director has been running the LSB since November 2019, along with Research Section II. This leadership change was a significant factor in the start of the more detailed development and implementation of the new concept. She is pushing ahead with the necessary comprehensive reform of the institute with great dedication and it is already starting to bear fruit. Worth highlighting are recent successes, like the establishment of a Leibniz Junior Research Group with third-party funding, for which a group leader has been recruited from Louvain in Belgium, and the establishment of a joint W2 professorship in Computational Pharmacology in partnership with TUM, which is being funded via the *Leibniz Programme for Women Professors* while awaiting a decision about tenure. From 2021 onwards, in a first for the institute, it has obtained funding for three DFG projects.

After just two years, the realignment process at the LSB is far from complete. In particular, section heads still need to be recruited for two of the three Research Sections. Only Research Section II on Metabolic Function, Chemoreception & Biosignals, which is headed by the Scientific Director, currently has a permanent head of section in place. Provided the advice and recommendations in this report are acted on, the review board believes there are best chances that the institute will continue to make good progress.

Special consideration should be given to the following main recommendations in the evaluation report (highlighted in **bold face** in the text):

Overall concept, results, changes and planning (chapter 2)

1. For the development of the LSB in the coming years, it remains essential to flesh out the concept of 'food systems biology' – the extremely broad and ambitious concept chosen in 2017 for the name of the institute. In the near future, additional **strategic questions** need to be clarified. For instance, a decision needs to be taken about which food groups the LSB wants to focus its research on. Until now, the choice has appeared arbitrary. In this context, the institute should consider focusing on foods that are of high importance for global basic nutrition or for a healthy diet. Work on luxury foods is less relevant. These prioritisation issues have already been broached at the LSB, but now need to be developed further in a strategic manner. It is good to see that the LSB aims to follow up its basic chemoreceptor-based studies with animal disease models and human intervention studies in future. How this important strategic goal can be implemented, in particular with partners at TUM, is something that now needs to be defined, moving beyond the announcements in the evaluation documents. The review board encourages the LSB to maintain a clear methodical focus in other areas too, and to bring in know-how through collaborations.
2. **Research Section III, In Silico Biology & Machine Learning,** is still in its infancy, both in terms of strategy and structure. The formulated goals must be broken down into concrete areas that are to be targeted. A strategy should also clearly define those areas (and fraction of staff) in which the section takes on the role of a bioinformatics service provider for other Research Sections, and where it plans to pursue independently initiated research. **Research Section I, Sensory Systems Chemistry,** is also still in a state of flux. The new conceptual approaches need to be given even more weight within the RS and be reflected structurally as well – in the distribution of resources and the development of strategic collaborations.
3. The further development, fleshing out and implementation of the LSB concept, which has been shaped in large part by the incumbent Director, presupposes that world-class **Section Heads** can be found for **Research Sections I and III** without delay. It is therefore important for the Bavarian department that is responsible for the LSB and chairs its Supervisory Board, to initiate procedures without delay for the planned joint appointments (W3 professorships) with TUM. Filling these positions is a prerequisite to enable the Director to further advance the reorientation of the LSB together with the other two section heads to push ahead with the realignment of the LSB and prepare an application to extend the institutional funding. According to the plans by the ministries responsible for the institute, a decision on the permanent extension of the LSB's institutional funding is to be made on the basis of this application in another procedure.

4. The Director is aligning the LSB's **publication and third-party-funding strategy** with the new concept. The publication strategy aims for an increased number of high-impact peer-reviewed and open access publications. This is already resulting in a significantly higher-impact publication record. The institute is encouraged to continue its activities in this area, specifically with focus on a broader range of journals and increased competitive and international funding.

Controlling and quality management (chapter 3)

5. The LSB's **institutional funding** for ongoing activities (core budget) was 3.76 M€ per year on average between 2018 and 2020. Against this backdrop, it makes sense that the responsible *Land* ministry has topped up the joint institutional funding by the federal and *Länder* governments for the years 2018 to 2024 by an additional 3.6 M€ per year on average – a *de facto* increase of the core budget – and is now striving to have this funding from the *Land* (Bavarian Stimulus Funds) converted into joint funding by the federal and *Länder* governments. A first application was not successful. Now the plan is to apply for an increase at the next possible opportunity. The joint federal and *Länder* funding process, through which the *Land* is currently planning to apply, requires preparations to take place as early as 2022.

   In the experts' view, it is not possible to implement the necessary structural and performance-related progress within this timeline. Instead, the Supervisory Board and, in particular, the responsible specialist departments of the host *Land* and federal government need to significantly improve and expand the structural conditions needed for the scientific development of the LSB. In view of the strong scientific capability and dedicated leadership skills of the Director, and the resources already invested by the *Land* through the Bavarian Stimulus Funds, an investment of this kind would make good sense. In a few years, it will be possible to make a robust scientific assessment of whether a permanent increase in joint funding by the federal and *Länder* governments is justified.

6. It is good to see that construction work on a **new building** will begin in late 2021 in the immediate vicinity of the current buildings (according to the information available to the review board at the time of the assessment, 04th Oct, 2021). The new building is scheduled to be ready in 2023/2024. This is an important step for the institute's consolidation and also has potential to increase the visibility and attractiveness of the LSB as a competitive employer.

7. The **Scientific Advisory Board** is currently in the process of being restructured in line with the institute's change of research focus since 2017. This is a highly welcome development as it is extremely important to have board members with expertise in the institute's new focus areas. New appointments to the SAB should also lead to a higher number of members from abroad (at present 3 of 11) and female scientists (1 of 11).

Cooperation and environment (chapter 5)

8. The possibilities for **collaboration with TUM** must be exploited further, as planned, for example in the area of human intervention studies. Collaboration should also take place in the field of data analysis and modelling. The ongoing joint DFG and Collaborative Research Centre (SFB) proposals by the LSB and TUM are promising.

2. Overall concept, results, changes and planning

Overall concept

According to the foundation charter of August 2017, the institute's mission is "to research the chemical composition of foods and their evaluation, taking into account the relevant microbiological, nutritional, physiological, toxicological, legal and other issues, and to promote science and research". The strategic aim derived from this mission is to reach an understanding of molecular networks and processes that drive food (processing)-related human biology and health. The LSB intends to follow a 'food systems biology' approach by integrating experiments with *in silico* biology and machine learning.

These highly ambitious aims are expanding the scientific focus of the institute considerably, in terms of content but also, above all, in terms of methodology. The new direction also led to the institute changing its name from the German Research Centre for Food Chemistry (*Deutsche Forschungsanstalt für Lebensmittelchemie*, DFA), a name it had held since it was founded in 1918 until the middle of 2017. The modernisation efforts are welcomed. They are a reaction to a major structural crisis that shook the LSB after the last evaluation.

Results

It is good to see that the research outputs are now being published in peer-reviewed journals to a much greater extent than at the time of the last evaluation (2011–2013: 58 articles, 2018–2020: 142 articles). These articles are increasingly being published via the open access route. It is worth highlighting that some results have been published in journals with a very high international reputation, e.g. *Nature* and *Nature Immunology.*

Following the realignment of the institute, the overall concept is being refined continuously. A few examples show how the concept planning is already producing results:

- The three Research Sections collaborated closely to produce results on structural characterisation of human bitter taste receptors in a combined approach involving experimental studies and computer modelling.
- RS II and RS III succeeded, together with other academic and industry partners, in characterising the impairment of odorant and taste receptors caused by SARS-CoV-2 infections.
- It is also good to see that a first human intervention study on the relationship between the sweet taste of sugar, energy intake, and hunger-satiety regulation was published in collaboration with partner institutions. The institute is encouraged to continue on this path of combining basic research and studies in animal models and humans (see below).
- Research-relevant databases are being developed and maintained, both in the Sections and in the technology platforms. Worth highlighting is an impressive prototype of the open access Food Systems Biology Database (FSBD) to collect scientific knowledge on food. In addition, for a long time the institute has been working on the comprehensive Souci-Fachmann-Kraut Food and Nutrition Tables (SFK), a definitive work in food chemistry.

Development since the previous evaluation

In July 2015, the Leibniz Association Senate pointed out that the institute's development was not yet keeping pace with the positive developments in food chemistry at TUM, the institute's partner university. At the time, the Senate stated: "The historically grown structures of the Institute must now be changed quickly in order to enable further scientific development of the Institute."

Other criticisms by the Senate led to an investigation into the use of funds at the institute. Against this backdrop, the Head of Administration offered his resignation at the end of 2015, followed shortly afterwards by the Director, who had been in post since 1995. Irregularities were found at the institute (called the DFA at that time) that made far-reaching financial restructuring of the institute unavoidable, including insolvency proceedings. The Supervisory Board installed an interim management team. The proceedings understandably placed the employees at the DFA under a lot of pressure and led to a reduction in output.

Halfway through 2017, the direction was set for the realignment: first, the mission and name of the institute were changed (see above). The institute is now organised into three Research Sections (RS), each of which currently has two or three Research Groups (RG). Three technology platforms work in tandem with the Research Sections. This basic structure makes good sense.

Secondly, in August 2017, a new Director was appointed. He was already Vice President of TUM and when he became President in October 2019, he gave up his position as Director of the LSB. The detailed development and implementation of the new concept only began in earnest under the leadership of the current Director, who has been in charge of the LSB and Research Section II since November 2019. She is pushing ahead with the necessary comprehensive reform of the institute with great dedication and energy, but, after just two years, it is far from complete.

Thirdly, the state of Bavaria almost doubled the institute's core budget (which was extremely small compared with other Leibniz Institutes in similar fields) from 2018 for a limited period of time. The *Land* is striving to put this additional funding (Bavarian Stimulus Funds) on a permanent footing via joint funding from the federal and *Länder* governments. A first application for this was initially submitted for the period from 2023 onwards. However, in January 2021 the German Council of Science and Humanities (*Wissenschaftsrat*, WR) decided there were not yet sufficient grounds for a permanent extension of the joint funding from the federal and *Länder* governments, despite approving of the reforms initiated at the LSB. Consequently, the state of Bavaria extended its additional funding: The Bavarian Stimulus Funds for the LSB now amounts to 25.4 M€ in total for 2018 to 2024 – an average of 3.6 M€ per year. Attempts are now being made to transfer the temporary *Land* financing into permanent joint funding by the federal and *Länder* governments from 2025 (application through the procedure for a strategic extraordinary item of expenditure, *kleiner strategischer Sondertatbestand*).

Strategic work planning for the coming years

In its statement of 22 January 2021, the WR noted that it was an ambitious goal of the LSB to "integrate the systems biology approach into food research". The "fundamentally convincing concept" is "unique worldwide" and has "great potential". However, the Institute "so far only partially has the prerequisites" for its implementation. According to the WR's assessment, successful implementation of the concept requires in particular that the LSB **(i)** clarifies its understanding of systems biology, develops the profile of Research Section III (*In Silico Biology & Machine Learning*) and expands interdisciplinary and international collaborations, **(ii)** fills the vacant leadership positions in two of the three Research Sections, and **(iii)** secures appropriate third-party funding and diversifies the publication strategies (see Status Report, p. A-9). The review board shares the WR's assessment that these are the key aspects for evaluating the strategic development of the LSB and follows this up with its assessments.

For the development of the LSB in the coming years, it remains essential to flesh out the concept of 'food systems biology' – the extremely broad and ambitious concept chosen in 2017 for the name of the institute. The Director of the LSB is aware of this, as became clear in the discussions with her. In the evaluation documents, the institute's strategic aim is limited to exploring "the complex networks and activities of biologically and sensory relevant ingredients of foods and their chemoreceptor-mediated effects in living organisms in order to make them systemically understandable and predictable in the long term". **In the near future, additional strategic questions need to be clarified.**

- **For instance, a decision needs to be taken about which food groups the LSB wants to focus its research on. Until now, the choice has appeared arbitrary. In this context, the institute should consider focusing on foods that are of high importance for global basic nutrition or for a healthy diet. Work on luxury foods is less relevant. These prioritisation issues have already been broached at the LSB, but now need to be developed further in a strategic manner**
- **It is good to see that the LSB aims to follow up its basic chemoreceptor-based studies with animal disease models and human intervention studies in future. How this important strategic goal can be implemented, in particular with partners at TUM, is something that now needs to be defined, moving beyond the announcements in the evaluation documents.** In doing so, the institute should consider from the outset how to translate the results to the consumer level.
- **The review board encourages the LSB to maintain a clear methodical focus in other areas too, and to bring in know-how through collaborations.** This applies in particular to the work on developing Research Section III, which started recently. The institute is advised to enter into a collaboration with the Leibniz research centres at TUM and, where relevant, with other potential partners outside Munich in the field of informatics/bioinformatics.

Research Section III, In Silico Biology & Machine Learning, is still in its infancy, both in terms of strategy and structure. The formulated goals must be broken down into

concrete areas that are to be targeted. A strategy should also clearly define those areas (and fraction of staff) in which the section takes on the role of a bioinformatics service provider for other Research Sections, and where it plans to pursue independently initiated research. At the beginning of 2020, there were 2.5 full time equivalent (FTE) available in the Research Section; in November 2021, there were nearly 6 FTE. It is a milestone for the Section's further development that a scientist from RS III will be appointed to a W2 professorship in Computational Pharmacology in 2022, initially for five years, through the *Leibniz Programme for Women Professors*. The appointment was made jointly with TUM. The development of RS III has been managed since November 2020 by a professor from the University of Rostock, who has outstanding credentials but is only able to devote 10 % of his working hours to this task, and only until a permanent Head of Section is appointed through a joint procedure with TUM.

Research Section I, Sensory Systems Chemistry, is also still in a state of flux. The new conceptual approaches need to be given even more weight within the RS and be reflected structurally as well – in the distribution of resources and the development of strategic collaborations. The position of Head of Section is still vacant. A long-standing habilitated employee of the institute is performing this role on an interim basis.

The further development, fleshing out and implementation of the LSB concept, which has been shaped in large part by the incumbent Director, presupposes that world-class Section Heads can be found for Research Sections I and III without delay. It is therefore important for the Bavarian department that is responsible for the LSB and chairs its Supervisory Board, to initiate procedures without delay for the planned joint appointments (W3 professorships) with TUM. Filling these positions is a prerequisite to enable the Director to further advance the reorientation of the LSB together with the other two section heads to push ahead with the realignment of the LSB and prepare an application to extend the institutional funding. According to the plans by the ministries responsible for the institute, a decision on the permanent extension of the LSB's institutional funding is to be made on the basis of this application in another procedure.

The Director is aligning the LSB's publication and third-party-funding strategy with the new concept. The publication strategy aims for an increased number of high-impact peer-reviewed and open access publications. This is already resulting in a significantly higher-impact publication record (see above, p. B-5). **The institute is encouraged to continue its activities in this area, specifically with focus on a broader range of journals and increased competitive and international funding.**

The portfolio of third-party funding was for a long time dominated by funds from the German Federation of Industrial Research Associations (*Arbeitsgemeinschaft industrieller Forschungsvereinigungen,* AiF), which funds research for small and medium-sized enterprises in Germany, and from a few large businesses. In 2021, in a first for the institute, scientists who had recently joined the LSB secured three DFG projects for the institute. Moreover, from 2022 onwards, a *Leibniz Junior Research Group* called "Mouthfeel – How texture makes flavor", which works primarily with biophysical methods, will be funded at the LSB and led by

a researcher who has been working in Louvain in Belgium. In addition, a researcher has secured funding through the *Leibniz Programme for Women Professors* (see above, p. B-8). It is good to see that the Director is very supportive of these efforts to secure third-party funds, and other applications are being prepared for submission to funding institutions that focus on basic research, including the EU.

3. Controlling and quality management

Facilities, equipment and funding

The LSB's institutional funding for ongoing activities (core budget) was 3.76 M€ per year on average between 2018 and 2020. Compared with other Leibniz institutions in the life sciences, this is an extremely low figure. For a *Land* or the federal government to apply for an institute to be accepted for joint funding by the federal and *Länder* governments as a Leibniz institution, the core budget currently has to be at least 5 M€.

Against this backdrop, it makes sense that the responsible *Land* ministry has topped up the joint institutional funding by the federal and *Länder* governments for the years 2018 to 2024 by an additional 3.6 M€ per year on average – a *de facto* increase of the core budget – and is now striving to have this funding from the *Land* (Bavarian Stimulus Funds) converted into joint funding by the federal and *Länder* governments. A first application was not successful (see chapter 2, p. B-6). **Now the plan is to apply for an increase at the next possible opportunity. The joint federal and *Länder* funding process, through which the *Land* is currently planning to apply, requires preparations to take place as early as 2022.**

In the experts' view, it is not possible to implement the necessary structural and performance-related progress within this timeline. Instead, the Supervisory Board and, in particular, the responsible specialist departments of the host *Land* and federal government need to significantly improve and expand the structural conditions needed for the scientific development of the LSB. In view of the strong scientific capability and dedicated leadership skills of the Director, and the resources already invested by the *Land* through the Bavarian Stimulus Funds, an investment of this kind would make good sense. In a few years, it will be possible to make a robust scientific assessment of whether a permanent increase in joint funding by the federal and *Länder* governments is justified.

In past years (2018–2020), the institute secured 1.3 M€ on average per year in **third-party funding** for research projects. This equates to 25 % of the budget for current expenditure (core budget plus third-party funding). If one includes the Bavarian Stimulus Funds as a *de facto* additional core budget (3.38 M€ per year for 2018–2020), the proportion represented by third-party funding is 15 %. The funds were almost all secured from the federal government and the *Länder* and from industry. This underlines how important it is to strategically realign the third-party funding portfolio as part of the reform of the entire LSB. It is good to see that in 2021, for the first time, three DFG projects were secured (with total funding of 892 k€ over three years, i.e. 212 k€ p.a.). These successes will be supplemented from 2022 onwards by two grants secured through the Leibniz Association's competition processes

(*Leibniz Junior Research Group* and *Leibniz Programme for Women Professors*). In the coming years, these successes should be consolidated as planned, and opportunities taken to apply for funds at European level.

For a long time, the LSB has occupied a TUM **building** on the Freising campus. Since the middle of 2020, additional premises have been rented in the immediate vicinity to meet the increased space requirements, especially for experimental work. **It is good to see that construction work on a new building will begin in late 2021 in the immediate vicinity of the current buildings (according to the information available to the review board at the time of the assessment, 04th Oct, 2021). The new building is scheduled to be ready in 2023/2024. This is an important step for the institute's consolidation and also has potential to increase the visibility and attractiveness of the LSB as a competitive employer.**

Organisational and operational structure

The fundamental reform of the LSB has led to clear changes in the internal structure. The new **organisation of the LSB** into Research Sections with Research Groups and technology platforms makes good sense.

A very positive development is that, since July 2018, the **Steering Board** includes the Head of Administration as well as the Scientific Director.

Internal collaboration is structured much better than it was at the time of the last evaluation. Three years ago, an **extended Management Board** was set up, in which the Steering Board, the heads of the Research Sections, Research Groups and technology platforms, and representatives of co-workers and doctoral candidates discuss the strategic development of the LSB and agree together on future plans.

Quality management

The institute has implemented a set of rules and strategies for quality management in recent years, ensuring compliance with the DFG and Leibniz guidelines for **good scientific practice**. An officer for genetic engineering and biodiversity monitors compliance with the Nagoya Protocol.

It was recently decided to implement a **performance-based funding (LOM)** system. This is welcomed. At a later stage, it will be possible to see how strong the impact is.

Quality management by advisory boards and supervisory board

The Scientific Advisory Board is currently in the process of being restructured in line with the institute's change of research focus since 2017. This is a highly welcome development as it is extremely important to have board members with expertise in the institute's new focus areas. New appointments to the SAB should also lead to a higher number of members from abroad (at present 3 of 11) and female scientists (1 of 11).

4. Human Resources

At 31 May 2021, the LSB employed 78 people (59.2 FTE). This number has increased from 56 (41.7 FTE) at the time of the last evaluation.

Leading scientific and administrative positions

After the last evaluation, the then Director and Head of Administration tendered their resignations (see chapter 2, p. B-6). The financial situation of the institute had to be fundamentally restructured. In 2017, the Supervisory Board set the direction for a new start and appointed a new Director. After he became President of TUM, the current **Director** took up her post in November 2019 and is now leading the institute with extreme dedication and a clear perspective for the scientific and structural requirements.

After a transition period, a new Head of Administration started working at the LSB in September 2017. She joined the Steering Board in 2018. In November 2021, a new **Managing Director** *(kaufmännischer Geschäftsführer)* was appointed who has experience in the administrative management of institutes.

For the further development of the LSB, it is now essential to fill the vacancies for scientific **heads of Research Sections I and III** through joint appointments with TUM in an international competitive process (see chapter 2, p. B-8).

Staff with a doctoral degree

The new Director has drawn dedicated researchers to the LSB, who completed their qualifications at other institutions, to take up positions as research group leaders. Successes in securing DFG funding and in Leibniz Association programmes are due in large part to this group of individuals. Accordingly, LSB employees are encouraged to move to other institutions after completing their qualifications. It is good to see that the Director supports the search for follow-on positions both nationally and internationally, partly with a view to developing a strong international network. In 2019, the head of a research group in Research Section I, a female LSB scientist who had habilitated, left to take up a position as an assistant professor at the Karlsruhe Institute of Technology (KIT), Germany.

Doctoral candidates

Since 2020, contracts with doctoral candidates have been based on current DFG regulations and follow the guidelines of the TUM Graduate School, in which all candidates participate. The procedures have been updated to a fully English-language education programme, leading to a cumulative thesis. This enables candidates to start writing their thesis at an earlier point in the process.

As a result, the average completion time for a doctoral degree has decreased significantly, but is still 4.7 years, this should remain a focus area and should be reduced further.

Equal opportunities and work-life balance

As of September 2021, 55 % of all scientists at the LSB are female. Among the doctoral candidates, the proportion is even higher, at 68 %.

The institute is led by a female scientist. She also heads one of the three Research Sections. The other two are currently being provisionally led by male scientists. From 2022 onwards, the Research Sections will comprise a total of nine research groups/junior research groups. Besides the Director, two other female scientists head research groups. The upcoming appointments to leadership positions offer opportunities to further increase the proportion of female scientists.

The LSB has implemented the regulations to which the member institutions of the Leibniz Association have committed themselves, and the regulations specified by the federal government and the *Länder* to ensure an appropriate gender equality policy.

5. Cooperation and environment

The LSB cooperates closely and successfully with the **Technical University of Munich (TUM)**. The institute's Scientific Director is jointly appointed by the LSB, TUM and a member of the *ZIEL Institute of Food and Health* at the *TUM School of Life Sciences*. More joint appointments to W3 professorships are planned for the heads of RS I and III. In addition, a third-party-funded joint W2 professorship with tenure track in Computational Pharmacology was recently set up with the university, initially for a period of five years, starting in 2022. **The possibilities for collaboration with TUM must be exploited further, as planned, for example in the area of human intervention studies. Collaboration should also take place in the field of data analysis and modelling. The ongoing joint DFG and Collaborative Research Centre (SFB) proposals by the LSB and TUM are promising**.

LSB scientists initiated together with scientists from TUM University Hospital, University of Vienna (Austria) and *Max Rubner Institute* (MRI, Karlsruhe, Germany) an expert network on "Sweet taste perception". The scientific cooperation with the MRI as the German Federal Institute on consumer health protection in the nutrition sector should be further developed. The MRI ensures already that LSB data from the *Souci-Fachmann-Kraut Food Composition and Nutrition Tables* (SFK) are transferred to the *German Nutrient Database* (BLS).

Within the **Leibniz Association**, the LSB already cooperates with other institutes, for example in two *Leibniz Research Networks*, but also in several prospective joint projects. When developing the LSB concept further and fleshing it out, it is important to keep an eye on the interfaces to other Leibniz Institutes, especially the German Institute of Human Nutrition *(Deutsches Institut für Ernährungsforschung*, DIfE).

Chemoreceptor-based studies are conducted in particular at the *Wageningen Food & Biobased Research Institute* (Wageningen University, The Netherlands) and at the *Monell Chemical Senses Center* (Philadelphia, USA) as part of comprehensive concepts for researching food and the relationship between food and human biology. Even if the LSB's institutional funding is increased permanently, its research opportunities will still be much more limited than at these centres. The scientific leaders at the LSB are aware that this competitive **international environment** must be taken into account in the further development of the institute's concept.

6. Subdivisions of the LSB

Research Section I: Sensory Systems Chemistry

[20.1 FTE, of whom 6.7 FTE research and scientific services staff, 7.1 FTE doctoral candidates, and 6.3 FTE service staff]

Research Section I (RS I) successfully combines the chemical analysis, identification and synthesis of key aroma substances in foods as well as in the human body after ingestion. These odorants and flavours are also studied in the context of human health responses. This broad research portfolio is based on a high level of expertise in method application and development. RS I uses a well-established set of techniques for quantification (mainly based on SAFE combined with GC-MS and SIDA[1]). However, there are much faster methods and sample preparation systems available, some of which are even more sensitive than this approach. In particular, it is essential that the RG on *Food Metabolome Chemistry*, which is by far the largest research group, works with the other Research Sections in future to develop innovative methodological approaches that go beyond the established methods. The establishment of the RG on *Transcriptome & Proteome Profiling* and the RG on *Biosystems Chemistry & Human Metabolism* in 2020 was a first effective step in broadening the portfolio of methods.

The very good research results are published appropriately. This also includes the output of the RG on *Functional Biopolymer Chemistry*, which came to an end at the LSB in 2019 when the leader moved to the Karlsruhe Institute of Technology (KIT). The results of the RG on *Food Metabolome Chemistry* appear primarily in journals that are co-edited by former directors of the institute, so the portfolio of journals should be diversified. Third-party funding is adequate, consisting mainly of federal and *Länder* government and industry funding. The RS also needs to secure revenue from the DFG and the EU. In this respect, it is good to see that a first DFG grant for research in the RG on *Transcriptome & Proteome Profiling* was recently approved. The number of completed doctorates (19 in the three-year-reporting period) is the highest of all Research Sections, but has fallen over recent years. The number of doctoral candidates needs to be increased again.

Future research should focus on foods that contribute significantly to daily nutrition or align expertise with natural foods and their associated sensory attributes to achieve a positive impact on industrial food production. This calls for close collaboration with partners both nationally and internationally. While the two new research groups set up in 2020 each have only three or four FTE, the RG on *Food Metabolome Chemistry*, which has existed since 1995, is much larger, with 12 FTE. The head of this research group is currently the provisional head of RS I.

On the whole, RS I is still in a state of flux. The new conceptual approaches now need to be given even more weight and be reflected structurally as well – in the distribution of resources and the development of strategic collaborations. For the further fruitful development of the Research Section, it is essential for the head of section position (W3 professorship) to be filled as planned with a world-class candidate without delay, in a joint appointment procedure with TUM.

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[1] SAFE = Solvent Assisted Flavour Evaporation; GC-MS = Gas Chromatography Mass Spectrometry; SIDA = Stable Isotope Dilution Assay

Research Section II: Metabolic Function, Chemoreception & Biosignals

[17 FTE, of whom 6 FTE research and scientific services staff, 5.2 FTE doctoral candidates, and 5.8 FTE service staff]

Research Section II (RS II) has been chaired since 2020 by the Scientific Director, and investigates molecular mechanisms of sensory perception of foods and their impact on chemoreceptor-associated human biology. The transformation from a strong and globally recognised taste and aroma chemistry unit to the new food systems biology concept started in 2018 and implementation of the approach is still in its infancy.

The very good research results are published in appropriate journals. For instance, in collaboration with RS III, insights were gained into the impairment of the sense of taste and smell following a SARS-CoV-2 infection. However, in collaboration with experts from different research fields, e.g. nutritional epidemiology and omics technologies, RS II has the potential to achieve even more publications in high-ranking journals recognised by a broader scientific community. It is good to see that third-party funding has increased since the evaluation of the WR in 2020/2021, coming from the federal and *Länder* governments and industry. For instance, a DFG grant was recently obtained for work in the RS. In the future, this trend needs to be continued, including EU funding as well as funding from the DFG. The number of completed doctoral degrees needs to be increased.

The future plans are ambitious and their implementation requires more resources and personnel. The research programme must be developed further and given greater focus. In this context, a more comprehensive approach to systems biology of whole foods is recommended, studying food patterns of 'natural' and sustainably produced foods in comparison to patterns of industrially produced foods composed mainly of semi-purified ingredients. The plans to target specific regions in the body or organs to trigger a certain response are supported and the receptors selected for investigation should be extended further.

It is good to see that human intervention studies will be carried out in collaboration with scientific partners. The LSB could add value to the research programmes of several high-quality and competitive European universities and research institutes by offering its cell lines and receptor models for complex food perception research. Research group heads should increase their visibility in the scientific community in Europe and beyond.

Research Section III: In Silico Biology & Machine Learning

[5.9 FTE, of whom 2.6 FTE research and scientific services staff, 2 FTE doctoral candidates, and 1.3 FTE service staff]

Research Section III (RS III) is crucial for implementing the overarching strategic focus of the LSB on systems biology. The Section is still in the process of being established. In November 2018, the RG on *Molecular Modeling* was set up. At the time of the evaluation, it had only 1.7 FTE. In November 2019, the RG on *Integrative Food Systems Analysis* was added to the Section. It currently has 4.1 FTE. The head of this research group has been working at the LSB since 2018 and, together with the Director, also runs the *Databases* technology platform. Since November 2020, RS III has been chaired by an interim head working on a part-time

basis (10 %), who is an expert with a strong track record in bioinformatics and systems biology.

The scientific goal is to investigate molecular mechanisms eliciting sensory perception and the comprehensive characterisation of complex food systems. For this purpose, the RS aims to develop molecular interaction networks and machine learning algorithms and to understand the molecular systems defining the functional properties of foods and their effects on human health and well-being.

A prototype of the Food Systems Biology Database (FSBI-DB) developed to collect knowledge about food is impressive. The Section should develop a long-term strategy to maintain the database and to enable partner organisations to integrate additional content. Given the recent establishment of RS III, the results it has achieved, such as the findings on the influence of SARS-CoV-2 on the sense of taste and smell, are commendable and are publicised adequately. However, the RS has the potential to achieve even more publications in a diverse spectrum of high-ranking journals.

The amount of third-party funding is still low, however an upward trend is visible, with the head of the RG on *Molecular Modeling* having secured a DFG project with funding from 2021. Future applications, especially for DFG and EU grants, should preferably be initiated in collaboration with external partners. RS III should also consider closer collaboration with institutions and infrastructure in the wider Munich area, e.g. the Leibniz Supercomputing Centre situated on the TUM campus, or with partners outside Munich. These centres would also profit from the Section's expertise in network modelling.

The future plans based on an integrated approach to studying molecule-based networks are very promising and have clear potential for excellent results, provided that the personnel resources of the RS increase substantially. In particular, collaboration between RS III and the other two Research Sections, which is important for the overall concept of the institute, needs to be fleshed out further. In this context, the balance between research and service must also be clarified, with clear definitions as to how much of the work of RS III should involve providing bioinformatic and other services to the other Research Sections, and how intensively it can pursue its own research profile.

The recruitment of two research group leaders has been very successful. Recently, the Leibniz Association decided to fund a tenure-track W2 professorship for a five year period, starting in 2022 (joint appointment of LSB and TUM). The further development of the Research Section presupposes that the vacancy at the head of RS III will be filled without further delay (see chapter 2, p. B-8).

7. Handling of recommendations of the last external evaluation

The LSB successfully addressed the recommendations made by the Leibniz Association Senate/the German Council of Science and Humanities (*Wissenschaftsrat*) in 2015/2021 (see Status Report, p. A-22f). The recommendations on publication (recommendation 1) and third-party funding (recommendation 2) still apply.

Appendix

1. Review Board

Chair (Member of the Leibniz Senate Evaluation Committee)

Evamarie **Hey-Hawkins**	Institute of Inorganic Chemistry, Leipzig University

Deputy Chair (Member of the Leibniz Senate Evaluation Committee)

Eva Inés **Obergfell**	Faculty of Law, Humboldt University Berlin

Reviewers

Tim **Clark**	Computer Chemistry Center, University of Erlangen-Nuremberg
Dolores **Corella Piquer**	School of Medicine, University of Valencia, Spain
Bert **de Groot**	Max Planck Institute for Biophysical Chemistry, Göttingen
Hans-Ulrich **Humpf**	Institute of Food Chemistry, University of Münster
Erich **Leitner**	Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Austria
Ulf **Leser**	Institute for Computer Science, Humboldt University Berlin
Michael **Müller**	Professor of Nutrigenomics and Systems Nutrition, University of East Anglia, UK
Mari **Sandell**	Department of Food and Nutrition, University of Helsinki, Finland
Michelle H. **Williams**	Department of Food Science, Aarhus University, Denmark

Representative of the federal government

Frank **Reifers**	Federal Ministry of Education and Research, Bonn

Representative of the Länder *governments (member of the Leibniz Senate Evaluation Committee)*

Marc **Brüser**	Ministry of Science and Health of Rhineland-Palatinate, Mainz

7 April 2022

Annex C: Statement of the Institution on the Evaluation Report

Leibniz Institute for Food Systems Biology
at the Technical University of Munich, Freising (Leibniz-LSB@TUM)

On behalf of all employees, we would like to thank the members of the evaluation committee for an open and constructive discussion during their virtual visit to our Institute on October 4th 2021, and for their highly valuable and supportive recommendations provided by their evaluation report.

Our statement on this evaluation report has been prepared in consultation with the members of the LSB's Extended Steering Board, its Scientific Advisory Board and the representatives of the funding bodies. Overall, the needs for action addressed in this report are stated correctly and are comprehensive.

We appreciate the positive comments on our visionary scientific program towards Food Systems Biology in terms of content and methodology, and on our scientific achievements documented by improvements of various performance indicators, namely publication quality and quantity, third-party funds (e.g. DFG projects, Leibniz Junior Research Group, Leibniz Women Professor being jointly appointed with the Technical University of Munich - TUM), and science transfer (e.g. databases).

The **Food Systems Biology approach was initiated** by Professor Thomas Hofmann in 2017. With this approach, the LSB no longer solely aims at an understanding of the composition and the hedonics of foods. The LSB now contributes to the development of a molecular systems biology understanding of chemosensory relevant food ingredients. According to the understanding of the LSB, Food Systems Biology means to explore and predict the composition and intrinsic interactions of dynamic food ingredient systems along the entire value chain, as well as to investigate their complex effects on biosystems, such as the human organism or the gastrointestinal microbiota, and to predict these effects using methodologies from bioinformatics, chemometrics and machine learning.

We fully agree with the members of the evaluation committee that **it will take some time to consolidate the Food Systems Biology approach** at the LSB, even though the members of the evaluation committee state that our approach is "already starting to bear fruit", highlighting several successes achieved since the implementation of this approach started in full swing at the end of 2019. The LSB appreciates this positive and encouraging comment, in particular because this transformation was challenged by transitions of the Steering Board in 2019 and 2021, one evaluation by the German Council of Science and Humanities in 2020, followed by the current subject evaluation in 2021, a re-location of about one half of the research facilities into another building in 2020, and the Corona pandemic starting in early 2020.

The overall concept of Food Systems Biology has been comprehensively discussed in several retreats and has already resulted in **four research publications, which demonstrate the implementation of the Food Systems Biology approach** by spanning over all of our three Research Sections.

In collaboration with the TUM, the LSB strives for integrating the Food Systems Biology approach also in academic education programs. From the winter semester 2022/2023, e.g., a lecture in Bioinformatics will be given by one of the RS III group leaders together with the TUM Chair of Bioinformatics, and a Food Systems Biology seminar is

scheduled starting in May 2022. Moreover, an international joint seminar series on Food Systems Biology with a federal research organization in New Zealand has been initiated. In addition, LSB researchers supervise Bachelor, Master and PhD theses. In order to keep our PhDs internationally competitive, the LSB seeks a shorter PhD duration (now: ~4.7 years; average duration at the TUM School of Life Sciences in 2021: 5.0 years)

In order to further implement the Food Systems Biology approach in our local environment, research collaborations with the TUM have been and will be further expanded in the future, following the evaluation committee's recommendation *"The possibilities for collaboration with TUM must be exploited further, as planned, for example in the area of human intervention studies."*

Following this strategy, the LSB director is member of the ZIEL-Institute for Food & Health at the TUM. Research collaborations between working group leaders of Research Section III (*In Silico* Biology and Machine Learning) and the TUM Chair of Biomolecular Dynamics were started in 2021. Group leaders of all Research Sections (I-III) are currently performing human intervention studies with the Chair of the ZIEL Core Facility for Human Studies at the TUM.

The members of the evaluation committee not only recommend to *"flesh out the concept of 'food systems biology'".* They also strongly emphasize the need *to strengthen Research Section III* (*In Silico* Biology & Machine Learning) since this Research Section *"is still in its infancy, both in terms of strategy and structure."*

The LSB's strategy for Research Section III derives from its understanding that Food Systems Biology is an interdisciplinary research approach that enables finding solutions for complex questions in food research. It combines food chemistry and molecular biological application-oriented basic research with *in silico* biology. The latter includes the areas of bioinformatics, machine learning, network modeling, and molecular analyses. The Food Systems Biology approach builds on the LSB's analytical strength, focusing on the formation of individual molecules and their chemical reactivity, to understand molecular network and processes driving food (processing) – related human biology and health in order to develop tasty foods for healthy people.

The LSB acknowledges this highly supportive **recommendation to strengthen Research Section III** and has already further increased the personnel resources of Research Section III by 3 FTEs during the past six months. This increase was mainly achieved by one of the group leaders of Research Section III, being granted DFG funding and a Leibniz Women Professorship at the end of 2021. The process of jointly appointing the candidate as a W3 Associate Professor at the TUM was started in January 2022, accompanied by two external offers for a permanent W3 professorship from the University of Oslo, which the candidate rejected.

In the last TUM management board meeting on March 15th 2022, the board members agreed on a fast-track procedure ("Leuchtturmverfahren", Bayerisches Hochschulperson-

algesetz/BayHSchPG [Bavarian University Staff Act] Art. 18.3[1]) to appoint the candidate following the Jülich Model[2].

In order to further consolidate the Food Systems Biology approach by reaching an understanding of molecular networks and processes that drive food(processing)-related human biology and health, and help consumers making a healthy food choice based on sensory preferences, the members of the evaluation committee recommend *"focusing on foods that are of high importance for global basic nutrition or for a healthy diet",* and to *"flesh out the concept of 'food systems biology'".*

By its statutes, the **LSB considers the quality of all foods,** and focuses its research on foods that constitute a dominant portion of a standard diet or respective food ingredients, such as plant proteins. The overall research portfolio might not have been comprehensively demonstrated during the visit of the evaluation committee, which had to be shortened from a 2-day onsite visit to a 1.5-hour virtual presentation because of the replacement procedure for evaluations in response to the Corona pandemic.

The national statistics published in early 2022 by Statista[3] demonstrate that the LSB focuses its research on the 20 most consumed food / food groups, e.g. coffee, cocoa or dairy products, and their constituents. Moreover, our recently launched, curated Food Systems Biology Database (FSBI DB[4]) includes research-based information on flavor-active molecules, their occurrence in almost all foods and their associated chemosensory receptors. To further focus on relevant food items, the LSB has initiated a collaboration with the Bavarian State Ministry of Food, Agriculture and Forestry (StMELF). This collaboration will enable the integration of Bavarian food consumption data[5] into the LSB's FSBI DB in order to evaluate the significance of flavor-active compounds for habitual dietary intakes.

In addition to this increase in personnel resources based on competitive third-party funds, the LSB fully **agrees with the members of the evaluation committee** that another important milestone for the LSB's future development is that *"world-class section heads can be found for Research Section I and III without delay".*

Attracting internationally leading scientists as Chairs for Research Section I and III will require financial resources that enable the permanent funding of these positions. For this funding, the LSB plans to apply for a minor extraordinary item of expenditure (STB B) at the Federal Joint Science Conference (GWK[6]) early 2023. Once this funding is approved, a permanent funding for these positions can be granted in 2025.

Apart from financial considerations, an attractive academic environment is one of the key factors to attract international leaders in their fields. The LSB considers its own academic leadership and the excellent academic reputation of the TUM as highly attractive and has

[1] https://www.gesetze-bayern.de/Content/Document/BayHSchPG-18
[2] https://www.leibniz-gemeinschaft.de/fileadmin/user_upload/Bilder_und_Downloads/%C3%9Cber_uns/Organisation/Dokumente/Guide_Joint_Appointments.pdf
[3] https://de.statista.com/prognosen/999889/deutschland-regelmaessig-konsumierte-lebensmittel
[4] https://fsbi-db.de/
[5] https://www.stmelf.bayern.de/ernaehrung/253378/index.php
[6] https://www.gwk-bonn.de/en/

already started negotiations with the president of the TUM to jointly appoint Chairs of Research Section I and III as W2 tenure track with fast track option (4-year period) to a W3 professorship at the TUM, according to the Jülich Model.

Specifically, the tender text for the Chair of Research Section III professorship position has already been discussed internally at the LSB, approved by the members of the Scientific Advisory Board this February, and forwarded to the TUM management board for further consideration this March. The position for the Chair of Research Section I will be generated, advertised and filled jointly between LSB and TUM, following the academic appeals process of the TUM.

In this respect, the evaluation committee states that, *"...the Supervisory Board and, in particular, the responsible specialist departments of the host Land and federal government need to significantly improve and expand the structural conditions needed for the scientific development of the LSB."*

In 2017, the Bavarian Ministry for Economic Affairs, Regional Development and Energy (StMWi) provided a stimulus package of 16.7 Mio Euros for initially 3 years. These funds have been extended until the end of 2024, with an additional amount of 10.5 Mio Euros (approved by the Bavarian State Parliament on April 6th 2022). In addition, the StMWi allocated a total amount of 12.35 Mio € for a new building to accommodate the LSB's expanded space requirements.

The LSB fully agrees with the perspective of the evaluation committee that additional funding is needed, and has been striving for adequate funds over the past 5 years. This effort was and still is extensively supported by its funding bodies.

In conclusion, the LSB's steering board will make all necessary efforts to realize all recommendations of the evaluation committee, especially with regard to further development of Food Systems Biology, diversification of third-party funding and publication strategy, and intensification of the collaboration with the TUM.