

Arbeitsbericht NAB 21-22

**TBO Bözberg-2-1:
Data Report**

**Dossier IV
Microfacies, Bio- and Chemo-
stratigraphic Analysis**

April 2022

**National Cooperative
for the Disposal of
Radioactive Waste**

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TB0 Bözberg-2-1: Data Report

Dossier IV Microfacies, Bio- and Chemo- stratigraphic Analysis

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stable carbon isotopes

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Nagra Arbeitsberichte ("Working Reports") present the results of work in progress that have not necessarily been subject to a comprehensive review. They are intended to provide rapid dissemination of current information.

This NAB aims at reporting drilling results at an early stage. Additional borehole-specific data will be published elsewhere.

In the event of inconsistencies between dossiers of this NAB, the dossier addressing the specific topic takes priority. In the event of discrepancies between Nagra reports, the chronologically later report is generally considered to be correct. Data sets and interpretations laid out in this NAB may be revised in subsequent reports. The reasoning leading to these revisions will be detailed there.

This Dossier was prepared by a project team consisting of:

S. Wohlwend (sampling, chemostratigraphy, conceptualisation and compilation)

H.R. Bläsi (microfacies)

S. Feist-Burkhardt (palynostratigraphy)

B. Hostettler, U. Menkveld-Gfeller, V. Dietze (ammonite stratigraphy)

G. Deplazes (project management and conceptualisation)

Editorial work: P. Blaser and M. Unger

The Dossier has greatly benefitted from technical discussions with, and reviews by, external and internal experts. Their input and work are very much appreciated.

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1 Introduction

1.1 Context

To provide input for site selection and the safety case for deep geological repositories for radioactive waste, Nagra has drilled a series of deep boreholes ("Tiefbohrungen", TBO) in Northern Switzerland. The aim of the drilling campaign is to characterise the deep underground of the three remaining siting regions located at the edge of the Northern Alpine Molasse Basin (Fig. 1-1).

In this report, we present the results from the Bözberg-2-1 borehole.

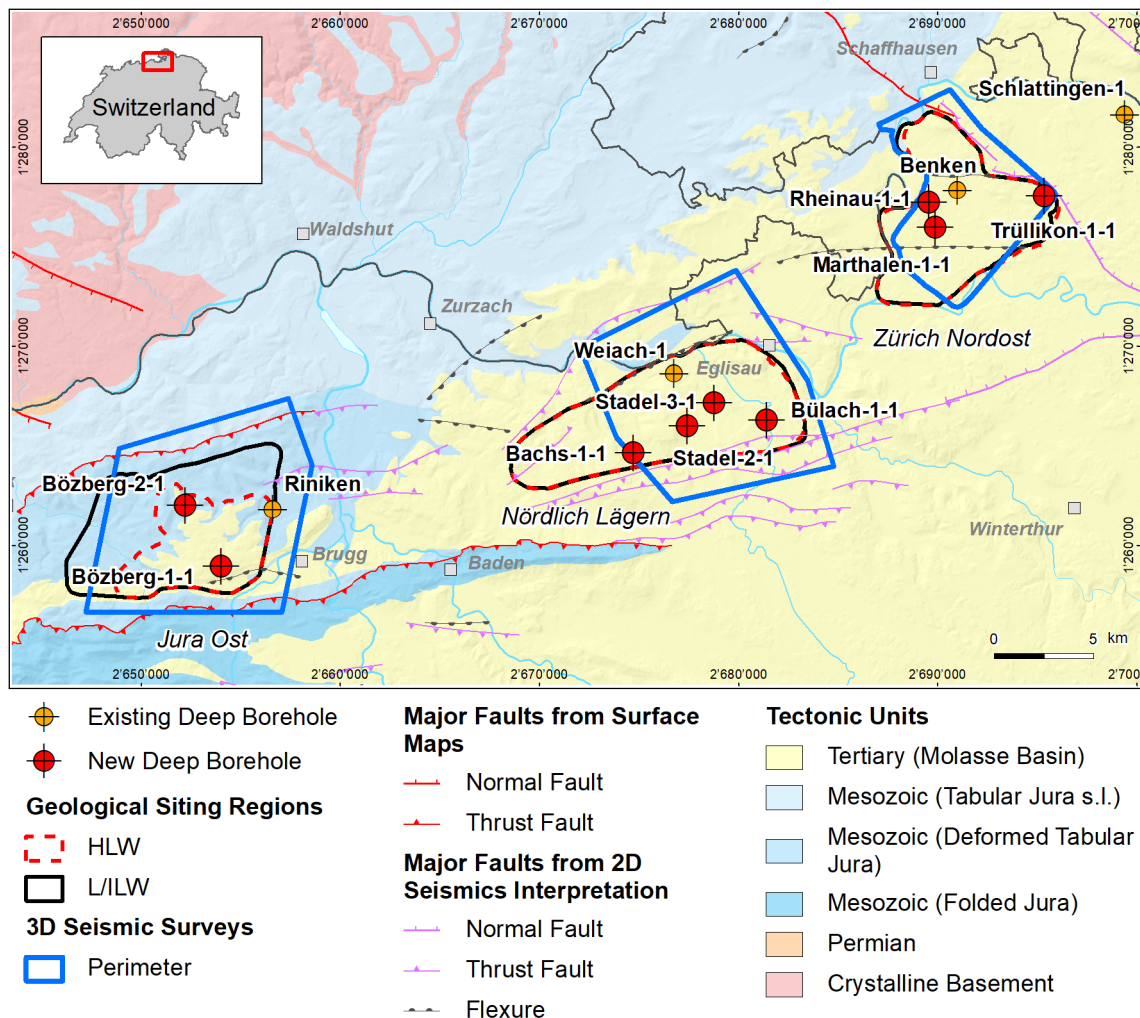


Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Bözberg-2-1 (BOZ2-1) exploratory borehole is the fifth borehole drilled within the framework of the TBO project. The drill site is located in the northern part of the Jura Ost siting region (Fig. 1-2). The vertical borehole reached a final depth of 829.11 m (MD)¹. The borehole specifications are provided in Tab. 1-1.

Tab. 1-1: General information about the BOZ2-1 borehole

Siting region	Jura Ost
Municipality	Bözberg (Canton Aargau / AG), Switzerland
Drill site	Bözberg-2 (BOZ2)
Borehole	Bözberg-2-1 (BOZ2-1)
Coordinates	LV95: 2'652'218.764 / 1'261'985.437
Elevation	Ground level = top of rig cellar: 624.33 m above sea level (asl)
Borehole depth	829.11 m measured depth (MD) below ground level (bgl)
Drilling period	11th August – 14th December 2020 (spud date to end of rig release)
Drilling company	Daldrup & Söhne AG
Drilling rig	Wirth B 152t
Drilling fluid	Water-based mud with various amounts of different components such as ² : 0 – 370 m: Bentonite & polymers 370 – 615 m: Potassium silicate & polymers 615 – 829.11 m: Pure-Bore®

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The main lithostratigraphic boundaries in the BOZ2-1 borehole are shown in Fig. 1-4.

¹ Measured depth (MD) refers to the position along the borehole trajectory, starting at ground level, which for this borehole is the top of the rig cellar. For a perfectly vertical borehole, MD below ground level (bgl) and true vertical depth (TVD) are the same. In all Dossiers depth refers to MD unless stated otherwise.

² For detailed information see Dossier I.

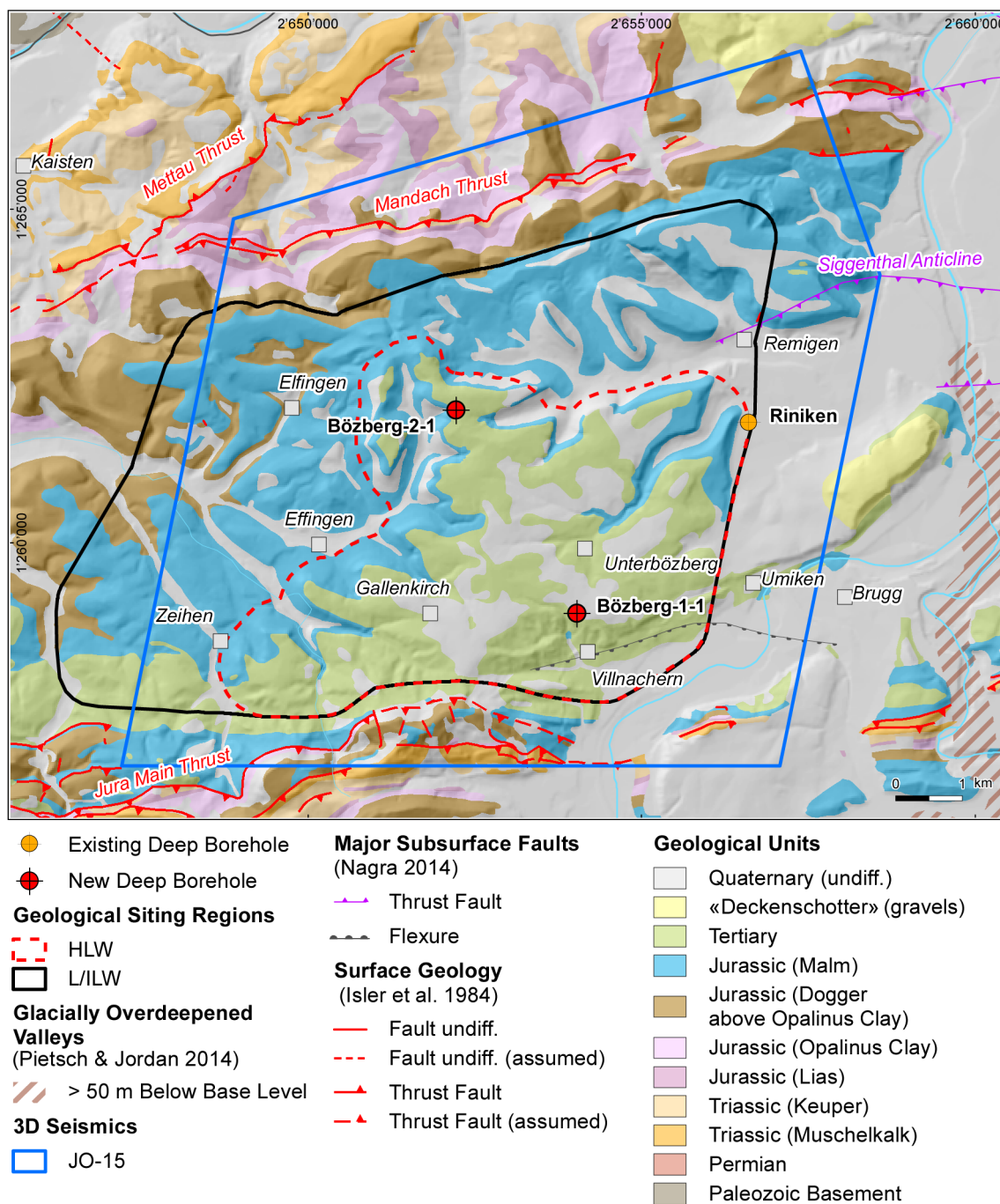


Fig. 1-2: Overview map of the investigation area in the Jura Ost siting region with the location of the BOZ2-1 borehole in relation to the boreholes Riniken and BOZ1-1

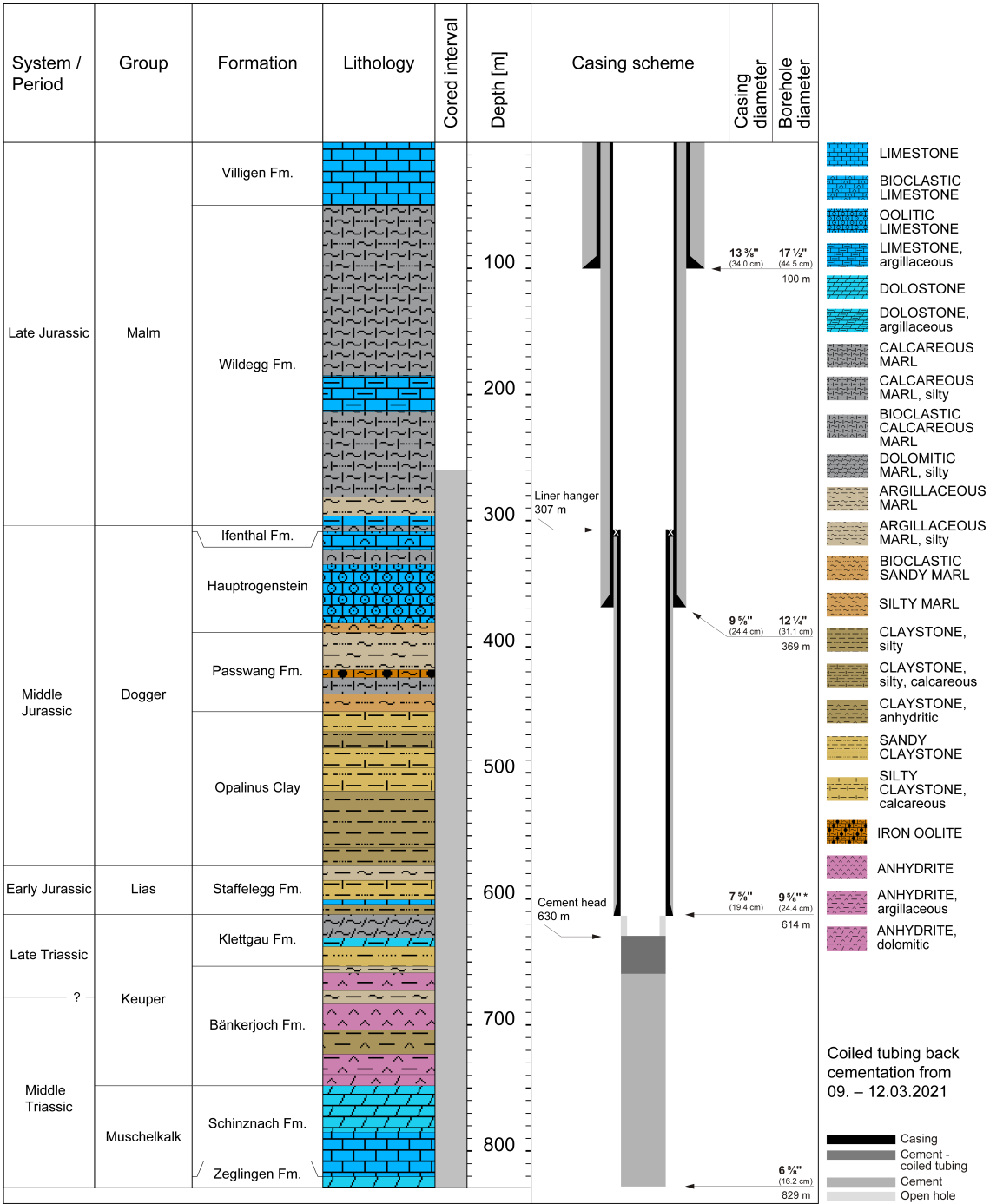


Fig. 1-3: Lithostratigraphic profile and casing scheme for the BOZ2-1 borehole³

³ For detailed information see Dossier I and III.

1.3 Documentation structure for the BOZ2-1 borehole

NAB 21-22 documents the majority of the investigations carried out in the BOZ2-1 borehole, including laboratory investigations on core material. The NAB comprises a series of stand-alone dossiers addressing individual topics and a final dossier with a summary composite plot (Tab. 1-3).

This documentation aims at early publication of the data collected in the BOZ2-1 borehole. It includes most of the data available approximately one year after completion of the borehole. Some analyses are still ongoing (e.g. diffusion experiments, analysis of veins, hydrochemical interpretation of water samples) and results will be published in separate reports.

The current borehole report will provide an important basis for the integration of datasets from different boreholes. The integration and interpretation of the results in the wider geological context will be documented later in separate geoscientific reports.

Tab. 1-3: List of dossiers included in NAB 21-22

Black indicates the dossier at hand.

Dossier	Title	Authors
I	TBO Bözberg-2-1: Drilling	P. Hinterholzer-Reisegger
II	TBO Bözberg-2-1: Core Photography	D. Kaehr & M. Gysi
III	TBO Bözberg-2-1: Lithostratigraphy	P. Jordan, P. Schürch, H. Naef, M. Schwarz, R. Felber, T. Ibele & M. Gysi
IV	TBO Bözberg-2-1: Microfacies, Bio- and Chemostratigraphic Analyses	S. Wohlwend, H.R. Bläsi, S. Feist-Burkhardt, B. Hostettler, U. Menkveld-Gfeller, V. Dietze & G. Deplazes
V	TBO Bözberg-2-1: Structural Geology	A. Ebert, L. Gregorczyk, S. Cioldi, E. Hägerstedt & M. Gysi
VI	TBO Bözberg-2-1: Wireline Logging, Micro-hydraulic Fracturing and Pressure-meter Testing	J. Gonus, E. Bailey, J. Desroches & R. Garrard
VII	TBO Bözberg-2-1: Hydraulic Packer Testing	R. Schwarz, M. Willmann, S. Reinhardt, S.M.L. Hardie, M. Voß & A. Pechstein
VIII	TBO Bözberg-2-1: Rock Properties, Porewater Characterisation and Natural Tracer Profiles	T. Gimmi, L. Aschwanden, L. Camesi, E. Gaucher, A. Jenni, M. Kiczka, U. Mäder, M. Mazurek, D. Rufer, H.N. Waber, P. Wersin, C. Zwahlen & D. Traber
IX	TBO Bözberg-2-1: Rock-mechanical and Geomechanical Laboratory Testing	E. Crisci, L. Laloui & S. Giger
X	TBO Bözberg-2-1: Petrophysical Log Analysis	S. Marnat & J.K. Becker
	TBO Bözberg-2-1: Summary Plot	Nagra

1.4 Scope and objectives of this dossier

The dossier at hand complements the lithostratigraphic report (Dossier III) on the BOZ2-1 borehole. The report documents data on microfacies analysis, ammonite- and palynostratigraphy as well as detailed geochemical (C, O and N isotopes) analyses. Preliminary results of these analyses already existed at data-freeze (02.03.2021), two months after the end of drilling operations and were integrated into the lithostratigraphic discussion and lithostratigraphic boundary definition (Dossier III).

The objectives of this report focusing on the Opalinus Clay and its confining units are:

- to specify the macroscopic description by a detailed microfacies analysis (components, matrix, cements),
- to allow a microfacies comparison of specific horizons, for example hardgrounds of the upper Opalinus Clay,
- to provide additional data on the diagenetic history of the sediment,
- to recover macrofossils from the stratigraphic interval of interest which are significant for facies changes and chronostratigraphic data,
- to compile an additional independent dataset of palynomorphs for chronostratigraphic data,
- to provide detailed geochemical (C, O and N isotopes) analyses with one metre spacing from the stratigraphic interval of interest,
- to allow a chemostratigraphic correlation (stable isotopes) with other deep boreholes in the three siting regions,
- to support the definition of the lithostratigraphic units.

The detailed stratigraphy of the BOZ2-1 borehole with core depth in metres can be found in Fig. 1-4. The stratigraphic intervals of interest for the different investigations (microfacies analysis, ammonite- and palynostratigraphy and geochemical analyses) and their specific sampling intervals are visualised in Fig. 1-5 with respect to the 1:5'000 lithostratigraphic profile.

All depths labelled with metres [m] in this report refer to "m MD core depth" if not stated otherwise.

TBO BÖZBERG-2-1				
System / Period	Group	Formation	Metres MD	Member / Sub-unit
Jurassic	Late	Malm	Villigen Fm.	
			50	
	Middle	Dogger	Wildeggen Fm.	Effingen Mb.
			300.25	Birmenstorf Mb.
			303.95	
			Ifenthal Fm.	
			308.70	«Movelier Beds» and «Spatkalk»
			Hauptrogenstein	
			334.83	
			388.54	Rothenfluh Mb.
			418.30	«Humphriesi-Schichten»
			424.40	Waldenburg and lower part of Bruggli Mb.
			450.53	«Cond. equivalents of the Sissach, Hauenstein and/or Hirnichopf Mb.»
			451.54	«Sub-unit with silty calcareous beds»
			480.56	«Upper silty sub-unit»
Triassic	Early	Lias	496.09	«Mixed clay-silt-carbonate sub-unit»
			559.75	«Clay-rich sub-unit»
			573.68	Gross Wolf Mb.
			576.57	Rietheim Mb.
			581.93	Grünschoholz Mb., Breitenmatt Mb. and Rickenbach Mb.
			585.24	Frick Mb.
			600.77	Beggingen Mb.
			604.27	Schambelen Mb.
			612.46	Gruhalde Mb.
			630.96	Gansingen Mb.
	Late	Keuper	637.82	Ergolz Mb.
			653.45	«Claystone with anhydrite nodules»
			683.23	«Cyclic sequence»
			704.07	«Thin-layered anhydrite and claystone sequence»
	Middle	Muschelkalk	739.32	«Banded massive anhydrite»
			748.27	Asp Mb.
			752.64	Stamberg Mb.
			785.00	Liedertswil Mb.
			793.79	Leutschenberg Mb. and Kienberg Mb.
			820.32	«Dolomitzone»
			Zeglingen Fm.	Final depth
			829.11	

Fig. 1-4: Bözberg-2-1 stratigraphy with core depth in metres [m MD]

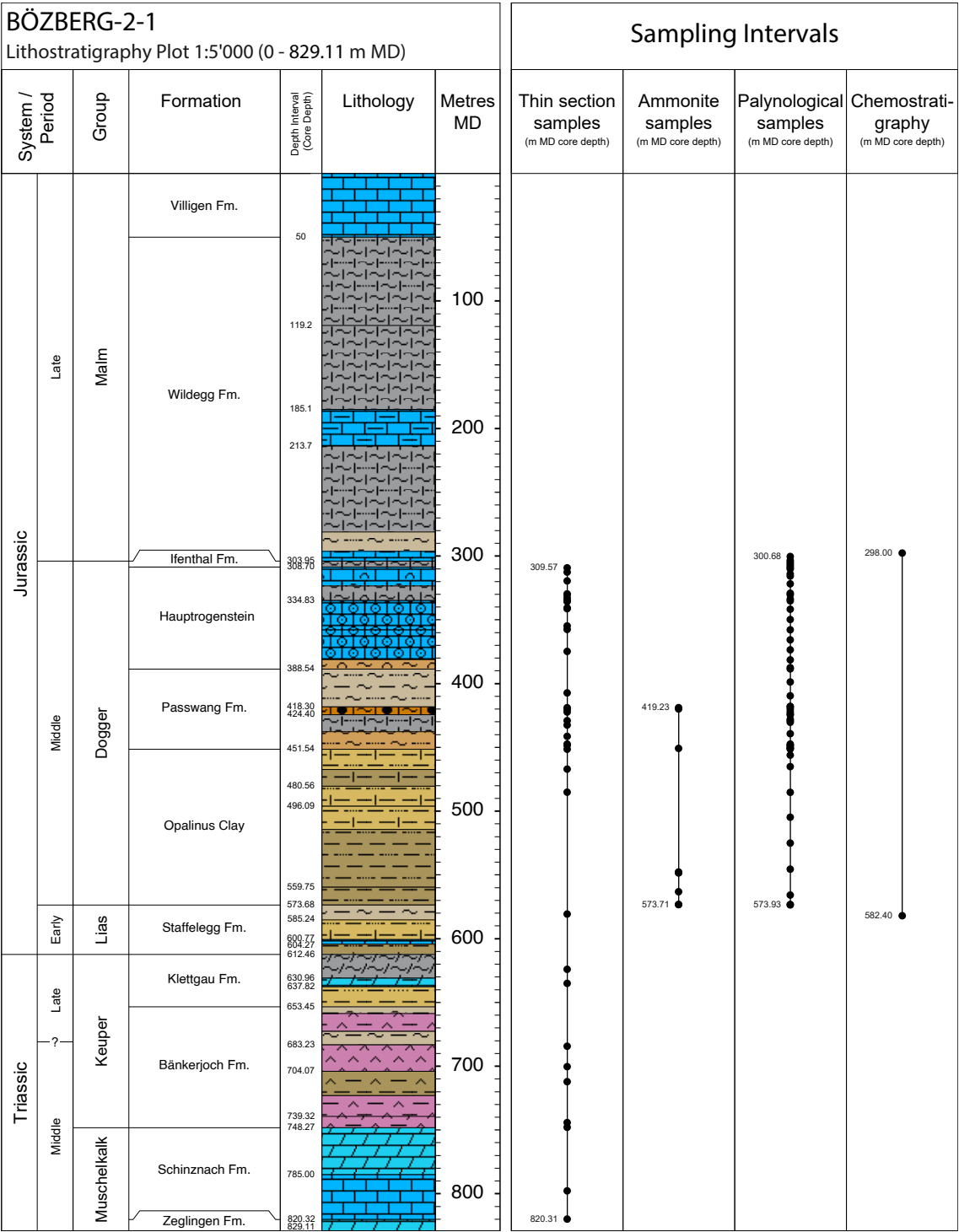


Fig. 1-5: Lithostratigraphy plot (1:5'000) from the Mesozoic succession with the individual sampling intervals for thin sections, macrofossils, palynological analysis and chemostratigraphy

1:5'000 stratigraphic plot modified from Dossier III.

2 Methods

2.1 Microfacies

Thin section preparation

All thin sections (TS) were cut edgewise from the core so that the long side is parallel to the coring direction and therefore covers as much of the stratigraphy as possible. The mean depth of the thin section corresponds to the Sample ID. Therefore, thin sections containing lithological boundaries may have Sample IDs that fall into only one of the two described intervals. However, the lower or upper range on the thin section still covers the interval. A list of all thin sections with their sampling range and Sample ID can be found in Appendix A1 of this report.

The thin sections from calcareous lithologies with a standard length of 4 cm were prepared at the University of Basel. Lithologies sensitive to water such as claystones and argillaceous sediments (swelling of clay minerals) or evaporates (dissolution of evaporitic minerals) were prepared by the Thin Section Lab (TSL) using petroleum, they are only 3 cm long. For better identification of the carbonate minerals calcite, Fe-calcite and Fe-dolomite, the left half of the thin sections was stained applying the technique of Dickson (1965). Thin sections with a macroscopic porosity were impregnated during preparation using a blue coloured epoxy resin to estimate the percentage of their porosity.

Thin section analyses

35 thin sections were analysed using a Zeiss polarisation microscope. First, all allochemical components, biogenic particles, siliciclastics, matrix and diagenetic alterations as neomorphic minerals, cements and replacements were studied. Then, to obtain the percentage of the components etc., 100 points were counted with a net micrometre ocular. For detrital quartz-bearing thin sections, the average grain size was evaluated in millimetres. To count inhomogeneous sediments, two different sections were looked at and averaged. A selection of 18 thin section photographs for microfacies analysis is documented in Appendix B (Figs. B-1 to B-18).

Components, matrix and cements (definitions)

To describe thin sections, several allochemical components (described below) were counted, and their numbers are documented in Section 3.1 ('Microfacies'). Some of the specific terms used for the components or matrix are explained as follows:

Clay matrix, micrite, microsparite (or pseudosparite): Sedimented mud consisting of clay minerals, other very small silicate grains, heavy minerals (i.e. clay matrix) and/or microcrystalline carbonate ooze (i.e. micrite). Microsparite is defined as a mosaic of small calcite crystals formed by aggrading neomorphism; originally, it was micrite and not a diagenetic pore-filling cement. Alternatively, microsparite could also be the product of dedolomitisation as seen in the «Felsenkalke» and «Massenkalk».

Dolomitic matrix: primary microcrystalline dolostone ooze.

Limonitic matrix: Calcite micrite mixed with microcrystalline limonitic grains grown during diagenesis.

Limonitic echinoderms, limonitic bivalves: Fragments, parts of echinoderms and bivalves, with limonite filling the skeletal structure of the fossil.

Pellets, peloids, aggregates: the column of pellets contains now aggregates (lumps) too; that means "carbonate grains of various kinds are clumped together to form compound grains" (Bathurst 1975) (see BOZ2-1-334.98, Fig. B-16, Appendix B)

Fe-stromatolites and stromatolitic clasts: Iron-mineralised microbial mats and/or microbial clasts.

Fe-ooids or iron-ooids: Limonitic/goethitic or chamositic ooids, with a visible concentric structure; some iron-ooids are replaced by calcite (calcitic iron-ooids), a few of them show relicts of iron mineral layers (see BOZ2-1-467.43, Fig. B-8, Appendix B).

Intraclasts: Rock fragments of early diagenetic cemented sediment, reworked and sedimented in the same sedimentary environment.

Calcite cement (sparite): "Normal" cement, calcite crystals grown – filled in – within the primary pore space or in leached components. In this column, the amount of calcite crystal pseudomorphs after gypsum was noted.

"Stellate cement": Calcite "cement" grown within the matrix and not filling primary or secondary pore space. The calcite crystals form small "stellates", i.e. a habitus typical for "hiatus beds" (firm-, hardgrounds; Wetzel & Allia 2000) or "hiatus concretions" (Voigt 1968).

Cone-in-cone calcite: Rows of piled calcite cones grown during diagenesis which were named "Tutenmergel" in the Swabian realm.

(Fe)-Dolomite: Normally dolomite rhombohedrons that originated during diagenesis; in special cases, the dolomite replaces gypsum crystals that were sedimented as detrital gypsum crystals. In some cases, the rhombohedrons consist of iron-dolomite, which are stained blue after the thin section staining.

Dedolomite: Calcite replacement of dolomite: each single dolomite rhombohedron is replaced by a few smaller calcite crystals. When it was a total dolostone and the calcitic replacement has been completed, the result is a thoroughly crystalline, sparitic/microsparitic limestone. In addition, another dedolomite type exists with larger calcite crystals jointly replacing a few dolomite crystals, thus forming a calcite mosaic similar to marble.

Anhydrite: Present in various forms: as a rock-forming mineral, as a vein mineral, mainly replacing "Fasergips", and as cement in sandstones (e.g. Ergolz Member of the Klettgau Formation).

Quartz cement: Authigenic quartz rims grown during diagenesis around detrital quartz grains; quartz/chalcedony in silicified bivalves (MAR1-1-569.18; Wohlwend et al. 2021c).

Porosity: Thin sections with a macroscopic porosity were impregnated during preparation using a blue coloured epoxy resin to estimate the volume percentage (vol.-%) of their porosity.

Hardground: Thin sections from hardgrounds document synsedimentarily cemented and lithified carbonate layers which have been exposed on the seafloor. During that time period, the hardgrounds are therefore mostly encrusted and bored by organisms and may consist of early marine calcite cements and are in parts mineralised by iron and manganese oxides or calcium phosphates.

2.2 Ammonite preparation

The BOZ2-1 cores were carefully examined for macrofossils at the Würenlingen (Canton Aargau) core storage facility. The cores were examined for ammonites and other macrofossils on the bedding and fractured surfaces as well as on the outer surface of the core; the core itself was not broken open. A list of all samples with their sampling range and Sample ID can be found in Appendix A2 of this report. In addition to ammonites, other conspicuous fossils were identified to the extent possible and entered in the list (Appendix A3), even when they were not subsequently, or only occasionally, recovered. The ammonites were then secured from the core and brought to the Natural History Museum in Bern, where they were prepared, documented, and afterwards archived in the earth sciences collection.

For the preparation, we used mechanical methods such as air tools and fine sandblasting equipment as well as a chemical etching method using potassium hydroxide (KOH). Sodium hydrogen carbonate was mainly used as abrasive. Residual material from sawing and preparing three ammonite samples (marked in grey in Appendix A4) was used as material for palynological samples. Before being photographed, we applied ammonium chloride steam to the fossils to compensate for variation in contrast caused by different colouring. A selection of ammonites is documented on two plates (Plate I – II) in Appendix C.

The names of several ammonite taxa are followed by a question mark, for example in *Pleydellia?* sp. The question mark after the genus name was used to indicate a question regarding the correct taxonomical assignment of the species to the genus.

2.3 Palynological sample preparation and quantitative analysis

Palynological processing of the rock samples was carried out by PLS Palynological Laboratory Services Ltd. (Holyhead, Anglesey, UK). Processing follows the standard protocol (Wood et al. 1996) using concentrated HCl and concentrated HF, followed by a short oxidation with HNO₃ and, if necessary, treatment with ultrasound. The residues are sieved at a mesh size of 15 µm. Residues are mounted on microscope slides and analysed using transmitted light microscopy. A list of all samples with their sampling range and Sample ID can be found in Appendix A4 of this report.

Two consecutive counts were carried out in the quantitative microscopic analysis. In a first count 200 grains of all palynomorphs were counted and the number of dinoflagellate cysts is noted (column 'DA *Dinocysts (count 1)*' in Appendix D1). In a second count, only dinoflagellate cysts are counted until a total of 100 dinoflagellate cysts is reached. The remainder of the slide is checked for additional, out-of-count species. Taxa recorded out of count are marked with a '+' in the range chart. Taxa only questionably identified are marked with a '?' in the range chart. Occurrences of fungal remains are recorded semi-quantitatively (R = Rare, O = Occasional, C = Common, A = Abundant, S = Superabundant).

Results are illustrated using the software package StrataBugs v2.1 (Appendices D1 and D2). Numerical age dates used for the Composite Standard and the Depth/Age plot are in line with those of the *Geologic Time Scale 2016* (Ogg et al. 2016). On the range chart Appendix D1 several abbreviations are used (AC = Acritarchs, ALBO = Algae, *Botryococcus* and *Pediastrum*, ALPR = Algae, Prasinophytes, ALZY = Algae, Zygnematophyceae, DA = Dinocyst abundance, DC = Dinoflagellate cysts, FT = Foraminiferal test linings, FU = Fungi, MP = Miscellaneous palynomorphs, SP = Spores and pollen. Several dinoflagellate cyst taxa contain a question mark in the name, as for example in *Evansia? eschachensis*. The question mark after the genus name indicates uncertainty regarding the correct taxonomical assignment of the species to the genus.

2.4 Chemostratigraphy

The sampling of the BOZ1-1 borehole focused primarily on the Dogger and Lias Groups and therefore primarily on clay mineral-rich layers of the Opalinus Clay. The sampling resolution was one metre, except for some intervals with denser sampling density (mainly hardgrounds, condensed intervals and the Rietheim Member of the Staffelegg Formation). All 323 samples were drilled with a micro-drill. In general, clay mineral-rich lithologies were sampled. Diagenetic calcite and siderite veins and nodules were avoided. The drilled powder amounted to around 1 g of material. A list of specific samples ($n = 15$) with results from calcareous beds, calcareous concretions, and macrofossils (e.g. belemnites) can be found in Appendix E1 of this report.

Inorganic (carbonate) analyses

The 323 samples were analysed for **stable carbon** ($\delta^{13}\text{C}_{\text{carb}}$) and **oxygen isotope** ($\delta^{18}\text{O}_{\text{carb}}$) of bulk carbonate, 308 continuous samples (roughly in metre resolution) and additional 15 samples mainly from specific calcareous beds and concretions in the Opalinus Clay (Appendix E1). Varying amounts of powder to reach approximately 120 μg of carbonate in the vial were weighed using a Mettler Toledo MT5 Fact microbalance in 12 ml vacutainers. The headspace was flushed with pure He, and then the samples were reacted with 100 % phosphoric acid at 72 °C in a ThermoFisher GasBench II carbonate device connected to a ThermoFisher Delta V PLUS mass spectrometer. The instrument is calibrated with international carbonate standards NBS19 and NBS18 distributed by the International Atomic Energy Agency (IAEA), Vienna and internal standards (MS2 "Carrara marble"; $\delta^{13}\text{C}_{\text{carb}} = 2.16 \text{ ‰}$, $\delta^{18}\text{O}_{\text{carb}} = -1.85 \text{ ‰}$). The reproducibility of the measurements based on replicated standards was $\pm 0.05 \text{ ‰}$ for $\delta^{13}\text{C}_{\text{carb}}$ and $\pm 0.06 \text{ ‰}$ for $\delta^{18}\text{O}_{\text{carb}}$. All isotope measurements were performed at the Stable Isotope Laboratory of the ETH Zurich (Geological Institute). The isotope values are reported in the conventional delta notation with respect to the Vienna Pee Dee Belemnite (VPDB).

The **Total Carbonate content** (TCarb) was calculated based on a calibration using extracted CO_2 from the known weight of the internal standard material (MS2), which is composed to 100% of carbonate (calcite). The mean area of the m/z 44 peak (corresponding to the most abundant isotopologue $^{12}\text{C}^{16}\text{O}_2$) in the mass spectrometer allows the carbonate content to be estimated from the individual bulk rock samples. The individual uncertainty for TCarb, represents the average from all standard deviations from the MS2 and is $\pm 5.14 \text{ ‰}$. However, the TCarb values calculated from the reaction of the phosphoric acid with the bulk rock, only reflect the carbonate that was able to react during the reaction time ($\sim 60 \text{ min}$). However, ankerite and especially siderite, for example, roughly require 60 h reaction time for full dissolution at 70 °C (Fernandez et al. 2016). Therefore, the calculated carbonate content (TCarb) does not completely represent the total amount of all different carbonates. The data reflect a mixed signal composed mostly of calcite and dolomite with a smaller component of the other more resistant carbonates (see also Wohlwend et al. 2019a).

Organic analyses

The powders remaining after inorganic analysis from 216 samples were decarbonated in quantities of less than 1 g in 10 ml of 3 M HCl for 12 h in 15 ml centrifuge tubes, to ensure the complete removal of carbonate. For neutralisation purposes, the residue was subsequently washed three times with deionised water, and then centrifuged and decanted. After drying at 70 °C in an oven for at least 72 h the samples were homogenised with a mortar and pestle. Depending on the organic carbon content of each specific sample, a different amount was weighed in a tin capsule using a Mettler Toledo MT5 Fact microbalance, so that approximately the same amount of organic carbon was always measured.

$\delta^{13}\text{C}_{\text{org}}$ and $\delta^{15}\text{N}_{\text{org}}$ were measured by flash combustion on a ThermoFisher Scientific FlashEA elemental analyser connected to a Delta V isotope ratio mass spectrometer (IRMS) operated in continuous flow mode. The samples were combusted in an O_2 atmosphere in a quartz reactor at 1'020 °C packed with $(\text{Co}_3\text{O}_4)\text{Ag}$ and Cr_2O_3 to form CO_2 , N_2 , NO_x and H_2O . These gases were then transferred through a reduction reactor containing elemental Cu at 600 °C to remove excess O_2 and to reduce NO_x to N_2 . H_2O and SO_x were subsequently removed using anhydrous $\text{Mg}(\text{ClO}_4)_2$ and elemental Ag. Then, N_2 and CO_2 were separated in a packed gas chromatographic column and analysed for their isotopic composition using the IRMS. Isotope ratios are reported in conventional delta notation with respect to atmospheric N_2 (AIR) and VPDB standards, respectively. The methods were calibrated with the International Atomic Energy Agency (IAEA)-N1 ($\delta^{15}\text{N} = 0.45 \text{ ‰}$), IAEA-N2 ($\delta^{15}\text{N} = +20.41 \text{ ‰}$) and IAEA-N3 ($\delta^{15}\text{N} = +4.72 \text{ ‰}$) reference materials for nitrogen, and NBS22 ($\delta^{13}\text{C} = -30.03 \text{ ‰}$) and IAEA-CH-6 ($\delta^{13}\text{C} = -10.46 \text{ ‰}$) for carbon. Reproducibility of the measurements is better than $\pm 0.2 \text{ ‰}$ for both nitrogen and carbon. Reproducibility and accuracy of the measurements are based on replicate analyses of the internal laboratory standards atropine, peptone and nicotinamide. All geochemical measurements were performed at the Stable Isotope Laboratory of the ETH Zurich (Geological Institute).

The **Total Organic Carbon** ($\text{TOC}_{\text{decarb}}$) and **Total Nitrogen** ($\text{TN}_{\text{decarb}}$) contents of the decarbonised samples were calculated based on the known carbon and nitrogen contents of atropine (70.56 wt.-% C, 4.84 wt.-% N). The individual uncertainty for $\text{TOC}_{\text{decarb}}$ represents the average from all standard deviations from atropine during that calculation and is $\pm 0.48 \text{ ‰}$, respectively $\pm 0.05 \text{ ‰}$ for the $\text{TN}_{\text{decarb}}$. The calculated $\text{TN}_{\text{decarb}}$ reflects a mixture of bound inorganic and organic nitrogen and therefore also contains ammonium, which substitutes for K^+ in the interlayer exchange sites of illite (Scheffer & Schachtschnabel 1984).

The **Carbon-to-Nitrogen ratio** (C/N ratio) is a ratio of the mass of carbon to the mass of nitrogen. In this study, the ratio was calculated using the $\text{TOC}_{\text{decarb}}$ and the $\text{TN}_{\text{decarb}}$. As mentioned above, the C/N ratios can also be influenced by inorganic nitrogen in the form of soil-derived ammonium (Scheffer & Schachtschnabel 1984). Due to this inorganic nitrogen, the C/N ratios of sediments containing additional inorganic nitrogen will decrease. Therefore, C/N ratios are referred to as organic carbon/total nitrogen ($\text{TOC}_{\text{decarb}}/\text{TN}_{\text{decarb}}$) giving the ratio of the C and N masses of the decarbonised samples ($\text{C}_{\text{org}}/\text{N}_{\text{org}}$). The calculated ratios allow to distinguish between marine ($\text{C/N} \leq 10$; Parsons 1975) *versus* terrigenous matter ($\text{C/N} \geq 12$; Kukal 1971) in marine sediments.

$$\frac{\text{C}_{\text{org}}}{\text{N}_{\text{org}}} = \frac{\text{TOC}_{\text{decarb}}}{\text{TN}_{\text{decarb}}} * \frac{\text{atomic mass (C)}}{\text{atomic mass (N)}} = \frac{\text{TOC}_{\text{decarb}}}{\text{TN}_{\text{decarb}}} * \frac{14.007}{12.011}$$

The **Total Organic Carbon** (TOC) of the whole/bulk sample was calculated using the semi-quantitative carbonate content (TCarb) and semi-quantitative $\text{TOC}_{\text{decarb}}$ content based on the following equation:

$$\text{TOC} = (1 - \text{TCarb}) * \text{TOC}_{\text{decarb}}$$

3 Results

3.1 Microfacies

Schinznach Formation (BOZ2-1-820.31, 798.17, 748.33)

The lowermost thin section of BOZ2-1 (BOZ2-1-820.31) comes from the basal bed of the Schinznach Formation. It is a pelletoidal limestone with small (0.05 – 0.1 mm) micritic components (35 vol.-% pellets; Tab. 3-1 for all vol.-% data in this section). Some of them have a small micritic rim and a microsparitic centre. These could eventually be ooids. Together with few biogene components (5 vol.-% echinoderms + bivalves) and codiacean algae (5 vol.-%), they are embedded in micrite matrix (25 vol.-%), calcite cement (15 vol.-%) and dolomite rhombohedrons (15 vol.-%).

BOZ2-1-798.17 is a bioclastic limestone or a bivalves-biopelsparite (Fig. B-1; Appendix B for all figures in this section), consisting of closely packed bivalves (37 vol.-%), echinoderms (10 vol.-%), other biogenes (2 vol.-%) and pellets (7 vol.-%) with micrite matrix (18 vol.-%), calcite cement (14 vol.-%) and dolomite (12 vol.-%). The last one can be found in burrows mainly.

The bed of BOZ2-1-748.33 looks, in a macroscopic view, like a grainy dolostone. But it is a dolomicrite (67 vol.-%) with swimming single anhydrite crystals (33 vol.-%) (Fig. B-2).

Bänkerjoch Formation (BOZ2-1-744.62, 712.56, 700.76, 684.75)

The four samples of the Bänkerjoch Formation, BOZ2-1-744.62, 712.56, 700.76 and 684.75 are all anhydrite rocks with different parts of anhydrite, dolomite and clay minerals and different habitus of the anhydrite minerals. BOZ2-1-744.62 is a blocky anhydrite (64 vol.-%) with small dolomite crystals (28 vol.-%) arranged in thin strings across the anhydrite, and clayey matrix (8 vol.-%).

Thin section BOZ2-1-712.56 shows a claystone (42 vol.-% clay matrix) with small anhydrite nodules (58 vol.-%), which are composed of blocky and acicular crystals (Fig. B-3).

BOZ2-1-700.76 is a chickenwire anhydrite, where the anhydrite nodules (68 vol.-% anhydrite) are closely joined, with a small argillaceous framework (14 vol.-% clay matrix). The dolomite rhombohedrons (18 vol.-%) are widespread within the anhydrite.

BOZ2-1-684.75 finally consists of a thin-layered alternation of anhydrite and claystone, whereat the anhydrite layers itself contain thin dolomite layers (Fig. B-4). The part of anhydrite makes 48 vol.-%, of dolomite 42 vol.-% and clay matrix 10 vol.-%.

Klettgau Formation (BOZ2-1-635.47, 624.43)

The two analysed samples of the Klettgau Formation concern once the Gansingen Member (BOZ2-1-635.47), and then we looked with BOZ2-1-624.43 if the Seebi Member is present.

Thin section BOZ2-1-635.47 shows a fully dolomitised, original (calcitic) oolitic, bioclastic limestone, consisting of layers of bivalves and layers of ooids. All could be counted as dolomite, but we differentiate as well as possible: bivalves (18 vol.-%), ooids (15 vol.-%) dolomite rhombohedrons (57 vol.-%) and porosity (10 vol.-%).

BOZ2-1-624.43 is a sandy, argillaceous dolostone with 18 vol.-% detrital quartz grains and rock fragments as well as intraclasts (4 vol.-%), sedimented with a clayey, dolomitic matrix (78 vol.-%) (Fig. B-5). So, the thin section documents a more siliciclastic interval, which was here included into the Gruhalde Member.

Staffelegg Formation (BOZ2-1-581.08)

The only studied thin section from the Staffelegg Formation belongs to the bed «Unterer Stein» of the Rietheim Member: BOZ2-1-581.08 is a microbial mat of a stromatolitic limestone (counted as other biogenes: 97 vol.-%) with pyrite (3 vol.-%).

Opalinus Clay (BOZ2-1-485.52, 467.43, 451.83)

Microfacies of several different Opalinus Clay sub-units and of iron-oolitic or calcareous beds has been analysed during the study of the sediments of BOZ1-1 (Wohlwend et al. 2022). So, we focussed here on an iron-oolitic hardground (BOZ2-1-467.43) and two biodetritic calcareous lenses respectively layers (BOZ2-1-485.52 and 451.83).

BOZ2-1-485.52 is composed of few calcareous layers of relatively big (up to 2 mm) crinoid skeletal elements (Fig. B-7) alternating with bioclastic bivalve layers and quartz sand layers. A part of these layers shows an intense pyritisation (Fig. B-6). The overall composition is 34 vol.-% echinoderms, 8 vol.-% bivalves and 2 vol.-% other biogenes, 18 vol.-% quartz, 11 vol.-% pyrite, 18 vol.-% clay matrix, 2 vol.-% micas and 7 vol.-% calcite cement.

Sample BOZ2-1-467.43 shows beautiful iron-oolids, whereat most of them are now calcitic recrystallised, few have their original chamosite mineralogy (Fig. B-8). Above the iron-oolite follows a bioclastic marl, thus the following composition results: iron-oolids (including calcitic iron-oolids) (16 vol.-%), echinoderms (21 vol.-%), bivalves (11 vol.-%), other biogenes (3 vol.-%), quartz (6 vol.-%), pyrite (5 vol.-%), limonitic grains (3 vol.-%) and micritic as well as marly matrix (35 vol.-%). The here mentioned calcitic iron-oolids have been noted in the "Fe-oolids" column in Tab. 3-1 with an asterisk behind the number.

BOZ2-1-451.83 was taken for analysing the grain composition of sand lenses. Is it composed of quartz grains or something else? So, the thin section consists of echinoderms (18 vol.-%), bivalves (12 vol.-%), other biogenes (4 vol.-%, e.g. different foraminifera), serpulids (1 vol.-%), pellets (15 vol.-%), with calcite cement (12 vol.-%) (Fig. B-9), as well as clay matrix (15 vol.-%) with quartz silt (14 vol.-%), siderite (5 vol.-%), pyrite (2 vol.-%) and mica (2 vol.-%). Biogene components, quartz grains and clay matrix are mixed by burrows and bioturbation.

Passwang Formation (BOZ2-1-448.81, 447.78, 441.73, 432.87, 429.43, 422.67, 420.59, 419.28, 407.67)

Most of the nine samples of the Passwang Formation are sandy, bioclastic limestones, two of them (BOZ2-1-448.81 and 422.67) contain iron-oolids and another two (BOZ2-1-420.59 and 419.28) are really iron-oolites. The latter three belong to the «Humphriesi-Schichten» of the Brüggl Member.

BOZ2-1-448.81, in the lower part of the Passwang Formation, is a bioclastic limestone with few iron-oolids (7 vol.-%, Fig. B-10). The dominant components are crinoid skeletal elements (37 + 4 (limonitic ones) vol.-%). They are relatively big (0.5 – 1.5 mm and up to 5 mm) and are accompanied by bivalves (7 vol.-%) and others biogenes, such as foraminifera (2 vol.-%), limonitic pellets (4 vol.-%) and quartz sand (13 vol.-%). These components are embedded in matrix and cement: micrite and limonitic matrix (13 vol.-%), calcite cement (6 vol.-%), "stellate cement" (3 vol.-%) and dolomite rhombohedrons (4 vol.-%).

The three samples BOZ2-1-447.78, 441.73 and 432.87 are sandy, bioclastic limestones (Fig. B-11) with nearly the same content of biogene components (26 – 35 vol.-%) as quartz grains (26 – 35 vol.-%). Microsparite (12 – 17 vol.-%), calcite cement (5 "stellate cement" (12 resp. 17 vol.-%, BOZ2-1-441.73 resp. 432.87) fill the last third of the thin sections. Echinoderms, bivalves, sponge spicules, foraminifera and serpulids, which are partly silicified (2 – 3 vol.-% quartz cement), are the biogene components.

BOZ2-1-429.43 is a limonitic, bioclastic limestone with limonitic biogene components (26 vol.-%), other echinoderms and bivalves (24 vol.-%), limonitic oncoids (6 vol.-%), limonitic pellets (4 vol.-%) and limonitic matrix (7 vol.-%) (Fig. B-12). Calcite cement (20 vol.-%) and iron-dolomite (11 vol.-%) are filling the space between the components.

Sample BOZ2-1-422.67, taken of a lower bed of the «Humphriesi-Schichten», is a limonitic, bioclastic limestone (iron-oolitic) with up to 12 vol.-% iron-oolids (Fig. B-13). Limonitic biogenes (18 vol.-%), bivalves (6 vol.-%), sponge spicules and foraminifera (5 vol.-%), limonitic pellets (5 vol.-%), as well as quartz sand (10 vol.-%) are further components. "Stellate cement" (15 vol.-%), closely connate with limonitic matrix (13 vol.-%) and components, gives evidence for a "hiatus bed". Iron-dolomite rhombohedrons (16 vol.-%) complete the microfacies.

The two thin sections BOZ2-1-420.59 and 419.28 are true iron-oolites of the «Humphriesi-Schichten». Iron-oolids (34, resp. 50 vol.-%) are the dominant components (Fig. B-14). They are accompanied by biogene components (totally 21 vol.-% (including serpulids + brachiopods), resp. 10 vol.-%), quartz silt (8, resp. 3 vol.-%) and mica (2, resp. 1 vol.-%). They have been sedimented with limonitic, calcareous (22 vol.-%, BOZ2-1-420.59) or marly matrix (31 vol.-%, BOZ2-1-419.28). Other minerals: iron-dolomite (6 vol.-%), pyrite (2 vol.-%), calcite cement (5 vol.-%) or anhydrite (5 vol.-%) appear in one or the other sample.

Then, the uppermost sample of the Passwang Formation, BOZ2-1-407.67, is a fine-grained limestone, composed of small biogene components, as for example sponge spicules (12 vol.-%) and bivalves (12 vol.-%), echinoderms (5 vol.-%) and others (3 vol.-%). Some pellets (5 vol.-%), pyrite (4 vol.-%), quartz (13 vol.-%) and microsparite (46 vol.-%) complete this limestone.

Hauptrogenstein (BOZ2-1-375.11, 357.90, 355.15, 341.63, 340.94, 336.09, 334.98, 333.20, 330.66, 330.02, 319.83, 312.93, 309.57)

The aim of these 13 thin sections is to verify if the numerous limestone beds of the Hauptrogenstein in BOZ2-1 have a similar microfacial composition as those of BOZ1-1. Namely with dominant oncoids, rather than many ooids. Seven samples (BOZ2-1-375.11, 357.90, 355.15, 341.63, 340.94, 336.09 and 334.98) have been chosen to resolve the microfacies. An additional goal was to test if the thin sections taken from the upper part («Movelier Beds» and «Spatkalk»; thin sections BOZ2-1-333.20, 330.66 and 330.02) show a comparable microfacies to the outcrops of the Movelier region further to the west. The uppermost three samples (BOZ2-1-319.83, 312.93 and 309.57) are limonitic beds, may correlate to the informal «Spatkalk», however, not individually eliminated here.

Effectively, the dominant components in the thin sections BOZ2-1-375.11, 355.15, 341.63, 340.94, 336.09 and 334.98 are oncoids (Fig. B-15) with a portion of 23 to 33 vol.-%. These samples contain furthermore, partly numerous, aggregate grains (Fig. B-16) (7 – 24 vol.-%, counted in the column of pellets) and some ooids (3 – 7 vol.-%). Biogene components: echinoderms (5 – 11 vol.-%), bivalves (4 – 12 vol.-%), others (1 – 4 vol.-%) are present too. BOZ2-1-375.11 is a micritic oncolitic limestone (34 vol.-% micritic matrix), whereas the others are calcite-cemented (17 – 28 vol.-%), contain no or little matrix (0 – 16 vol.-%), but Fe-dolomite rhombohedrons (2 – 18 vol.-%). BOZ2-1-357.90 comes from a bed with less oncoids (8 vol.-%), but numerous biogene components: bivalves (23 vol.-%), echinoderms (18 vol.-%), other biogenes (4 vol.-%) and aggregates (7 vol.-%), sedimented with micrite (5 vol.-%) and cemented by calcite (31 vol.-%) and dolomite (4 vol.-%).

The two samples BOZ2-1-333.20 and 330.66 of the lower part of the «Movelier Beds» and «Spatkalk» are limonitic, bioclastic limestones, consisting of limonitic echinoderms + bivalves (33, resp. 36 vol.-%), limonitic serpulids (6, resp. 5 vol.-%), other biogenes (4, resp. 0 vol.-%). Iron-ooids (5 vol.-%, BOZ2-1-330.66) or limonitic pellets (5 vol.-%, BOZ2-1-333.20) are present too. The components are embedded in a limonitic, marly and micritic matrix (46 vol.-%, BOZ2-1-333.20, Fig. B-17) or in limonitic (10 vol.-%, BOZ2-1-330.66) and non-limonitic micrite matrix (14 vol.-%) and calcite cement (20 vol.-%), as well as few iron-dolomites (3, resp. 10 vol.-%).

Thin section BOZ2-1-330.02 shows much more serpulids (23 vol.-%), than echinoderms (24 vol.-%), bivalves (14 vol.-%), sedimented with micritic (15 vol.-%), partly limonitic matrix (4 vol.-%) and cemented by calcite (20 vol.-%) in one half.

The sample of the upper part of the «Movelier Beds» and «Spatkalk», BOZ2-1-319.83, is a bioclastic limestone with echinoderms (33 vol.-%), bivalves (17 vol.-%), other biogenes (3 vol.-%) and pellets with micritic matrix (24 vol.-%), limonitic matrix (4 vol.-%) and calcite cement (13 vol.-%).

BOZ2-1-312.93 and 309.57 are limonitic, bioclastic limestones. Most of the fossils and the matrix are limonitic: limonitic echinoderm + bivalves (45, resp. 48 vol.-%), however in BOZ2-1-312.93 also 8 vol.-% non limonitic echinoderms were present, additionally 3, resp. 14 vol.-% other biogenes (where most of them are limonitic bryozoans; Fig. B-18) can be found. BOZ2-1-312.93 contains limonitic matrix (21 vol.-%) and calcite cement (19 vol.-%), whereas BOZ2-1-309.57 is a grainstone with only sparite cement (28 vol.-%). Both contain Fe-dolomite (4 resp. 10 vol.-%) too.

3.2 Ammonite stratigraphy

From BOZ2-1 nine macrofossil specimens were recovered, eight of them were ammonites and one specimen (depth 548.68 m) with brachiopods (list in Appendix A2). From these ammonite specimens, only one (depth 573.71 m) could not be extracted because of poor preservation. Another specimen (depth 451.19 m) was unfortunately truncated by the drilling such that only a part of the ventral side was present. This was not sufficiently diagnostic for determination.

In the formations drilled in BOZ2-1, ammonites are generally rather sparsely represented except for the lower part of the Opalinus Clay, the «Humphriesi-Schichten» of the Passwang Formation and the Ifenthal Formation. The ammonites from the latter formation, however, were not recovered due to incompleteness. Four additional ammonites (depths 576.19 m, 574.21 m, 411.29 m, 304.56 m; listed in Appendix A3) were also not recovered because these could not have been further identified due to poor preservation or incompleteness, even with extensive preparation. In contrast, the core sample (depth 548.68 m, Opalinus Clay) is remarkable: four inarticulate brachiopods of the genus *Discinisca* are preserved on the bedding surface.

We documented a selection of ammonites and additional macrofossils with photographs on two plates (Plates I – II) in Appendix C. In addition to ammonites, other conspicuous fossils were identified to the extent possible (Appendix A3), even when they were not subsequently, or only occasionally, recovered.

In general, the more ammonites are present in a specific profile section, the more precisely the biostratigraphic classification of that section can be determined (Tab. 3-2). Due to the generally small sample size and the poor, often incomplete preservation of the ammonites, a more-or-less large uncertainty in the determination must be expected, which may affect the biostratigraphic classification. Furthermore, it must be considered that not all ammonites have the same index value. The uncertainty in the determination is in the range of about one ammonite Subzone (SZ) but can be as high as one ammonite Zone (Z), when the available data are insufficient.

Staffelegg Formation

- 576.19 m: *Pseudogrammoceras* ex gr. *fallaciosum* (Bayle, 1878). Steinkern preservation. Age: the species is common in the Late Toarcian, Thouarsense Zone, Fallaciosum Subzone. Lithology: light- to dark-grey bioclastic limestone. The ammonite could not be recovered.
- 574.21 m: *Pleydellia* sp. Ammonites and ammonite fragments. Age: Aalensis Zone. The ammonites could not be recovered.
- 573.71 m: Ammonite indet. Due to poor preservation, it could not be identified. Lithology: dark-grey bioclastic claystone (with shell fragments). The ammonite is not illustrated.

Opalinus Clay

- 573.58 m: *Leioceras* ex gr. *subglabrum* (Buckman, 1902). Flattened argillaceous steinkern. Age: Opalinum Zone, Opalinum Subzone. Lithology: dark-grey claystone with bioclasts. Another fossil: *Bositra buchi*? The ammonite is illustrated on Plate I, Fig. 1.
- 563.60 m: *Leioceras* ex gr. *opalinum* (Reinecke, 1818). Flattened specimen with partially preserved calcitic shell. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark-grey, mica-bearing claystone. Other fossils are ammonites and a bivalve. The ammonite is illustrated on Plate I, Fig. 2.
- 548.85 m: *Leioceras* ex gr. *opalinum* (Reinecke, 1818). Flattened specimen with partially preserved calcitic shell. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark-grey, mica-bearing claystone. The ammonite is illustrated on Plate I, Fig. 3.
- 548.68 m: *Discinisca* sp. (brachiopods identified by H. Sulser). Partially preserved shell. Age: occurs in the Toarcian and Early Aalenian. Lithology: dark-grey mica-bearing claystone. Another fossil: a bivalve. The brachiopods are illustrated on Plate I, Fig. 4.
- 548.09 m: *Leioceras* ex gr. *opalinum* (Reinecke, 1818). Flattened specimen with partially preserved calcitic shell. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark-grey, mica-bearing claystone. The ammonite is illustrated on Plate I, Fig. 5.

Passwang Formation

- 451.19 m: Graphoceratidae indet. Incomplete, truncated specimen in steinkern preservation. Only a part of the venter is preserved. Age: probably Late Aalenian, Concavum Zone? Lithology: dark-grey to rust-brown marl (iron-oolitic). Other fossils are bivalve fragment and belemnites. The ammonite is not illustrated.
- 420.28 m: *Dorsetensia* sp. Incomplete, truncated specimen in steinkern preservation. Age: Humphriesianum Zone, Romani Subzone? Lithology: dark, rust-brown limestone (iron-oolitic). The iron-oooids reach ca. 0.8 mm in diameter and are limonitic/goethitic. Other fossils are indeterminate shell fragments. The ammonite is illustrated on Plate II, Figs. 1a and 1b.
- 419.23 m: *Itinsaites* sp.? Incomplete, truncated specimen in steinkern preservation. Age: Humphriesianum Zone, Humphriesianum Subzone. Lithology: dark, rust-brown marl (iron-oolitic). Diameter of the iron-oooids up to ca. 0.8 mm. The oooids are limonitic/goethitic. Other fossils are an ammonite at depth 419.21 m, a belemnite (*Belemnopsis* sp.; identified by R. Weis), a terebratulid, and indeterminate shell fragments. The ammonite is illustrated on Plate II, Figs. 2a, 2b and 2c. The belemnite is illustrated on Plate II, Figs. 2a and 2d.
- 411.92 m: *Teloceras* sp.? Ammonite fragment on the bedding surface. Age: probably Humphriesianum Zone, Blagdeni Subzone. The ammonite was not recovered.

Ifenthal Formation

304.56 m: *Oxycerites* sp. Incomplete specimen, only a whorl cross section is preserved. Age: probably Bathonian. The ammonite was not recovered.

Tab. 3-2: Ammonite and other macrofossil determination from BOZ2-1

Depth [m MD]	Identification	Ammonite Zone (Subzone) or Age
304.56	<i>Oxycerites</i> sp.	Bathonian?
411.92	<i>Teloceras</i> sp.?	Humphriesianum Z (Blagdeni SZ) ?
419.23	<i>Itinsaites</i> sp.? and <i>Belemnopsis</i> sp.	Humphriesianum Z (Humphriesianum SZ)
420.28	<i>Dorsetensia</i> sp.	Humphriesianum Z (Romani SZ ?)
451.19	Graphoceratidae indet.	Concavum Zone?
548.09	<i>Leioceras</i> ex gr. <i>opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum Subzone)
548.68	<i>Discinisca</i> sp.	Toarcian to Early Aalenian
548.85	<i>Leioceras</i> ex gr. <i>opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum Subzone)
563.60	<i>Leioceras</i> ex gr. <i>opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum Subzone)
573.58	<i>Leioceras</i> ex gr. <i>subglabrum</i> (Buckman, 1902)	Opalinum Zone (Opalinum Subzone)
573.71	Ammonite indet.	
574.21	<i>Pleydellia</i> sp.	Aalensis Zone
576.19	<i>Pseudogrammoceras</i> ex gr. <i>fallaciosum</i> (Bayle, 1878)	Thouarsense Zone (Fallaciosum Subzone)

System	Stage	Zone	Subzone
Jurassic	Late	Oxfordian	Bifurcatus
			Grossouvrei
			Stenocycloides
			Rotoides
			Schilli
			Luciaeformis
			Parandieri
			Plicatilis
			Antecedens
			Vertebrale
	Middle	Callovia	Cordatum
			Costicardia
			Bukowski
			Praecordatum
			Scarburgense
			Lamberti
			Henrici
			Spinosum
			Proniae
			Phaeinum
	Early	Bathonian	Coronatum
			Grossouvrei
			Obductum
			Jason
			Medea
			Enodatum
			Calloviense
			Koenigi
			Galilaei
			Curtilobus
	Late	Bajocian	Gowerianus
			Kamptus
			Terebratus
			Keppleri
			Discus
			Hollandi
			Hannoveranus
			Blanazense
			Hodsoni
			Morrisi
	Middle	Pliensbachian	Subcontractus
			Progracilis
			Zigzag
			Tenuiplicatus
			Yeovilensis
			Macrescens
			Convergens
			Bomfordi
			Truellei
			Acris
	Early	Sinemurian	Tetragona
			Garantiana
			Dichotoma
			Baculata
			Polygyralis
			Banksii
			Niortense
			Humphriesianum
			Blagdeni
			Romani
	Late	Toarcian	Pinguis
			Macrum
			Kumaterum
			Laeviuscula
			Trigonalis
			Ovale
			Discites
			Concavum
			Formosum
			Concavum
Jurassic	Early	Pliensbachian	Bradfordensis
			Gigantea
			Murchisonae
			Haugi
			Bifidatum *
			Opalinum
	Late	Toarcian	Aalensis
			Torulosum
			Aalensis
			Moorei
			Levesquei
			Levesquei
			Dispansum
			Insigne
			Thouarsense
			Fallaciosum
	Early	Pliensbachian	Thouarsense
			Variabilis
			Crassum
			Fibulatum
			Commune
			Falcifer
			Elegans
			Exaratum
			Elegantulum
			Semicelatum
	Late	Toarcian	Clevelandicum
			Paltum
			Spinatum
			Hawskerense
			Apyrenum
			Gibbosus
			Subnodosus
			Stokesi
			Davoei
			Figulinum
	Early	Pliensbachian	Capricornus
			Maculatum
			Luridum
			Valdani
			Masseanum
			Ibex
			Jamesoni
			Jamesoni
			Brevispina
			Polymorphus
	Late	Toarcian	Taylori
			Raricostatum
			Aplanatum
			Macdonnelli
			Raricostatum
			Densinodulum
			Oxynotum
			Simpsoni
			Obtusum
			Denotatus
	Early	Pliensbachian	Stellare
			Obtusum
			Turneri
			Sauzeanum
			Scipionanum
			Charlesi
			Bucklandi
			Rotiforme
			Conybeari
			Angulata
	Late	Toarcian	Complanata
			Extranodosa
			Liasicus
			Laquaues
			Portlocki
			Johnstoni
			Planorbis
			Planorbis
			Planorbis
			Planorbis

BOZ2-1

Grey highlighted zones and subzones are documented in the drill core with ammonites. Fields with additional interrogation points are not surely proven with ammonites.

Biostratigraphy modified after Cariou & Hanzpergue (1997)

* after Dietze et al. (2021), former «Comptum» Subzone

Fig. 3-1: Zones and subzones which are documented by ammonites in BOZ2-1

3.3 Palynostratigraphy

The studied samples yielded mostly a good palynological residue with rich and diverse palynofloras. Preservation is good. The palynomorph assemblages are composed of mainly dinoflagellate cysts and pollen and spores. Minor components are prasinophytes, acritarchs, fungal remains, foraminiferal test linings and green algae (e.g. *Botryococcus*). A total of 169 dinoflagellate cyst taxa, 22 other aquatic palynomorphs and 50 pollen and spore taxa are recorded.

Some reworked sporomorphs (*Densosporites* spp.) indicate erosion of Triassic sediments in the source area. Other reworking is indicated by the occurrence of a few single specimens of the dinoflagellate cyst *Luehndea spinosa*, a typical Early Jurassic species with a main distribution in the Late Pliensbachian and earliest Toarcian.

The studied samples from BOZ2-1 cores are dated to span the interval from the latest Toarcian to the Oxfordian. There are 16 sample intervals differentiated and, where possible, assigned to ammonite biostratigraphy. A list of the analysed samples and the age dating of each sample is given in Tab. 3-3. The indicated ages, zones (Z) and subzones (SZ) for each sample are the result of the palynostratigraphical analysis and interpretation. The results of the quantitative analysis are illustrated in a Range Chart (Appendix D1). A Depth/Age plot is illustrated in Appendix D2.

Sample 573.93 m (1 sample): Late Toarcian, Aalensis Zone to Early Aalenian, Opalinum Zone, Opalinum Subzone

The palynoflora in this sample is characterised by the very high abundance of one dinoflagellate cyst species, *Evansia*? cf. *granochagrinata*. The species dominates the palynoflora, reaching 70% of all palynomorphs counted. Other dinoflagellate cysts present, though in low numbers, are a few representatives of the families Phallocystaceae (*Dodekovia pseudochytroides*, *Reutlingia hirsuta*) and Valvaeodiniaceae (*Valvaeodinium cavum*, *V. sphaerechinatum*, *V. vermipellitum*) as well as *Hystriochodinium*? sp., *Kallosphaeridium praussii*, *Mancodinium semitabulatum*, *Nannoceratopsis* spp., *Nannoceratopsis gracilis* s.l., *Scrinioicassis limbicavatus* and *S. weberi*.

The sample interval is defined by the dominant occurrence (superabundance) of *Evansia*? cf. *granochagrinata*.

The composition of the dinoflagellate cyst assemblage is typical for the interval straddling the Toarcian/Aalenian boundary. *Evansia*? cf. *granochagrinata* has its FAD (First Appearance Datum) in the Late Toarcian, probably Levesquei Zone. *Kallosphaeridium praussii* first appears in the Late Toarcian Aalensis Zone. The very high abundance or dominance of *Evansia*? cf. *granochagrinata* is typical for an age of the sample straddling the Toarcian/Aalenian boundary (Aalensis Zone to Opalinum Zone, Opalinum Subzone). This characteristic bioevent at the Early to Middle Jurassic boundary defines the palynostratigraphic unit A of Feist-Burkhardt & Pross (2010).

Sample interval 573.57 – 485.64 m (6 samples): Early Aalenian, Opalinum Zone, Opalinum Subzone

Dinoflagellate cyst assemblages of this sample interval are rich and diverse. They are composed of common to abundant *Evansia*? cf. *granochagrinata*, diverse Phallocystaceae (*Andreodinium* sp. 2, *A. aff. elongatum*, *Dodekovia* spp., *D. bullula*, *D. knertensis*, *D. pseudochytroides*, *D. syzygia*, *Ovalicysta hiata*, *Parvocysta bjaerkei*, *P? tricornuta*, *Phallocysta? frommernensis*, *Reutlingia cardobarbata*, *R. hirsuta*, *R. nasuta*, *Susadinium scrofoides*) and Valvaeodiniaceae

(*Comparodinium aquilonium*, *Valvaeodinium* spp., *V. cavum*, *V. sphaerechinatum*, *V. vermipellitum*), species of *Nannoceratopsis* (*Nannoceratopsis* spp., *N. sp. 1*, *N. sp. B*, *N. dictyambonis*, *N. gracilis* s.s. and s.l., *N. triangulata*) and *Scriniocassis* (*S. limbicavatus*, *S. priscus*, *S. weberi*) as well as *Bradleyella* sp. 2, *Hystriochodinium*? sp. in Feist-Burkhardt & Pross (2010), *Kallosphaeridium praussii*, *Mancodinium semitabulatum* and *Wallodinium laganum*. The species *Evansia*? cf. *granochagrinata* is very abundant in the samples at the base of the interval but its abundance decreases up section. *Phallocysta*? *frommernensis* is fairly common throughout the interval and shows an acme up to the basal sample in the interval above.

The interval is defined by the first occurrence of *Phallocysta*? *frommernensis* to the first occurrences of questionable *Batiacasphaera* sp. A in Feist-Burkhardt & Pross (2010) and several subspecies of *Nannoceratopsis plegas* in the sample interval above.

According to Feist-Burkhardt & Pross (2010) there are four marker species for the Early Aalenian Opalinuston Formation (Germany stratigraphy): *Kallosphaeridium praussii*, *Phallocysta*? *frommernensis*, *Nannoceratopsis triangulata* and *Wallodinium laganum*. All four marker species occur in this interval. The genus *Batiacasphaera* has its FAD in the upper part of the Opalinum Zone with *Batiacasphaera* sp. A often being abundant in the Bifidatum Subzone of the Opalinum Zone. The acme of *Phallocysta*? *frommernensis* defines the palynostratigraphical unit B of Feist-Burkhardt & Pross (2010) of the Opalinuston Formation.

The sample interval is interpreted Early Aalenian Opalinum Zone, Opalinum Subzone, and corresponds largely to palynostratigraphic unit B of Feist-Burkhardt & Pross (2010).

The occurrence of *Luehndea spinosa* (545.90 m and 485.64 m) indicates reworking of Early Jurassic Late Pliensbachian to earliest Toarcian sediments in the source area.

Sample interval 465.47 – 451.65 m (3 samples): Early Aalenian, Opalinum Zone, probably Bifidatum Subzone

Assemblages in this interval are reduced in the diversity of phallocystacean dinoflagellate cysts. The base of the interval is characterised by the first occurrences of questionable *Batiacasphaera* sp. A and several subspecies of *Nannoceratopsis plegas* (*N. plegas brevicornis*, *N. plegas plegas*). Last occurrences in this interval include *Evansia*? cf. *granochagrinata*, *Nannoceratopsis triangulata* and *Phallocysta*? *frommernensis*, and at the top of the interval *Scriniocassis priscus*, *S. weberi* and *Wallodinium laganum*.

The interval is defined from the first occurrence of questionable *Batiacasphaera* sp. A to the last occurrences of *Scriniocassis weberi* and *Wallodinium laganum*.

The genus *Batiacasphaera* has its FAD in the upper part of the Opalinum Zone with *Batiacasphaera* sp. A often being abundant in the Bifidatum Subzone of Opalinum Zone. The LADs (Last Appearance Datum) of *Scriniocassis weberi* and of *Wallodinium laganum* are considered to be at the top of the Opalinum Zone.

The interval is interpreted Opalinum Zone, probably Bifidatum Subzone (previously «Comptum» Subzone; Dietze et al. 2021).

The occurrence of *Luehndea spinosa* (465.47 m) indicates reworking of Early Jurassic Late Pliensbachian to earliest Toarcian sediments in the source area.

Sample interval 451.19 – 449.11 m (3 samples): Early Bajocian, Discites Zone

The dinoflagellate cyst assemblages in this interval differ a lot from the samples below. Representatives of the genus *Dissiliodinium* are abundant. There are numerous first occurrences at the base of the interval, i.a. *Andreedinium elongatum*, *Batiacasphaera* spp., *Dissiliodinium* spp., *D. lichenoides*, *D. aff. giganteum*, *Evansia? eschachensis*, *E? spongogranulata*, *Moesiodinium raileanui* and *Pareodinia* spp. The species *Pareodinia* sp. 4 occurs only in the sample at 450.80 m. Last occurrence at the top of the interval has *Nannoceratopsis* sp. B.

The interval is defined from the first occurrence of *Dissiliodinium* aff. *giganteum* and to the last occurrence of *Nannoceratopsis* sp. B.

Dissiliodinium aff. *giganteum* and *Nannoceratopsis* sp. B have their FADs in the Discites Zone. *Pareodinia* sp. 4 has so far only been observed in the Discites Zone.

The interval is dated Discites Zone.

Sample interval 448.81 – 447.78 m (2 samples): Early Bajocian, Ovale Zone

In addition to species known from below, the dinoflagellate cyst assemblages are characterised by the first occurrences of *Dissiliodinium giganteum*, *Durotrigia* spp. and *Gongylodinium erymnoteichon*. Last occurrences in this interval show *Andreedinium elongatum* and *Evansia? eschachensis*.

The interval is defined from the first occurrence of *Dissiliodinium giganteum* to the last occurrences of *Andreedinium elongatum* and *Evansia? eschachensis*.

The FAD of *Dissiliodinium giganteum* is in the Ovale Zone. The LADs of *Andreedinium elongatum* and *Evansia? eschachensis* are also in the Ovale Zone.

The sample is dated Ovale Zone.

Sample interval 439.68 – 428.43 m (4 samples): Early Bajocian, Laeviuscula Zone

Assemblages in this interval show the first occurrences of *Batiacasphaera laevigata*, *Cavatodissiliodinium hansgochtii* and *Durotrigia daveyi*. Last occurrences in this interval have *Dissiliodinium giganteum*, *Evansia? spongogranulata*, *Moesiodinium raileanui*, *Nannoceratopsis dictyambonis* and *N. plegas plegas*.

The interval is defined from the first occurrence of *Cavatodissiliodinium hansgochtii* at the base of the interval to the last occurrences of *Nannoceratopsis dictyambonis* and *N. plegas plegas* at the top and the first occurrence of *Kallosphaeridium hypornatum* in the interval above.

The FAD of *Cavatodissiliodinium hansgochtii* is in the Laeviuscula Zone. The LADs of *Nannoceratopsis dictyambonis* and *N. plegas plegas* are in the Laeviuscula Zone. The FAD of *Kallosphaeridium hypornatum* is in the Sauzei Zone.

The interval is dated Laeviuscula Zone.

Sample interval 424.96 – 424.08 m (2 samples): Early Bajocian, Sauzei Zone

Assemblages in this interval show the first occurrence of *Kallosphaeridium hypornatum*.

The interval is defined from the first occurrence of *Kallosphaeridium hypornatum* to the first occurrences of questionable *Durotrigia filapicata* and *Wanaea* sp. 1 in the interval above.

The FAD of *Kallosphaeridium hypornatum* is in the Sauzei Zone. The FADs of *Durotrigia filapicata* and *Wanaea* sp. 1 are in the Humphriesianum Zone.

The interval is dated Sauzei Zone.

Sample 422.39 m (1 sample): Early Bajocian, Sauzei to Humphriesianum Zone

The assemblage in this sample shows the first occurrences of questionable *Durotrigia filapicata* and *Wanaea* sp. 1 and the last occurrence of *Cavatodissiliodinium hansgochtii*, which is common.

The interval is defined by the co-occurrence of questionable *Durotrigia filapicata* and *Wanaea* sp. 1 on one hand and *Cavatodissiliodinium hansgochtii* on the other.

The FADs of *Durotrigia filapicata* and *Wanaea* sp. 1 are considered to be early in the Humphriesianum Zone. The LAD of *Cavatodissiliodinium hansgochtii* was so far considered to be in the late Sauzei Zone.

Based on the co-occurrence of the taxa mentioned, the interval is interpreted Sauzei to Humphriesianum Zone.

Sample interval 418.68 – 418.18 m (2 samples): Early Bajocian, Humphriesianum Zone, Blagdeni Subzone

The assemblages in this interval are characterised by numerous first occurrences including common *Acanthaulax crista*, *Atopodinium* sp. 1, *Atopodinium polygonale*, questionable *Meiourogoniaulax valensii*, *Nannoceratopsis spiculata*, *Rhynchodiniopsis?* sp. 1 and abundant *Valensiella/Ellipsoidictyum* spp. *Nannoceratopsis gracilis* s.l. has its last occurrence at the top of the interval.

The interval is defined from the first occurrences of *Atopodinium* sp. 1 and *Rhynchodiniopsis?* sp. 1 to the first occurrence of *Valvaeodinium spinosum* in the interval above.

The FADs of *Acanthaulax crista*, *Atopodinium* sp. 1, *Meiourogoniaulax valensii*, *Nannoceratopsis spiculata*, *Rhynchodiniopsis?* sp. 1 and *Valensiella/Ellipsoidictyum* spp. are all in the Humphriesianum Zone, those of *Atopodinium* sp. 1 and *Rhynchodiniopsis?* sp. 1 are considered to be in the Blagdeni Subzone of the Humphriesianum Zone. The FAD of *Valvaeodinium spinosum* is in the Niortense Zone.

The interval is dated Blagdeni Subzone of the Humphriesianum Zone.

Sample interval 409.94 – 335.49 m (11 samples): Late Bajocian, Niortense to Garantiana Zone

The assemblages in this interval are characterised by numerous first occurrences. In the lower part of the interval these include *Endoscrinium asymmetricum*, unquestionable *Gongylodinium hocneratum*, *Gonyaulacysta pectinigera*, *Korystocysta gochtii*, questionable *Rosswangia simplex*, *Valvaeodinium spinosum*, *Wanaea indotata* and higher up section *Aldorfia aldorfensis*, *Batiacaspheera* sp. 1, *Carpathodinium predae*, *Carpathodinium* sp. 2, *Chytroeisphaeridia chytroeides*, *Ctenidodinium* spp., *Ct. continuum*, *Ct. sellwoodii* group, *Mikrocysta* spp. and *Rhynchodiniopsis? regalis*. Representatives of the genus *Ctenidodinium* are present but not common. *Durotrigia daveyi* is common in most samples and shows its last occurrence at the top of the interval. The last occurrence of *Mancodinium semitabulatum* with a single specimen in the sample at 387.88 m may be reworked.

The interval is defined by the first occurrence of *Valvaeodinium spinosum* to the last occurrence of *Durotrigia daveyi* and the first occurrences of unquestionable *Orobodinium automobile* and *Sirmiodiniopsis* sp. in the interval above.

The FADs of most of the first occurring species are in the Niortense Zone (*Carpathodinium predae*, *Ctenidodinium continuum*, *Gonyaulacysta pectinigera*, *Korystocysta gochtii*, *Rosswangia simplex*, *Valvaeodinium spinosum*) and higher within the Niortense Zone (*Endoscrinium asymmetricum*, *Gongylodinium hocneratum*), that of *Ctenidodinium sellwoodii* group is in the Garantiana Zone. The LAD of *Durotrigia daveyi* is in the Garantiana Zone. The FADs of *Orobodinium automobile* and *Sirmiodiniopsis* sp. are in the Parkinsoni Zone.

The interval is interpreted Niortense to Garantiana Zone.

Sample 334.07 m (1 sample): Late Bajocian, Parkinsoni Zone

The dinoflagellate cyst assemblage is quite similar to those from below, with *Acanthaulax crispa* consistently occurring up to the top of the interval. Representatives of the genus *Ctenidodinium* are abundant. *Ctenidodinium combazii* does not yet occur but is recorded at the base of the interval above. First occurrences in this sample include *Endoscrinium luridum*, *Meiourogoniaulax* sp. 1, unquestionable *Orobodinium automobile* and *Sirmiodiniopsis* sp. of Feist-Burkhardt & Wille (1992).

The interval is defined from the first occurrences of *Orobodinium automobile* and *Sirmiodiniopsis* sp. to the last occurrence of *Acanthaulax crispa*.

The FADs of *Orobodinium automobile* and *Sirmiodiniopsis* sp. are in the Parkinsoni Zone. The LAD of *Acanthaulax crispa* is in the Parkinsoni Zone.

The interval is dated Parkinsoni Zone.

Sample interval 330.57 – 314.46 m (5 samples): Early Bathonian, Zigzag Zone

Assemblages in this interval are characterised by abundant and diverse representatives of the genus *Ctenidodinium*, including common *Ct. combazii*. First occurrences at the base of the interval include *Ctenidodinium combazii*, *Gonyaulacysta eisenackii*, *Lithodinia jurassica* and *Tubeutubercella dangeardii*. Later there is also *Dissiliodinium minimum*. The chorate dinoflagellate cyst

Cleistosphaeridium spp. Has a first occurrence with a questionable specimen in this interval. Unquestionable *Cleistosphaeridium* spp. Occurs in the interval above. The species *Meiourogonyaux valensii* has its last occurrence at the base of the interval.

The interval is defined from the first occurrences of *Lithodinia jurassica* and *Tubotuberella dangeardii* to the first unquestionable occurrence of *Cleistosphaeridium* spp. in the interval above.

The FAD of *Ctenidodinium combazii* is within the upper part of the Parkinsoni Zone, those of *Lithodinia jurassica* and *Tubotuberella dangeardii* are in the Zigzag Zone. The LAD of *Meiourogonyaux valensii* is in the Zigzag Zone. The FAD of *Cleistosphaeridium* spp. is in the Tenuiplicatus Subzone of the Zigzag Zone.

The interval is dated Zigzag Zone.

Sample interval 310.47 – 308.07 m (3 samples): Early Bathonian, Zigzag Zone, Tenuiplicatus Subzone to Late Bathonian, Hodsoni Zone

The assemblages are quite similar to those from below with abundant and diverse representatives of the genus *Ctenidodinium*. Abundance of *Ctenidodinium* increases up section. There are several first occurrences within the interval including *Ambonosphaera* sp. 2, *Cleistosphaeridium* spp. (unquestionable), *Ctenidodinium cornigerum*, *Gonyaulacysta jurassica*, *Nannoceratopsis pellucida* (questionable) and the first complex skolochorate dinocysts indeterminate. Last occurrences in this interval include *Carpathodinium predae*, *Dissilodinium minimum* (questionable) and *Gongylodinium erymnoteichon*.

The interval is defined from the first unquestionable occurrence of *Cleistosphaeridium* spp. to the first occurrence of *Atopodinium prostaticum* in the interval above.

The FAD of the first chorate dinoflagellate cyst, *Cleistosphaeridium ehrenbergii*, is in the Tenuiplicatus Subzone of the Zigzag Zone, those of *Gonyaulacysta jurassica* and *Nannoceratopsis pellucida* are in the Progracilis Zone. The LAD of *Carpathodinium predae* is in the Morrisi Zone. The FAD of *Atopodinium prostaticum* is in the Hodsoni Zone.

The interval is interpreted Tenuiplicatus Subzone of the Zigzag Zone to Hodsoni Zone.

Sample interval 306.58 – 305.17 m (2 samples): Late Bathonian, Hodsoni to Discus Zone

The assemblages are similar to below with abundant and diverse representatives of the genus *Ctenidodinium*. In addition, there are the first occurrences of *Atopodinium prostaticum*, *Eodinia* spp., *Rigaudella filamentosa* and *Sirmiodiniopsis orbis*. Last occurrences in this interval are i.a. *Atopodinium polygonale*, *Ctenidodinium combazii*, *Gongylodinium hocneratum* (questionable), *Gonyaulacysta pectinigera*, *Rhynchodiniopsis? regalis* and *Valvaeodinium spinosum*.

The interval is defined from the first occurrence of *Atopodinium prostaticum* to the last occurrence of *Valvaeodinium spinosum*.

The FADs of *Atopodinium prostaticum*, *Rigaudella filamentosa* and *Sirmiodiniopsis orbis* are in the Hodsoni Zone. The LAD of *Rhynchodiniopsis? regalis* is in the Hodsoni Zone, that of *Valvaeodinium spinosum* is in the Discus Zone.

The interval is dated Hodsoni to Discus Zone.

Sample 303.77 m (1 sample): Oxfordian, probably Plicatilis to Transversarium Zone

Composition of the dinoflagellate cyst assemblage in this sample is very different to below. Complex skolochorate dinocysts are abundant, specimens of *Ctenidodinium* are rare. There are numerous first occurrences. These include *Acanthaulax* spp., *Amphorula dodekova*, *Cleistosphaeridium iaculigerum*, *Compositosphaeridium polonicum*, *Dingodinium tuberosum* (questionable), *Endoscrinium galeritum*, *Glossodinium dimorphum*, *Leptodinium arcuatum*, *L. mirabile* (questionable), *L. subtile* (questionable), *Mendicodinium* sp. A of Brenner (1988), *Rhynchodiniopsis cladophora*, *Rigaudella aemula*, *Scriniodinium crystallinum*, *S. dictyotum*, *Sentusidinium rioultii*, *Sirmiodinium grossii*, *Stephanelytron redcliffense*, *Systematophora areolata* and *Wallodinium* sp. 1. Last occurrences in this sample are *Dingodinium tuberosum* (questionable), *Rigaudella aemula* and *Scriniodinium crystallinum*.

There are species with FADs considered to be in the Plicatilis Zone (*Glossodinium dimorphum*, *Leptodinium arcuatum*, *L. mirabile*, *Systematophora areolata*), in the Transversarium Zone (*Leptodinium subtile*) and in the Bifurcatus Zone (*Amphorula dodekova*, *Dingodinium tuberosum*). There are species with LADs considered to be in the Plicatilis Zone (*Scriniodinium crystallinum*) and in the Transversarium Zone (*Compositosphaeridium polonicum*, *Endoscrinium galeritum*, *Rigaudella aemula*, *Sirmiodiniopsis orbis*).

The co-occurrence of the taxa mentioned does not allow for an unambiguous age interpretation. The sample is definitely Oxfordian in age. In terms of ammonite zones it corresponds probably to the Plicatilis to Transversarium Zone.

Sample 300.68 m (1 sample): Middle Oxfordian, Transversarium to Late Oxfordian, Bifurcatus Zone

Composition of the dinoflagellate cyst assemblage in this sample is quite similar to below. In addition, there are the first occurrences of i.a. *Cribroperidinium* spp., *Lithodinia arcanitabulata* (questionable), *Neuffenia willei*, *Occisucysta balios*, *Stephanelytron caytonense*, *S. scarburghense* and *Tehamadinium* spp. Important taxa present in this sample are i.a. *Compositosphaeridium polonicum*, *Ctenidodinium ornatum*, *Endoscrinium galeritum*, *Gonyaulacysta eisenackii*, *Nannoceratopsis pellucida* and *Sirmiodiniopsis orbis*.

There are species with LADs considered to be in the Transversarium Zone (*Compositosphaeridium polonicum*, *Ctenidodinium ornatum*, *Endoscrinium galeritum*, *Gonyaulacysta eisenackii*, *Nannoceratopsis pellucida*, *Sirmiodiniopsis orbis*), and there are species with FADs considered in the Bifurcatus Zone (*Lithodinia arcanitabulata*, *Occisucysta balios*).

The sample is interpreted Transversarium to Bifurcatus Zone.

Tab. 3-3: List of analysed palynology samples from BOZ2-1

The indicated ages, zones and subzones for each sample are the result of the palynostratigraphical analysis and interpretation.

Depth [m MD]	Age	Zone & Subzone
300.68	Late – Middle Oxfordian	Bifurcatus – Transversarium Zone
303.77	Oxfordian	Probably Transversarium – Plicatilis Zone
305.17	Late Bathonian	Discus – Hodsoni Zone
306.58	Late Bathonian	Discus – Hodsoni Zone
308.07	Late – Early Bathonian	Hodsoni – Zigzag Zone (Tenuiplicatus SZ)
309.49	Late – Early Bathonian	Hodsoni – Zigzag Zone (Tenuiplicatus SZ)
310.47	Late – Early Bathonian	Hodsoni – Zigzag Zone (Tenuiplicatus SZ)
314.46	Early Bathonian	Zigzag Zone
316.04	Early Bathonian	Zigzag Zone
322.13	Early Bathonian	Zigzag Zone
329.49	Early Bathonian	Zigzag Zone
330.57	Early Bathonian	Zigzag Zone
334.07	Late Bajocian	Parkinsoni Zone
335.49	Late Bajocian	Garantiana – Niortense Zone
342.05	Late Bajocian	Garantiana – Niortense Zone
350.12	Late Bajocian	Garantiana – Niortense Zone
358.18	Late Bajocian	Garantiana – Niortense Zone
366.06	Late Bajocian	Garantiana – Niortense Zone
373.89	Late Bajocian	Garantiana – Niortense Zone
381.77	Late Bajocian	Garantiana – Niortense Zone
387.88	Late Bajocian	Garantiana – Niortense Zone
388.82	Late Bajocian	Garantiana – Niortense Zone
399.09	Late Bajocian	Garantiana – Niortense Zone
409.94	Late Bajocian	Garantiana – Niortense Zone
418.18	Early Bajocian	Humphriesianum Zone (Blagdeni SZ)
418.68	Early Bajocian	Humphriesianum Zone (Blagdeni SZ)
422.39	Early Bajocian	Humphriesianum – Sauzei Zone
424.08	Early Bajocian	Sauzei Zone
424.96	Early Bajocian	Sauzei Zone
428.43	Early Bajocian	Laeviuscula Zone
429.43	Early Bajocian	Laeviuscula Zone
430.72	Early Bajocian	Laeviuscula Zone
439.68	Early Bajocian	Laeviuscula Zone
447.78	Early Bajocian	Ovale Zone
448.81	Early Bajocian	Ovale Zone
449.11	Early Bajocian	Discites Zone
450.80	Early Bajocian	Discites Zone
451.19	Early Bajocian	Discites Zone
451.65	Early Aalenian	Opalinum Zone (probably Bifidatum SZ)
456.47	Early Aalenian	Opalinum Zone (probably Bifidatum SZ)
465.47	Early Aalenian	Opalinum Zone (probably Bifidatum SZ)
485.64	Early Aalenian	Opalinum Zone (Opalinum SZ)
505.16	Early Aalenian	Opalinum Zone (Opalinum SZ)
525.45	Early Aalenian	Opalinum Zone (Opalinum SZ)
545.90	Early Aalenian	Opalinum Zone (Opalinum SZ)
566.19	Early Aalenian	Opalinum Zone (Opalinum SZ)
573.57	Early Aalenian	Opalinum Zone (Opalinum SZ)
573.93	Early Aalenian – L. Toarcian	Opalinum Zone (Opalinum SZ) – Aalensis Zone

3.4 Chemostratigraphy

The sampling of the BOZ2-1 cores focused primarily on the upper part of the Lias Group (Figs. 3-2 and 3-3) and Dogger Group (Figs. 3-4 to 3-7) and, therefore inter alia on clay mineral-rich layers of the Opalinus Clay. The summary Figs. 3-8 and 3-9 illustrate the fully analysed interval from the upper part of the Staffelegg Formation up to the lowermost part of the Wildeggen Formation (582.40 – 298.00 m). The data presented here (applies for all subsequent figures in this section) is shown in comparison to other data collected during the drilling campaign: Stratigraphic profile after Dossier III, DryClay (values in wt.-% vertical axis in m MD log depth; cf. Dossier X), XRD measurements (horizontal bars; calcite: blue, dolomite and ankerite: green, siderite: red; cf. Dossier VIII) and C(org) measurements also with blue horizontal bars (cf. Dossier VIII). In addition, formation boundaries were highlighted with black lines and other formal or informal subintervals with grey lines. The following stratigraphic abbreviations were used in Figs. 3-2 to 3-9: F. = Frick Member; G.B.R = Grünschholz Member, Breitenmatt Member and Rickenbach Member; R. = Rietheim Member; G. W. = Gross Wolf Member; OPA = Opalinus Clay; W. & l.B. = Waldenburg and lower part of the Bruggli Member; «H.-S.» = «Humphriesi-Schichten»; Bi. = Birmenstorf Member; Ef. = Effingen Member.

In addition to the continuous samples (roughly in metre resolution), some specific samples were taken (Appendix E1) to complete the information about the calcareous beds and macrofossils. Some of the firm- to hardground samples were drilled directly from the remaining thin section blocks to correlate the bulk geochemical data with the microfacies analysis. All these data points are distinguished in different colours on Figs. 3-2, 3-4 and 3-6 (in light blue: calcareous samples (firm- and hardgrounds, "hiatus beds", "hiatus concretions", calcareous concretions); in violet: septarian nodules; in green: macrofossils) but may not be shown on the individual plots because of the data ranges (see Appendix E1 for data).

The data will be discussed in three intervals: Lias Group, the lower part of the Dogger Group – mainly Opalinus Clay and the upper part of the Dogger Group. Not all data are discussed to the same extent as for example the $\delta^{18}\text{O}_{\text{carb}}$ and $\delta^{15}\text{N}_{\text{org}}$ data. The oxygen isotopes are strongly influenced by diagenesis. This can be exemplarily shown with the measured belemnites in the Lias Group in MAR1-1 (green points in Fig. 3-2 in Wohlgend et al. 2021c). These are 3 to 4 ‰ more positive than the marlier bulk rock and therefore much less diagenetically overprinted. The nitrogen isotopes may not be as meaningful in some cases, because the combined $\delta^{13}\text{C}_{\text{org}}$ and $\delta^{15}\text{N}_{\text{org}}$ measurements showed a too low concentration of N in most of the measurements.

Although, the calculated carbonate content (TCarb) is only a semi-quantitative method, the values presented here correspond quite good to the XRD values measured at the University of Bern (cf. Dossier VIII). The XRD data are illustrated in the following Figs. 3-2, 3-4 and 3-6 to provide a visual comparison between the data presented here and those from Dossier VIII. As discussed in Wohlgend et al. (2019b) based on measurements from the BDB-1 borehole at the Mont Terri Rock Laboratory, the values calculated here follow nicely the calcite and dolomite wt.-% with an additional mixed signal from the other carbonates (mainly siderite). Because during the reaction time of 60 min at 72 °C, a complete reaction for example for siderite does not take place. The TCarb values are slightly too low in siderite-rich successions (red bars in the XRD data), which is for example often the case in the «Mixed clay-silt-carbonate sub-unit» (559.75 – 496.09 m; Fig. 3-4).

In contrast to the carbonate measurements (bulk samples), the organic measurements were not always measured in metre resolution, depending on the variability of the expected isotope data. If no major isotope changes occur over longer stratigraphic successions, as can be expected in the middle part of the Opalinus Clay as well as from the Rothenfluh Member (Passwang Formation) up to the Hauptrogenstein, only every second sample (mainly 2 m interval) was analysed.

Lias Group

Starting from the bottom up (Fig. 3-2), the oldest sediments measured belong to the Early Jurassic (probably Late Pliensbachian). The lowermost three measurements (582.40 m, 582.20 m and 582.00 m) belong to the uppermost combined Grünschholz Member, Breitenmatt Member and Rickenbach Member. The following ones, between 581.90 m and 574.60 m, represent the upper two members of the Staffelegg Formation. They show larger variations in their individual data, which can be explained by the overall higher sampling resolution in the Lias Group (some intervals in the Rietheim Member with around 10 cm spacing) as well as by the nodular calcareous lithology of the Gross Wolf Member.

The semi-quantitative carbonate content (TCarb, Fig. 3-2) represents the lithological variations in the Rietheim Member and the hanging Gross Wolf Member up to the Opalinus Clay. In the Rietheim Member the TCarb values show an increasing trend from around 16 wt.-% to values slightly above 50 wt.-%. The interval between the base of the Rietheim Member and the «Unterer Stein» (581.93 – 581.10 m) clearly contains less carbonate than the hanging interval to the top of the Rietheim Member. The whole succession of the member is interrupted by higher values measured from the three calcareous interbeds in the middle part of the member («Unterer Stein»: 581.10 – 580.88 m, «Homogene Kalkbänke»: 580.59 – 580.32 m and «Oberer Stein»: 579.71 – 579.47 m). The uppermost calcareous interbed was not sampled (questionable «Monotisbank»: 576.66 – 576.63 m). The nomenclature of these beds is *sensu* Kuhn & Etter (1994). The TCarb data from these three beds is documented in Appendix E1 and marked by blue dots in the Fig. 3-2. The overlying Gross Wolf Member shows similar values as below, measured mostly from the marly sediment. The calcareous nodules to nodular beds clearly would show higher values, however they were not sampled in this study.

The $\delta^{13}\text{C}_{\text{carb}}$ values document at the base of the Rietheim Member a negative trend with the most negative value (-3.5 ‰ at 581.12 m) just below the «Unterer Stein». The negative trend is subsequently followed by a rapid increase. The most positive $\delta^{13}\text{C}_{\text{carb}}$ values thereafter were documented just above the «Oberer Stein» with 1.8 ‰ at 579.00 m. The values stabilise afterwards to the top of the Gross Wolf Member and show a continuous decreasing trend to around -1.7 ‰. The discussed negative excursion below the «Unterer Stein» represents one of the major Mesozoic negative carbon-isotope excursions (CIE) – the Toarcian-Oceanic Anoxic Event (T-OAE).

The negative CIE of the T-OAE can also be seen by the $\delta^{13}\text{C}_{\text{org}}$ values (Fig. 3-3). The most negative one, with a value of -32.5 ‰ at 581.40 m, is slightly lower than the most negative one from the $\delta^{13}\text{C}_{\text{carb}}$. The following rapid positive shift is also clearly documented in the organic matter, where the most positive value (-26.4 ‰) was measured between the «Homogene Kalkbänke» and the «Oberer Stein» at 579.92 m. The $\delta^{13}\text{C}_{\text{org}}$ curve shows great similarity with the data documented from the Riniken cores by Fantasia et al. (2018, 2019). The $\delta^{13}\text{C}_{\text{org}}$ values document at the very base of the Rietheim Member a fast shift to negative values, not like in BOZ1-1 where it is documented by an abrupt jump, probably indicating an erosive phase or a short time of condensation (Wohlwend et al. 2022).

The Rietheim Member is very bituminous and is itself defined by the occurrence of bituminous shale. The TOC as well as the C/N ratio (both Fig. 3-3) limit the range of the member. Both proxies show very increased values. The highest TOC value with 15.4 wt.-% was measured slightly below the «Unterer Stein» at 581.20 m. The average range of the semi-quantitative TOC content lies between 2.3 and 9.8 wt.-%, whereby the four calcareous beds were not analysed during this report. The hanging Gross Wolf Member has an obvious different lithological composition which is nicely documented by the very stable but much lower TOC content, which is clearly below 0.5 wt.-%.

The C/N ratios show the same trend as the TOC with the highest ratios measured contemporaneous with the bituminous lower and middle part of the Rietheim Member (ratios between 20 and 41), compared to the overlying Gross Wolf Member with a much lower C/N ratio (8 – 12). Such high C/N ratios, measured in the Rietheim Member, are normally rather unusual for marine organic matter, which usually has values between 5 and 8 (e.g. Emerson & Hedges 1988, Meyers 1997) and would therefore pretend that the organic material would be of terrigenous source. However, such high C/N ratios were also reported from mid-Pleistocene sapropels from the Tyrrhenian Basin (Meyers & Bernasconi 2005) which are also clearly produced by marine organic matter. Van Mooy et al. (2002) proposed a model for these very unusual C/N ratios in which they determined from sediment trap studies that suboxic microbial degradation via denitrification preferentially utilises nitrogen-rich amino acids and hence leaves a larger proportion of the nitrogen-poor organic matter components intact than under oxic conditions. C/N values of the surviving organic matter necessarily rise.

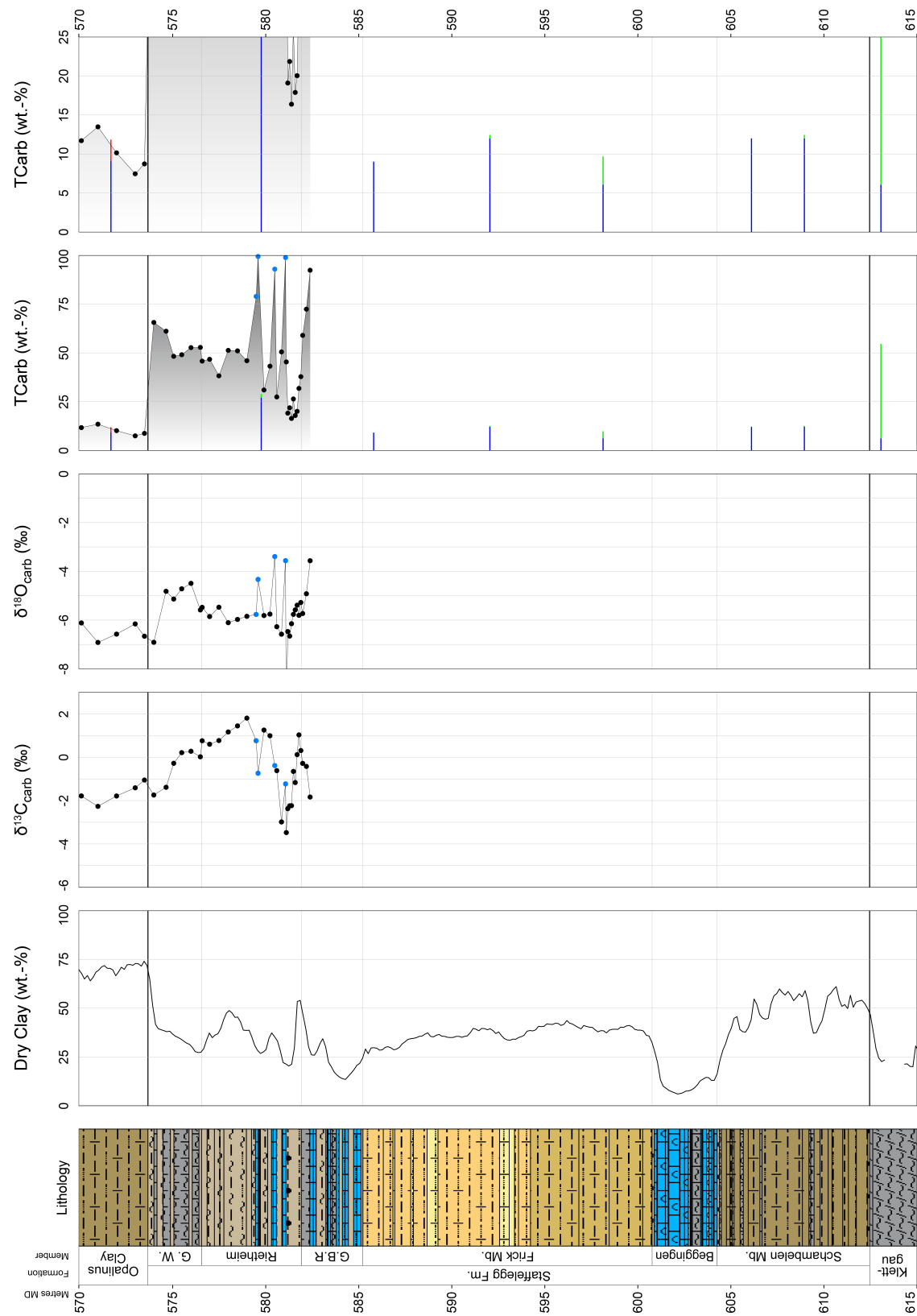


Fig. 3-2: Bulk rock (carbonate) isotopic data from the Lias Group
Geochemical data from 582.40 – 570.11 m, additional explanations and references see text at the beginning of Section 3.4.

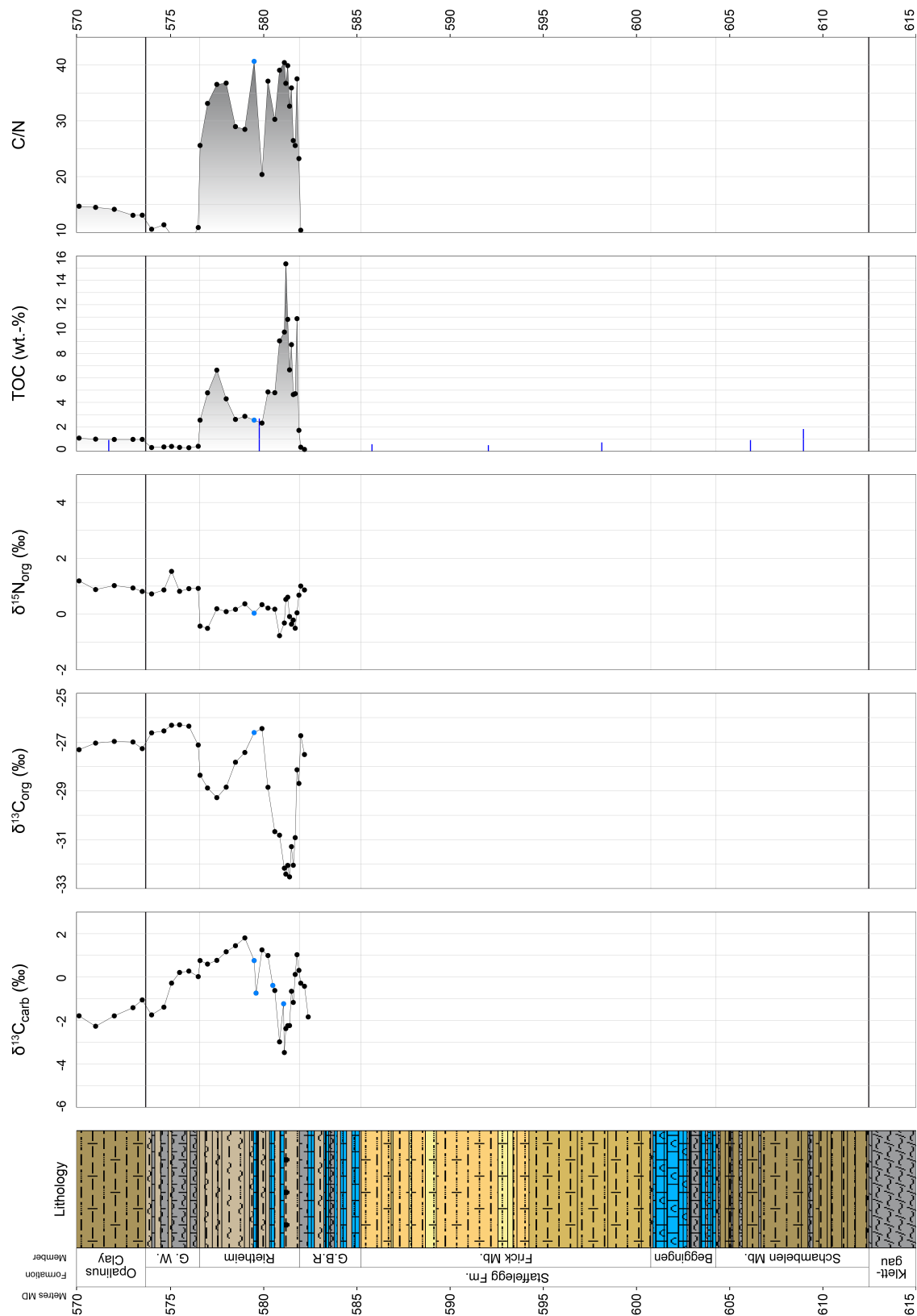


Fig. 3-3: Organic isotopic data from the Lias Group

Geochemical data from 582.40 – 570.11 m, additional explanations and references see text at the beginning of Section 3.4.

Lower part of the Dogger Group – mainly Opalinus Clay

The interval described in the following section, the lower part of the Dogger Group (the Opalinus Clay and the transition into the lower part of the Passwang Formation), is also the interval at the main focus of these investigations (Figs. 3-4 and 3-5).

The semi-quantitative carbonate content (TCarb) values from the more homogeneous clay mineral-dominated lithologies are rather low and very stable compared to those from the underlying Staffelegg Formation (Fig. 3-4). In the lowermost succession of the Opalinus Clay the average TCarb values decrease from around 14 wt.-% to values around 5 wt.-% at 556.00 m. Upsection, the TCarb documents a slightly increasing trend to values around 13 wt.-% at around 538.00 m (one more calcareous sample at 536.00 m with 22 wt.-%), followed by a decreasing trend up to the sample at 515.16 m, reaching again low TCarb values around 5 wt.-%. Between the two samples from 515.16 m to 514.06 m an obvious shift to more calcareous values is documented, reaching the highest values of 17 wt.-% at 498.00 m, almost at the top of the «Mixed clay-silt-carbonate sub-unit» (559.75 – 496.09 m). The above hanging «Upper silty sub-unit» (496.09 – 480.56 m) and the «Sub-unit with silty calcareous beds» (480.56 – 451.54 m) document several trends to increased carbonate contents. Two of them are clearly topped by calcareous beds (472.28 – 472.18 m and 467.56 – 467.28 m). The individual trends are then overlain by less calcareous sediments. In the hanging Passwang Formation, with the very thin «Condensed equivalents of the Sissach, Hauenstein and Hirnichopf Members» (451.54 – 450.53 m) and in the lowermost succession of the Waldenburg Member and lower part of the Brüggli Member, the TCarb values vary strongly due to the very different lithologies. Although, the very base of the Waldenburg Member and lower part of the Brüggli Member is clearly represented by a sediment interval with a very low carbonate content (around 5 wt.-% between 450.50 – 449.00 m).

The above-mentioned uppermost informal «Sub-unit with silty calcareous beds» comprises several calcareous beds, mainly firm- to hardgrounds (see Appendix E1 for data and Section 3.1 for microfacies description). Two of them are illustrated in Fig. 3-4 by thicker light blue lines ending with blue dots marking the TCarb values. Some of the analysed samples are classified as measurements from "hiatus concretions" and calcareous (one of them slightly sideritic) concretions. In addition, also several questionable septarian nodules (or just calcareous nodules) were measured, illustrated in violet. The calcareous beds comprise TCarb values that are typical for calcareous marl (50 – 75 wt.-%) and limestone (75 – 100 wt.-%). The lowermost calcareous concretions, or here questionable septarian nodules, between 564.42 m and 563.74 m (marked in violet), belong to a level in the «Clay-rich sub-unit» (573.68 – 559.75 m), which can be correlated over several boreholes and siting regions (e.g. BUL1-1: Wohlwend et al. 2021a; TRU1-1: Wohlwend et al. 2021b; BOZ1-1: Wohlwend et al. 2022).

The $\delta^{13}\text{C}_{\text{carb}}$ data reveal two negative CIE or intervals (Fig. 3-4): a lower CIE in the «Clay-rich sub-unit» and an upper CIE in the «Sub-unit with silty calcareous beds», maybe starting already in the upper part of the «Upper silty sub-unit». The lower negative CIE is represented by a clear decreasing trend, reaching the most negative value (-3.5 ‰ at 564.05 m) within the horizon with the calcareous (slightly sideritic) concretions or questionable septarian nodules between 564.42 m and 563.74 m. The above following overall increasing trend up to the upper part of the «Upper silty sub-unit» (up to 485.15 m) is only interrupted by the slightly positive shift between 554.00 m to 546.00 m with the most positive value at 551.00 m with a $\delta^{13}\text{C}_{\text{carb}}$ value of -0.7 ‰. The upper negative CIE shows around 1.5 ‰ more negative $\delta^{13}\text{C}_{\text{carb}}$ values and is somehow bounded by two calcareous beds below and above (less prominent then in BOZ1-1; Wohlwend et al. 2022). The two bounding calcareous beds are located at: 480.56 – 479.94 m and 467.42 – 467.28 m (cf. Dossier III). From 467.00 m to the top of the Opalinus Clay the $\delta^{13}\text{C}_{\text{carb}}$ values show again a slightly increasing trend, reaching the most positive value in the uppermost sub-unit just below the top of the Opalinus Clay (+0.3 ‰ at 452.00 m). Crossing the lithological boundary to the

hanging Passwang Formation, the overlying hardground documents an even more positive $\delta^{13}\text{C}_{\text{carb}}$ value (+1.1 ‰ at 451.50 m). The $\delta^{13}\text{C}_{\text{carb}}$ data, analysed from the interval with the very low carbonated content at the base of the Waldenburg Member and lower part of the Brüggli Member (450.50 – 449.00 m), start again by lower $\delta^{13}\text{C}_{\text{carb}}$ values, documenting then an increasing trend in the following 4 m (-1.5 ‰ at 451.00 m to +1.1 ‰ at 447.00 m).

The $\delta^{13}\text{C}_{\text{carb}}$ data from the calcareous beds and/or bored and reworked intraclasts document possibly an early diagenetic signal (e.g. Wetzel & Allia 2000). The calcareous concretions to questionable septarian nodules are the only macroscopic features with very negative $\delta^{13}\text{C}_{\text{carb}}$ values (-12.9 to -27.5 ‰, Appendix E1). However, very fine authigenic calcite was probably also precipitated in the very fine primary porosity of the Opalinus Clay, which would lead to the more negative $\delta^{13}\text{C}_{\text{carb}}$ values in the lower and upper negative excursions, discussed above (see also Wohlwend et al. 2016.).

The $\delta^{13}\text{C}_{\text{org}}$ data (Fig. 3-5) show a different picture compared to the $\delta^{13}\text{C}_{\text{carb}}$ values. The curve is in the main part relatively stable. The Opalinus Clay succession can be subdivided, based on $\delta^{13}\text{C}_{\text{org}}$ values, into three subintervals: The lowermost interval (573.50 – 560.00 m) can be described from the base of Opalinus Clay with a slight increasing trend followed by an abrupt negative shift, reaching the most negative value at 561.00 m with -28.5 ‰. The middle interval follows from 559.00 m to 514.06 m. The interval documents a very gradual increasing trend from -26.9 ‰ to -26.5 ‰. The uppermost interval (512.00 – 452.00 m) can be described by a gradual decreasing trend, a part with lower values (504.00 – 490.00 m around -27 ‰), followed by an increasing trend to the top of the Opalinus Clay. The increasing part is interrupted by a positive $\delta^{13}\text{C}_{\text{org}}$ value with -26.1 ‰ at 466.00 m. Crossing the lithological boundary to the hanging Passwang Formation, the $\delta^{13}\text{C}_{\text{carb}}$ values jump from -26.3 ‰ at 452.00 m to -25.8 ‰ just above at 451.00 m. The lithological boundary is therefore also nicely visible by the clear shift in the $\delta^{13}\text{C}_{\text{org}}$ data between the values below (top Opalinus Clay) and above from the Passwang Formation.

The TOC as well as the C/N ratio will be discussed in the same paragraph. Both proxies document rather stable conditions throughout the lower part of the Opalinus Clay up to 494.00 m (TOC: around 1 wt.-%, C/N ratio between 12 and 14). Only one exception has to be mentioned at 561.00 m (TOC: 1.4 wt.-%, C/N: 15.4). From 492.00 m upwards, both proxies start to vary more. The obvious largest shift in the C/N ratio is documented from the sediment below to above the uppermost calcareous bed (467.56 – 467.28 m). There, the C/N ratio jumps from 17 (468.00 m) to a ratio close to 24 (467.00 m). A similar obvious jump can also be observed by the TOC content, although the jump is slightly higher in stratigraphy between the samples 466.00 m (0.6 wt.-%) to 465.00 m (1.5 wt.-%). The TOC as well as the C/N ratios document a clear change in the sediment input to the hanging Passwang Formation.

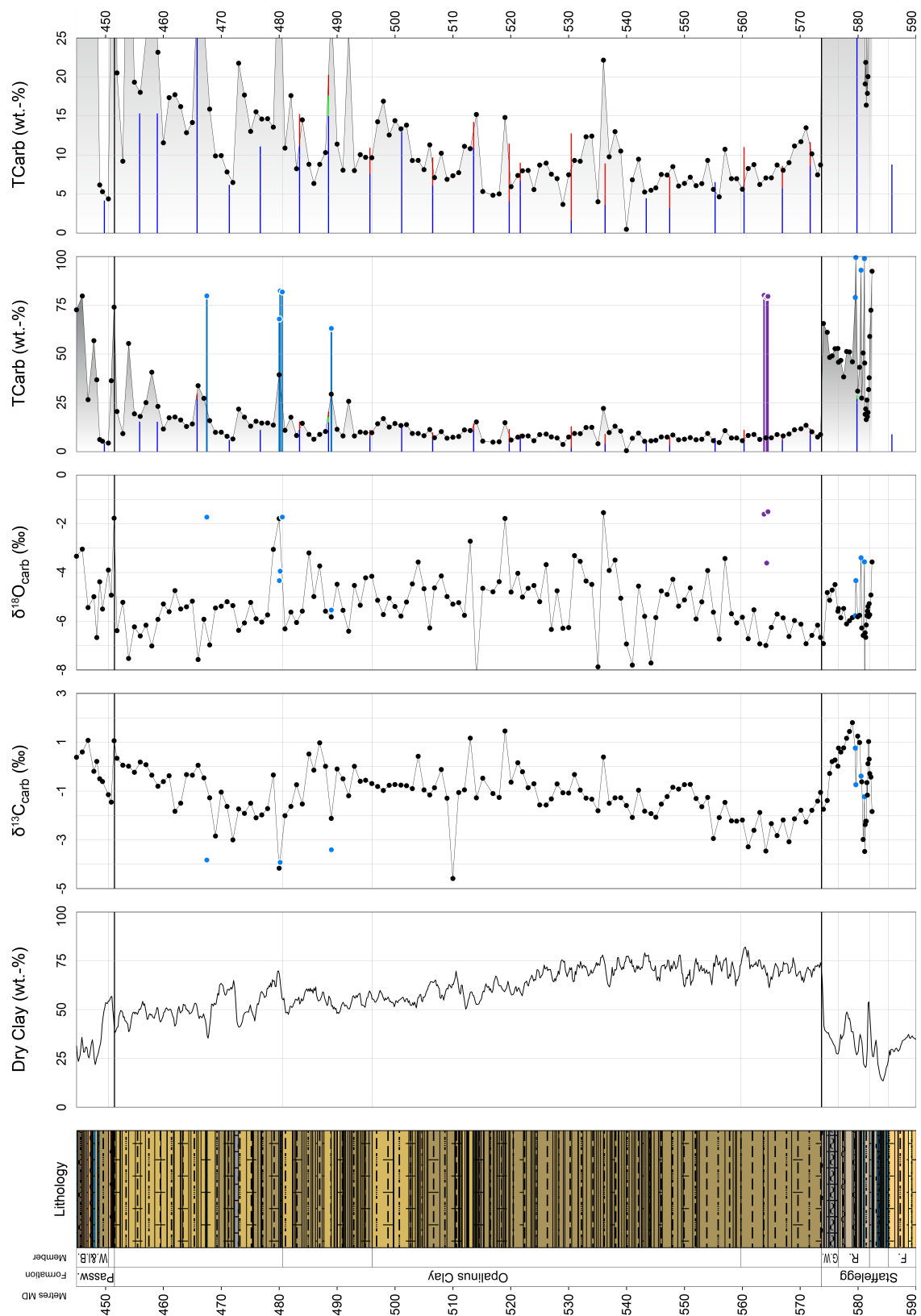


Fig. 3-4: Bulk rock (carb.) isotopic data from the lower Dogger Group – mainly Opalinus Clay
 Geochemical data from 582.40 – 445.00 m, additional explanations and references see text
 at the beginning of Section 3.4.

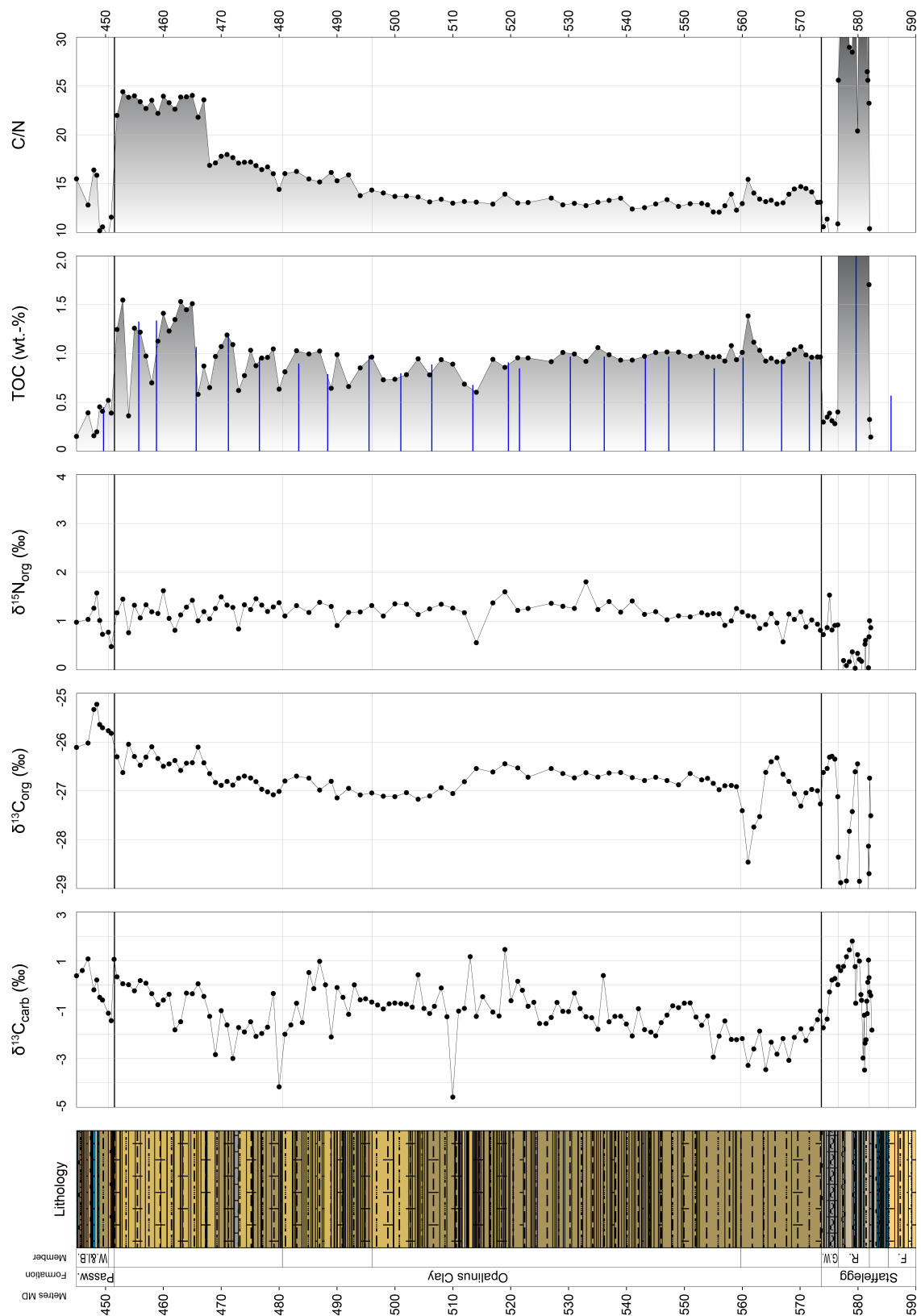


Fig. 3-5: Organic isotopic data from the lower Dogger Group – mainly Opalinus Clay
 Geochemical data from 582.40 – 445.00 m, additional explanations and references see text at the beginning of Section 3.4.

Upper part of the Dogger Group

The following described interval, the upper Dogger Group (Passwang Formation, Hauptrogenstein, Ifenthal Formation and Wildegge Formation), covers in time the whole Middle Aalenian to Middle Oxfordian substages (Figs. 3-6 and 3-7).

The semi-quantitative TCarb (Fig. 3-6) represents the alternation of silty claystone, argillaceous to calcareous marl and limestone in the upper part of the Dogger Group. The here documented TCarb contents represent clearly the most calcareous succession in comparison to other locations from the same age interval (e.g. MAR1-1: Wohlwend et al. 2019c, BOZ1-1: Wohlwend et al. 2022). BOZ2-1 was cored (same as BOZ1-1) in the Celtic ("Rauracian") facies of the Dogger (calcareous facies) in comparison to the more eastern location, which were cored in the Swabian facies (basinal facies equivalent). The TCarb curve reflects quite nicely the inverse DryClay content curve (*cf.* Dossier X) and thus documents the varying lithologies from the Passwang Formation with many calcareous interbeds to the hanging carbonate-rich platform sediments from the Hauptrogenstein.

Based on the TCarb content (same as in BOZ1-1: Wohlwend et al. 2022), the lower part of the Passwang Formation (below the «Humphriesi-Schichten») can be divided into three subintervals, representing three different lithologies: The lowermost one is characterised by the very low carbonated content at the base of the Waldenburg Member and lower part of the Bruggli Member (450.50 – 449.00 m). The second or middle one (448.50 – 432.00 m) includes several calcareous marl to limestone beds in an argillaceous to silty marl. The large scatter in the TCarb data can be explained by random sampling of calcareous interbeds and argillaceous to marly intervals (background sediment). The sampling spacing was strictly one metre not to generate an artefact by only measuring one lithology. The third interval (430.98 – 425.00 m) is marked by very low carbonate contents of around 5 – 20 wt.-%. However, one calcareous measurement stands out (68 wt.-% at 429.00 m) belonging to the uppermost of three limonitic, maybe slightly iron-oolitic limestone beds (429.95 – 428.90 m). Thereafter, TCarb data follow nicely the lithological description (*cf.* Dossier III). The hanging «Humphriesi-Schichten» as well as the Rothenfluh Member differ from the lying successions. The «Humphriesi-Schichten» document a more calcareous succession overlain by argillaceous marl of the Rothenfluh Member. The transition to the hanging Hauptrogenstein is documented by a trend to more and more calcareous lithologies from argillaceous to calcareous marl. The Hauptrogenstein is very calcareous and remains from 360.06 m upsection almost exclusively above 90 wt.-% until 334.83 m and is therefore significantly more calcareous than BOZ1-1 (Wohlwend et al. 2022). The uppermost interval of the Hauptrogenstein (334.83 – 308.70 m) is represented by slightly lower carbonate contents, also nicely recognisable in the DryClay content curve.

As already mentioned above, the $\delta^{13}\text{C}_{\text{carb}}$ data (Figs. 3-6 and 3-7) show an overall positive trend from the top of the Opalinus Clay upsection. This trend is interrupted by six analyses from the «Humphriesi-Schichten» with $\delta^{13}\text{C}_{\text{carb}}$ values close to 0 ‰. The trend toward more positive values continues steadily before stabilising in the lower part of the Hauptrogenstein with values slightly above 2.0 ‰. Approximately around 344.98 m, the $\delta^{13}\text{C}_{\text{carb}}$ data shift again to more negative values, reaching a first negative minimum at 330.02 m (+0.7 ‰) followed by a second negative trend in the uppermost part of the Hauptrogenstein with the lowest value at 311.00 m (+0.6 ‰). In the uppermost part of the Ifenthal Formation (+0.7 ‰ at 305.00 m and +1.8 ‰ at 304.00 m) to the hanging Wildegge Formation (+2.7 ‰ at 303.83 m), a jump by +2 ‰ is documented. The striking positive shift of +2 ‰ to values around +2.7 ‰ is typical for the Callovian/Oxfordian boundary and was already documented by Rais et al. (2007) in other locations and the Weiach borehole and was for example also documented in the BUL1-1 borehole (Wohlwend et al. 2021a). The most positive $\delta^{13}\text{C}_{\text{carb}}$ values found by Rais et al. (2007) are from the Middle Oxfordian (Transversarium Zone).

The $\delta^{13}\text{C}_{\text{org}}$ data (Fig. 3-7) show a somehow similar overall increasing trend throughout the lower part of the Passwang Formation as discussed above for the $\delta^{13}\text{C}_{\text{carb}}$ data. The positive shift ends in a prominent positive peak of -24.0 ‰ at 427.89 m. The $\delta^{13}\text{C}_{\text{org}}$ values thereafter decrease through the «Humphriesi-Schichten» into the Rothenfluh Member. The same evolution was already described from the BOZ1-1 core (Fig. 3-7; Wohlwend et al. 2022). However, in BOZ1-1 the negative trend can be followed until the Klingnau Formation. In BOZ2-1 the $\delta^{13}\text{C}_{\text{org}}$ data document already in the lower part of the Hauptrogenstein a reversal, documenting a slightly increasing trend up to 336.09 m, followed by a clear shift to lower values around -27 ‰.

The uppermost four samples, taken from the Hauptrogenstein (313.88 m, 312.00 m, 309.88 m and 309.00 m) and subordinate also in the «Humphriesi-Schichten» (422.00 m), document a strange positive peak or "excursion", marked in Fig. 3-7 by dashed lines. Similar strange positive values in the $\delta^{13}\text{C}_{\text{org}}$ data were also analysed at the same stratigraphic interval («Spatkalk») of the Hauptrogenstein and subordinate also in the «Humphriesi-Schichten») in BOZ1-1 (Wohlwend et al. 2022). There the samples were taken, like the ones here in BOZ2-1, from very reddish, iron-oolitic and limonitic intervals. Like in BOZ1-1, the samples in question (also including two additional ones at 427.89 m and 304.00 m), have been decarbonised a second time for 12 h, but this time at 70 °C. The additional remeasurements document lower $\delta^{13}\text{C}_{\text{org}}$ values (marked by open data points and connected with solid lines). Therefore, the assumption of incomplete decarbonisation of ankerite and/or other iron-carbonates thus seems to be confirmed.

Finally, the $\delta^{13}\text{C}_{\text{org}}$ data also document the striking positive shift close to the Callovian/ Oxfordian boundary from -26.7 ‰ at 305.00 m to -23.9 ‰ at 303.90 m. The shift is almost +3 ‰.

The semi-quantitative TOC content is in principle below 0.5 wt.-%, reaching never more than 0.8 wt.-% from the Passwang Formation to the Wildegg Formation. The lowest TOC values were documented from the lower part of the Passwang Formation (lower succession of the Waldenburg Member and lower part of the Brüggli Member).

The C/N ratios document very nicely a gradual shift from the Passwang Formation into the lower part of the Hauptrogenstein, reaching the highest ratio of 22 at 344.98 m. The lower boundary of the informal interval of the «Movelier Beds» and «Spatkalk» is clearly marked by an abrupt shift to much lower C/N ratios (ratio of 13 at 334.00 m). Similar to the analyses in BOZ1-1 (Wohlwend et al. 2022), the shift from ratios around 22 to around 13 could document a change in facies to more marine or more basinal (less terrigenous). This could therefore indicate a transgressive phase.

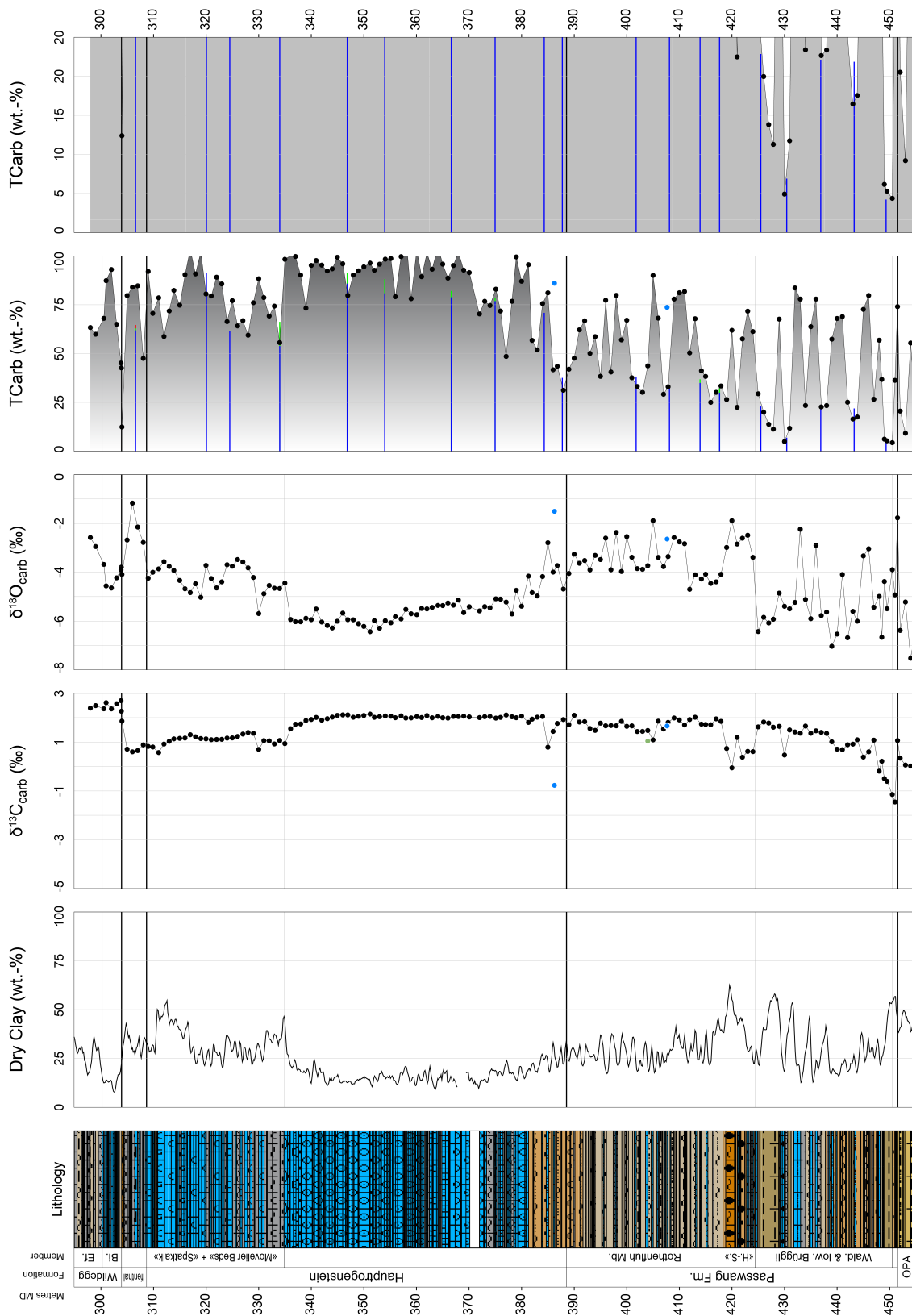


Fig. 3-6: Bulk rock (carbonate) isotopic data from the upper part of the Dogger Group
 Geochemical data from 445.00 – 298.00 m, additional explanations and references see text at the beginning of Section 3.4.

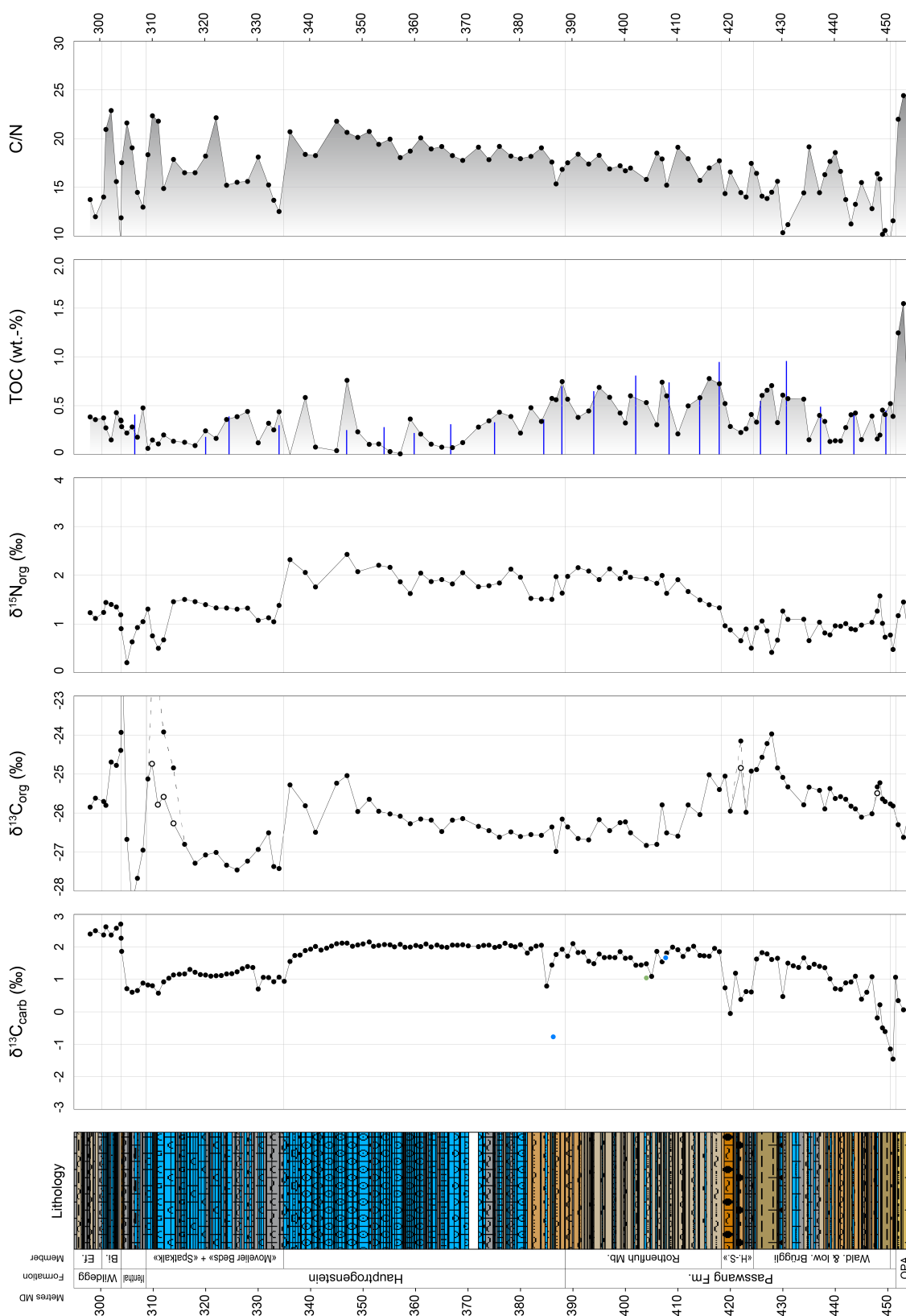


Fig. 3-7: Organic isotopic data from the upper part of the Dogger Group

Geochemical data from 445.00 – 298.00 m, additional explanations and references see text of Section 3.4.

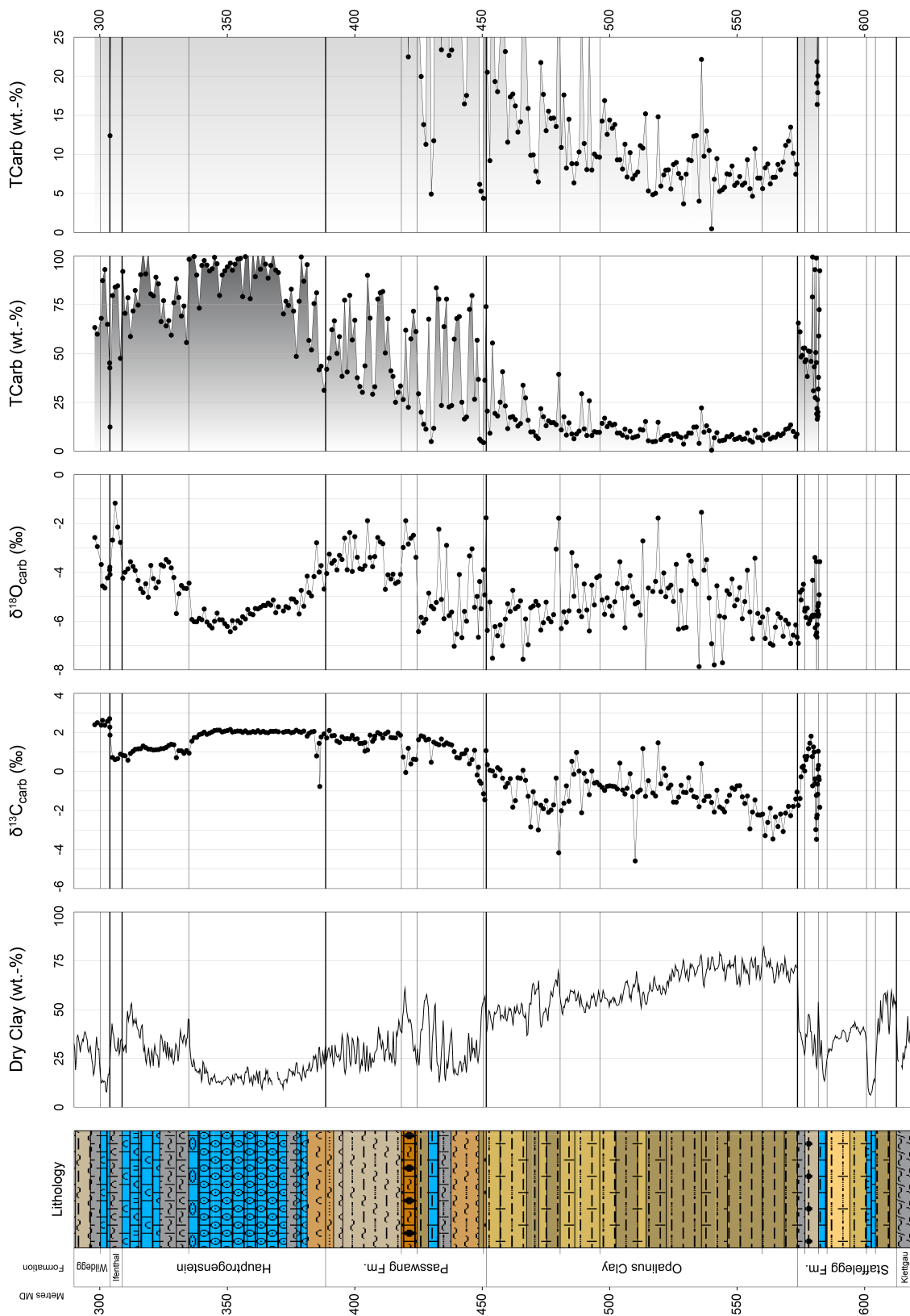


Fig. 3-8: Whole bulk rock (carbonate) isotopic data from BOZ2-1

Geochemical data from 582.40 – 298.00 m, additional explanations and references see text at the beginning of Section 3.4.

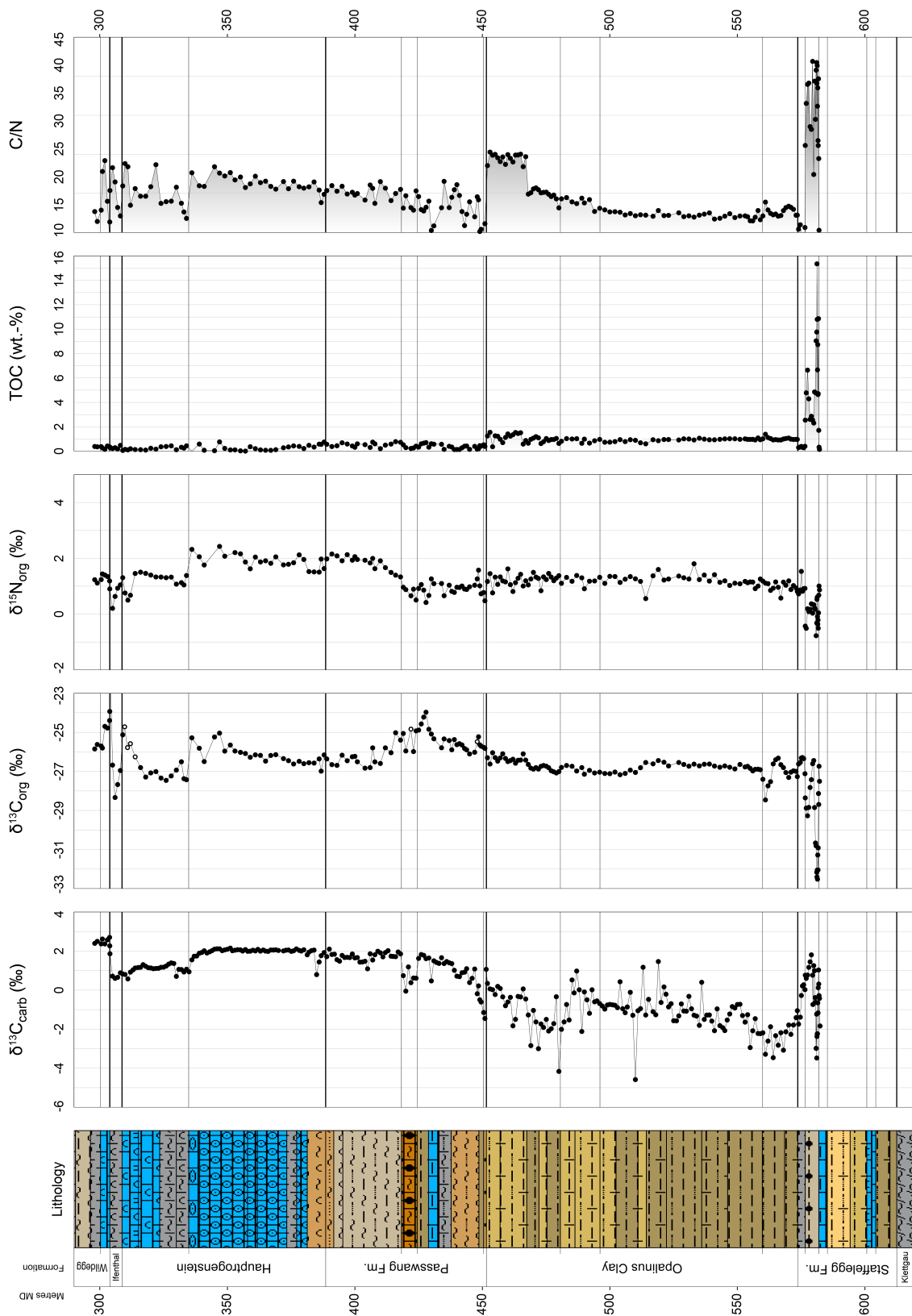


Fig. 3-9: Whole organic isotopic data from BOZ2-1

Geochemical data from 582.40 – 298.00 m, additional explanations and references see text at the beginning of Section 3.4.

4 Definition of specific lithostratigraphic boundaries

The boundaries between stratigraphical units, as also shown in the stratigraphical logs of the lithostratigraphy report (Dossier III), were mostly defined by using lithological criteria. According to the guidelines on stratigraphical nomenclature of Remane et al. (2005), the definition of lithostratigraphical units should be based, both vertically and horizontally, on lithological variations regardless of their age. In fact, the formation boundaries, as used by Nagra for the ongoing borehole campaign of Stage 3 of the Sectoral Plan for Geological Repositories (Jordan & Deplazes 2019), were not always obvious in the borehole and definitions were difficult to apply, either because of the small core diameter or because of differences in facies. The exact location of some of the formation boundaries caused discussions during core description and the process of quality control. Most of the important data for questionable boundaries were already present before the data-freeze (02.03.2021) and were used for the log descriptions and drawings. In the following paragraphs, the underlying considerations are explained for providing a better understanding of how boundaries were demarcated. We are aware of the fact that several boundaries are no longer based on lithological criteria alone and that chronostratigraphic criteria (ammonite, palyno- and chemostratigraphy) are included in the definitions.

Opalinus Clay (573.68 – 451.54 m)

The *lower boundary* of the Opalinus Clay is set at 573.68 m at the uppermost surface of a fossiliferous argillaceous and calcareous marl succession from the underlying Staffelegg Formation (*cf.* Dossier III). The lithological boundary is therefore evident above all in the carbonate content (TCarb: Figs. 3-2 and 3-4). The value decreases from 66 wt.-%, measured from the uppermost sample (574.00 m) of the Gross Wolf Member, to values between 8 and 14 wt.-% in the basal Opalinus Clay (Fig. 3-2). The lithological change between the Gross Wolf Member and the Opalinus Clay is also visible in the slight increase in TOC from values < 0.5 wt.-% to values around 1 wt.-% in the Opalinus Clay (Fig. 3-5). The described ammonites (Section 3.2) document that the lithological boundary is very close to the Toarcian / Aalenian stage boundary. The uppermost ammonite (*Pleydellia* sp.) from the Gross Wolf Member, taken at 574.21 m, yields Aalensis Zone. The lowermost ammonite (*Leioceras* ex gr. *subglabrum*) from the Opalinus Clay from 573.58 m can be dated as Opalinum Zone (Opalinum Subzone).

The *upper boundary* of the Opalinus Clay is set at 451.54 m at the base of the overlying very condensed succession of iron-oolites and limestone (iron-oolitic) interval with many dark reddish encrusted intraclasts and iron-stromatolites (451.54 – 450.53 m) (*cf.* Dossier III). Placing the boundary at this level was not based on lithological reasons alone. The claystone (silty) from 450.53 m to 448.92 m, which directly overlays the condensed succession with iron-oolid, cannot clearly be distinguished from intervals from the upper part of the Opalinus Clay. Iron-oolids alone are not a reliable indication of the definition, because they have already been identified in several beds in the Opalinus Clay (e.g. BUL1-1; Wohlwend et al. 2021a). However, the TCarb measurement from the sample 450.50 m documents a very low carbonate content of only 4.4 wt.-%, which is also compared to the upper part of the Opalinus Clay very low. The boundary was also placed at this level by comparison with the newly adapted stratigraphy in the Rinken borehole and other outcrops of the Jura Ost siting region (Wohlwend et al. 2019a). A similar condensed bed from the Wasserflue outcrop (Wohlwend et al. 2019a), where palynological samples and ammonites were taken directly from the hardground, has given an age from the Bradfordensis to Concavum Zone. The cores from BOZ1-1 shows almost the same succession (Wohlwend et al. 2022).

In BOZ2-1 no ammonites were determined from the upper part of the Opalinus Clay. However, the palynological sample, taken from the uppermost part of the Opalinus Clay at 451.65 m, documents with the LADs of *Scrinocassis weberi* and *Wallodinium laganum* to be at the top of the Opalinus Zone, probably Bifidatum Subzone. From the hanging succession at 451.19 m an incomplete, truncated specimen of a Graphoceratidae indet. was described yielding probably Concavum Zone?. Residual material from the preparation of that specimen was used as a palynological sample. The quantitative analysis documents the presence of *Dissiliodinium* aff. *giganteum* and *Nannoceratopsis* sp. B. Both have their FADs in the Discites Zone.

These biostratigraphic findings confirm the correlation to similar beds in the Jura Ost siting region. Placing the boundary at this level therefore fits the lithological as well as the biostratigraphical description of the base of the Passwang Formation by Burkhalter (1996) and the new findings by Wohlwend et al. (2019a).

The positive chemostratigraphic shift or even jump with an amplitude of around +0.5 ‰ in the $\delta^{13}\text{C}_{\text{org}}$ values, discussed above in Section 3.4, also fits to similar shifts found in the same intervals (e.g. Wohlwend et al. 2021a).

Passwang Formation (451.54 – 388.54 m)

The *lower boundary* of the Passwang Formation is set at 451.54 m at the base of the very condensed succession of iron-oolites and limestone (iron-oolitic) interval with many dark reddish encrusted intraclasts and iron-stromatolites (451.54 – 450.53 m) (cf. Dossier III). The hard-ground, as already discussed above, covers several ammonite zones. The palynological sample, taken from the uppermost part of the underlying Opalinus Clay at 451.65 m is dated Opalinus Zone (probably Bifidatum Subzone). The incomplete, truncated specimen of a Graphoceratidae indet. from the discussed condensed bed at 451.19 m yields probably Concavum Zone?. The palynological sample from the residual material is interpreted as Discites Zone.

The original definition of the individual members of the Passwang Formation (Burkhalter 1996) would indicate that the condensed succession (451.54 – 450.53 m) covers the equivalent sedimentation time of the Sissach Member to possibly Hirnichopf Member. Therefore, the bed was named «**Condensed equivalents of the Sissach, Hauenstein and/or Hirnichopf Members**». This condensation fits into the regional expression of the evolution during that time in the Jura Ost siting region (Wohlwend et al. 2019a).

The **Waldenburg Member and lower part of Brüggli Member** was combined during the work of Wohlwend et al. (2019a) by several reasons. The lithological separation into two individual members is especially for the Jura Ost siting region not feasible. Although, the lithological expression fits with the observed and studied outcrops. The *lower boundary*, as discussed above, is set at the top of the condensed succession at 450.53 m. The *upper boundary* is set at 424.40 m at the only pure lithological defined boundary to the «Humphriesi-Schichten». The onset of the iron-oolites and limonitic components define the boundary. Dating with palynomorphs yields for the informally combined interval Discites Zone to Sauzei Zone.

The «**Humphriesi-Schichten**» are purely defined on lithological criteria with the on- and offset of iron-oolites and/or limonitic components (Burkhalter 1996). The *lower boundary* is set at 424.40 m and the *upper boundary* at 418.30 m (cf. Dossier III). The two ammonites, from this interval, are both incomplete and truncated specimens in steinkern preservation. The lower one at 420.28 m (*Dorsetensia* sp.), is typical for the Romani Subzone? of the Humphriesianum Zone. The upper one at 419.23 m (*Itinsaites* sp.?) indicates a slightly younger age (Humphriesianum Subzone of the Humphriesianum Zone). The palynological samples taken at 424.08 m, 422.39 m and 418.68 m are interpreted as Sauzei to Humphriesianum Zone (Blagdeni Subzone).

The **Rothenfluh Member**, in the hanging of the iron-oooid-rich interval, is set with the *lower boundary* at the offset of the iron-oooids and/or limonitic components at 418.30 m (*cf.* Dossier III). The *upper boundary*, which is as well the upper boundary of the Passwang Formation, is defined at the base of the lowermost, more than 10 cm thick bed containing (calcitic) oooids from the hanging Hauptrogenstein. The boundary was set therefore at the base of the oolitic bed at 388.54 m (*cf.* Dossier III). Individual (calcitic) oooids are already found little below it. The age of the Rothenfluh Member can be ranged by a palynological sample (418.18 m) and a fragment of a *Teloceras* sp.? (411.92 m), both from the Blagdeni Subzone of the Humphriesianum Zone. The upper part (409.94 – 388.82 m) is interpreted palynologically as Niortense – Garantiana Zone.

Hauptrogenstein (388.54 – 308.70 m)

The drilling BOZ2-1 is situated in the transition area between the carbonate platform of the Hauptrogenstein in the west and the more basinal Klingnau Formation in the east. The two formations are interlocking and therefore a separation is not always straightforward. The BOZ2-1 drilling is more to the west than BOZ1-1 and Riniken and therefore also more proximal to the carbonate platform, which is documented by the clearly more calcareous facies (Fig. 3-6). The bioclastic calcareous marl, which is found above 334.83 m, does not reach a total thickness of more than 15 m, which serves as a criterion for the delimitation of the Klingnau Formation (see discussion of the Klingnau Formation in BOZ1-1 in Wohlwend et al. 2022). Therefore, the whole succession from 388.54 m to 308.70 m was defined as Hauptrogenstein.

The *lower boundary* is set at the base of the lowermost more than 10 cm thick oolitic bed at 388.54 m (*cf.* Dossier III). The onset of calcareous oooids goes hand in hand with a marked decrease in the TCarb value to around 31 wt.-% at 387.95 m (Fig. 3-6) followed by a clear increase to higher TCarb values in the lower part of the Hauptrogenstein. In addition, the TOC content and C/N ratio (Fig. 3-7) also mimic this lithological transition with a very fine but noticeable excursion in both plots just above the lithological boundary.

The *upper boundary* is documented by an erosive hardground with reworking lithoclasts at 308.70 m, separating an overlying bioclastic limestone from a limestone grading downwards into bioclastic limestone (limonitic) with some iron-oooids (*cf.* Dossier III).

The age of the Hauptrogenstein, as it is lithologically defined in BOZ2-1, is dated by palynological samples from the Niortense – Garantiana Zone to the Zigzag (Tenuplicatus Subzone) – Hodsoni Zone. The lithological subboundary in the Hauptrogenstein between the lower part of the Hauptrogenstein and the informal part of the «Movelier Beds» and «Spatkalk» (334.83 m) coincides with the ammonite zone boundary between the Niortense – Garantiana Zone (335.49 m) and the Parkinsoni Zone (334.07 m). Just above begins with the next palynological sample at 330.57 m the Zigzag Zone of the Early Bathonian. This sample was taken from a limonitic, bioclastic limestone bed (330.94 – 329.97 m) with few iron-oooids (thin section BOZ2-1-330.66). A similar lithological succession of calcareous marl with limonitic bioclasts and limonitic pellets is documented in BOZ1-1 (437.90 – 435.84 m), coinciding also with the Parkinsoni to Zigzag Zone boundary (Wohlwend et al. 2022). As already outlined in the report for BOZ1-1, the beds described in there show lithological similarities to the condensed beds from the profile Acheberg – Klingnau (bed 34 to 38; Wohlwend et al. 2019a). There, the ammonites from the Parkinsoni Zone (Acris and Truellei Subzones) allow a correlation with either one or both «Parkinsonien Beds» by Schmassmann (1945). As it is described in the lithostratigraphic report from BOZ2-1 (Dossier III, Fig. 3-1), the interval from 334.83 m to 329.97 m seems to be associated to the «Movelier Beds» from the nearby Sulz – Cheisacher Profile of Schmassmann (1945).

5 Conclusion

The present study documents data on microfacies analysis, ammonite stratigraphy and palynostratigraphy as well as detailed geochemical analyses (C, O and N isotopes). With this data collection, it was possible to predict the delimitation of the Mesozoic strata more accurately. Most of the important data for the boundaries in question were already present at the data-freeze (02.03.2021). Therefore, the present report complements the lithostratigraphic report of Dossier III for the deep borehole Bözberg-2-1. The lithological boundaries, and therefore the stratigraphic profile, were mostly defined by lithological criteria. Nevertheless, the customary formal and informal formation boundaries were not always obvious in the drill cores, either because of the small core diameter or changing facies conditions. The exact location of specific formation boundaries led to discussions requiring additional data to determine the exact profile description and illustration. We are aware that certain boundaries are thus no longer based solely on lithological criteria, and that the definitions therefore also include chronostratigraphic criteria (ammonite stratigraphy, palyno- and chemostratigraphy).

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Appendix A: List of all samples

Appendix A1:	List of all thin sections from BOZ2-1 (820.31 – 309.57 m).....	A-2
Appendix A2:	List of all sampled macrofossils from BOZ2-1 (573.71 – 419.23 m).....	A-3
Appendix A3:	List of other provisionally determined conspicuous macrofossils from BOZ2-1 (608.02 – 301.71 m).....	A-4
Appendix A4:	List of all palynological sample from BOZ2-1 (573.93 – 300.68 m).....	A-5

Appendix A1: List of all thin sections from BOZ2-1 (820.31 – 309.57 m)

For the description and individual counting of the thin sections see Section 3.1; selected photos can be found in Appendix B.

Top [m]	Bottom [m]	Avg. depth [m]	Formation	Retrieval date [dd.mm.yyyy]	Sample ID
309.55	309.59	309.57	Hauptrogenstein	14.12.2021	BOZ2-1-309.57-TS
312.91	312.95	312.93	Hauptrogenstein	14.12.2021	BOZ2-1-312.93-TS
319.81	319.85	319.83	Hauptrogenstein	14.12.2021	BOZ2-1-319.83-TS
330.00	330.04	330.02	Hauptrogenstein	14.12.2020	BOZ2-1-330.02-TS
330.64	330.68	330.66	Hauptrogenstein	14.12.2020	BOZ2-1-330.66-TS
333.18	333.21	333.20	Hauptrogenstein	14.12.2020	BOZ2-1-333.20-TS
334.96	335.00	334.98	Hauptrogenstein	14.12.2020	BOZ2-1-334.98-TS
336.07	336.11	336.09	Hauptrogenstein	14.12.2020	BOZ2-1-336.09-TS
340.92	340.96	340.94	Hauptrogenstein	14.12.2020	BOZ2-1-340.94-TS
341.61	341.65	341.63	Hauptrogenstein	14.12.2020	BOZ2-1-341.63-TS
355.13	355.17	355.15	Hauptrogenstein	14.12.2020	BOZ2-1-355.15-TS
357.88	357.92	357.90	Hauptrogenstein	27.11.2020	BOZ2-1-357.90-TS
375.09	375.13	375.11	Hauptrogenstein	14.12.2020	BOZ2-1-375.11-TS
407.64	407.69	407.67	Passwang Fm.	14.12.2020	BOZ2-1-407.67-TS
419.26	419.29	419.28	Passwang Fm.	14.12.2020	BOZ2-1-419.28-TS
420.57	420.60	420.59	Passwang Fm.	14.12.2020	BOZ2-1-420.59-TS
422.65	422.69	422.67	Passwang Fm.	14.12.2020	BOZ2-1-422.67-TS
429.41	429.45	429.43	Passwang Fm.	12.01.2021	BOZ2-1-429.43-TS
432.85	432.89	432.87	Passwang Fm.	12.01.2021	BOZ2-1-432.87-TS
441.71	441.75	441.73	Passwang Fm.	12.01.2021	BOZ2-1-441.73-TS
447.76	447.80	447.78	Passwang Fm.	12.01.2021	BOZ2-1-447.78-TS
448.79	448.83	448.81	Passwang Fm.	12.01.2021	BOZ2-1-448.81-TS
451.81	451.85	451.83	Opalinus Clay	12.01.2021	BOZ2-1-451.83-TS
467.41	467.45	467.43	Opalinus Clay	12.01.2021	BOZ2-1-467.43-TS
485.50	485.53	485.52	Opalinus Clay	12.01.2021	BOZ2-1-485.52-TS
581.06	581.10	581.08	Staffellegg Fm.	12.01.2021	BOZ2-1-581.08-TS
624.41	624.44	624.43	Klettgau Fm.	10.03.2021	BOZ2-1-624.43-TS
635.45	635.49	635.47	Klettgau Fm.	10.03.2021	BOZ2-1-635.47-TS
684.73	684.76	684.75	Bänkerjoch Fm.	10.03.2021	BOZ2-1-684.75-TS
700.74	700.77	700.76	Bänkerjoch Fm.	10.03.2021	BOZ2-1-700.76-TS
712.54	712.57	712.56	Bänkerjoch Fm.	10.03.2021	BOZ2-1-712.56-TS
744.60	744.63	744.62	Bänkerjoch Fm.	10.03.2021	BOZ2-1-744.62-TS
748.31	748.35	748.33	Schinz nach Fm.	10.03.2021	BOZ2-1-748.33-TS
798.15	798.19	798.17	Schinz nach Fm.	10.03.2021	BOZ2-1-798.17-TS
820.29	820.33	820.31	Schinz nach Fm.	10.03.2021	BOZ2-1-820.31-TS

Appendix A2: List of all sampled macrofossils from BOZ2-1 (573.71 – 419.23 m)

For the definitive determination of the individual macrofossils see Section 3.2 (Tab. 3-2).

Top [m]	Bottom [m]	Sample depth [m]	Formation	Retrieval date [dd.mm.yyyy]	Sample ID
419.20	419.26	419.23	Passwang Fm.	14.12.2020	BOZ2-1-419.23-BS(MF)
420.26	420.30	420.28	Passwang Fm.	14.12.2020	BOZ2-1-420.28-BS(MF)
451.17	451.21	451.19	Opalinus Clay	12.01.2021	BOZ2-1-451.19-BS(MF)
548.06	548.09	548.09	Opalinus Clay	12.01.2021	BOZ2-1-548.09-BS(MF)
548.66	548.68	548.68	Opalinus Clay	12.01.2021	BOZ2-1-548.68-BS(MF)
548.81	548.85	548.85	Opalinus Clay	12.01.2021	BOZ2-1-548.85-BS(MF)
563.575	563.60	563.60	Opalinus Clay	12.01.2021	BOZ2-1-563.60-BS(MF)
573.56	573.58	573.58	Opalinus Clay	12.01.2021	BOZ2-1-573.58-BS(MF)
573.705	573.72	573.71	Staffelegg Fm.	12.01.2021	BOZ2-1-573.71-BS(MF)

Appendix A3: List of other provisionally determined conspicuous macrofossils from BOZ2-1 (608.02 – 301.71 m)

Top [m]	Bottom [m]	Fossil	Determination (provisional)
301.71		Ammonite	Oppelidae indet.
302.36		Ammonite	<i>Perisphinctes</i> sp.
302.59		Ammonite	<i>Ochetoceras</i> ? sp.
304.79	304.93	Ammonites	<i>Opeliidae</i> indet.
386.47		Bivalve	<i>Trigonia costata</i>
390.92		Bivalve	<i>Trigonia costata</i>
410.18		Bivalve	<i>Modiolus</i> sp.
419.20	419.26	Ammonite	<i>Stephanoceras</i> sp.
419.41		Ammonites	<i>Stephanoceras</i> sp.
548.06	548.09	Ammonite	<i>Leioceras</i> sp.
553.95		Ammonite	<i>Leioceras</i> sp.
554.51		Ammonite	<i>Leioceras</i> sp.
554.56		Bivalves	<i>Bositra buchi</i>
556.62		Ammonite	<i>Leioceras</i> sp.
559.17	559.22	Ammonites	<i>Leioceras</i> sp.
560.02		Ammonite	<i>Leioceras</i> sp.
575.95		Bivalves	<i>Plagiostoma</i> sp.
578.46		Fragment of Ammonite	indet.
579.37		Ammonite	<i>Lytoceras</i> sp.
581.37		Bivalve	<i>Pseudomytiloides</i> sp.
581.69		Fragment of Ammonite	<i>Lytoceras</i> sp. ?
583.10		Ammonite	<i>Lytoceras</i> sp.
608.02		Bivalve	<i>Modiolus</i> sp.

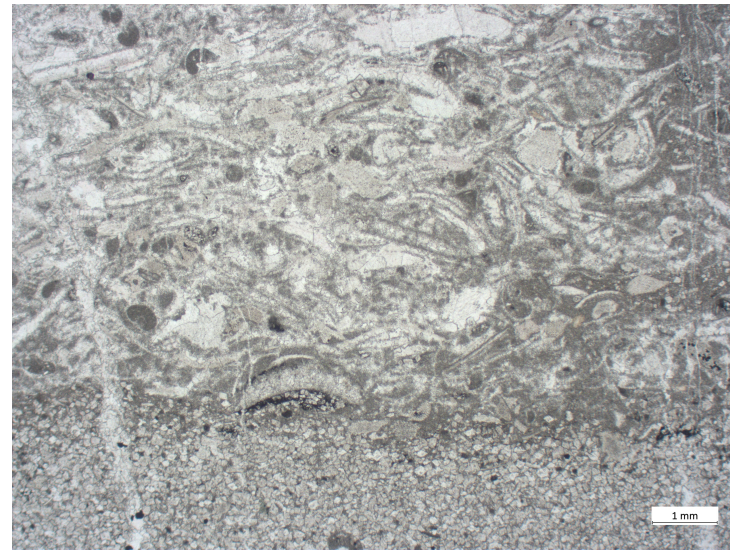
Appendix A4: List of all palynological samples from BOZ2-1 (573.93 – 300.68 m)

Palynological samples in grey are taken from ammonite samples retrieved at specific depths. Sampling was always as close as possible to the ammonite.

Top [m]	Bottom [m]	Avg. Depth [m]	Formation	Retrieval date [dd.mm.yyyy]	Sample ID
300.67	300.69	300.68	Wildeggen Fm.	14.12.2020	BOZ2-1-300.68-BS(PA)
303.76	303.78	303.77	Wildeggen Fm.	14.12.2020	BOZ2-1-303.77-BS(PA)
305.16	305.18	305.17	Ifenthal Fm.	14.12.2020	BOZ2-1-305.17-BS(PA)
306.57	306.59	306.58	Ifenthal Fm.	14.12.2020	BOZ2-1-306.58-BS(PA)
308.06	308.08	308.07	Ifenthal Fm.	14.12.2020	BOZ2-1-308.07-BS(PA)
309.48	309.50	309.49	Hauptrogenstein	14.12.2020	BOZ2-1-309.49-BS(PA)
310.46	310.48	310.47	Hauptrogenstein	14.12.2020	BOZ2-1-310.47-BS(PA)
314.45	314.47	314.46	Hauptrogenstein	14.12.2020	BOZ2-1-314.46-BS(PA)
316.03	316.05	316.04	Hauptrogenstein	14.12.2020	BOZ2-1-316.04-BS(PA)
322.12	322.14	322.13	Hauptrogenstein	14.12.2020	BOZ2-1-322.13-BS(PA)
329.48	329.50	329.49	Hauptrogenstein	14.12.2020	BOZ2-1-329.49-BS(PA)
330.56	330.58	330.57	Hauptrogenstein	14.12.2020	BOZ2-1-330.57-BS(PA)
334.06	334.08	334.07	Hauptrogenstein	14.12.2020	BOZ2-1-334.07-BS(PA)
335.48	335.50	335.49	Hauptrogenstein	14.12.2020	BOZ2-1-335.49-BS(PA)
342.04	342.06	342.05	Hauptrogenstein	14.12.2020	BOZ2-1-342.05-BS(PA)
350.11	350.13	350.12	Hauptrogenstein	14.12.2020	BOZ2-1-350.12-BS(PA)
358.17	358.19	358.18	Hauptrogenstein	14.12.2020	BOZ2-1-358.18-BS(PA)
366.05	366.07	366.06	Hauptrogenstein	14.12.2020	BOZ2-1-366.06-BS(PA)
373.88	373.90	373.89	Hauptrogenstein	14.12.2020	BOZ2-1-373.89-BS(PA)
381.76	381.78	381.77	Hauptrogenstein	14.12.2020	BOZ2-1-381.77-BS(PA)
387.87	387.89	387.88	Hauptrogenstein	14.12.2020	BOZ2-1-387.88-BS(PA)
388.81	388.83	388.82	Passwang Fm.	14.12.2020	BOZ2-1-388.82-BS(PA)
399.08	399.10	399.09	Passwang Fm.	14.12.2020	BOZ2-1-399.09-BS(PA)
409.93	409.95	409.94	Passwang Fm.	14.12.2020	BOZ2-1-409.94-BS(PA)
418.17	418.19	418.18	Passwang Fm.	14.12.2020	BOZ2-1-418.18-BS(PA)
418.67	418.69	418.68	Passwang Fm.	14.12.2020	BOZ2-1-418.68-BS(PA)
420.26	420.30	420.28	Passwang Fm.	14.12.2020	BOZ2-1-420.28-BS(PA)
422.38	422.40	422.39	Passwang Fm.	14.12.2020	BOZ2-1-422.39-BS(PA)
424.07	424.09	424.08	Passwang Fm.	12.01.2021	BOZ2-1-424.08-BS(PA)
424.95	424.97	424.96	Passwang Fm.	12.01.2021	BOZ2-1-424.96-BS(PA)
428.42	428.44	428.43	Passwang Fm.	12.01.2021	BOZ2-1-428.43-BS(PA)
429.41	429.45	429.43	Passwang Fm.	12.01.2021	BOZ2-1-429.43-BS(PA)
430.71	430.73	430.72	Passwang Fm.	12.01.2021	BOZ2-1-430.72-BS(PA)
439.67	439.69	439.68	Passwang Fm.	12.01.2021	BOZ2-1-439.68-BS(PA)
447.76	447.80	447.78	Passwang Fm.	12.01.2021	BOZ2-1-447.78-BS(PA)
448.79	448.83	448.81	Passwang Fm.	12.01.2021	BOZ2-1-448.81-BS(PA)
449.10	449.12	449.11	Passwang Fm.	12.01.2021	BOZ2-1-449.11-BS(PA)
450.79	450.81	450.80	Passwang Fm.	12.01.2021	BOZ2-1-450.80-BS(PA)
451.17	451.21	451.19	Passwang Fm.	12.01.2021	BOZ2-1-451.19-BS(PA)
451.64	451.66	451.65	Opalinus Clay	12.01.2021	BOZ2-1-451.65-BS(PA)
456.46	456.48	456.47	Opalinus Clay	12.01.2021	BOZ2-1-456.47-BS(PA)
465.46	465.48	465.47	Opalinus Clay	12.01.2021	BOZ2-1-465.47-BS(PA)
485.63	485.65	485.64	Opalinus Clay	12.01.2021	BOZ2-1-485.64-BS(PA)
505.15	505.17	505.16	Opalinus Clay	12.01.2021	BOZ2-1-505.16-BS(PA)
525.44	525.46	525.45	Opalinus Clay	12.01.2021	BOZ2-1-525.45-BS(PA)
545.89	545.91	545.90	Opalinus Clay	12.01.2021	BOZ2-1-545.90-BS(PA)
566.18	566.20	566.19	Opalinus Clay	12.01.2021	BOZ2-1-566.19-BS(PA)
573.56	573.58	573.57	Opalinus Clay	12.01.2021	BOZ2-1-573.57-BS(PA)
573.92	573.94	573.93	Staffellegg Fm.	12.01.2021	BOZ2-1-573.93-BS(PA)

Appendix B: Photos microfacies

Fig. B-1:	Thin section BOZ2-1-798.17, Schinznach Fm.	B-2
Fig. B-2:	Thin section BOZ2-1-748.33, Schinznach Fm.	B-2
Fig. B-3:	Thin section BOZ2-1-712.56, Bänkerjoch Fm.	B-2
Fig. B-4:	Thin section BOZ2-1-684.75, Bänkerjoch Fm.	B-3
Fig. B-5:	Thin section BOZ2-1-624.43, Klettgau Fm. (Gruhalde Mb.)	B-3
Fig. B-6:	Thin section BOZ2-1-485.52 (lower part), Opalinus Clay	B-3
Fig. B-7:	Thin section BOZ2-1-485.52 (upper part), Opalinus Clay	B-4
Fig. B-8:	Thin section BOZ2-1-467.43, Opalinus Clay	B-4
Fig. B-9:	Thin section BOZ2-1-451.83, Opalinus Clay	B-4
Fig. B-10:	Thin section BOZ2-1-448.81, Passwang Fm. (Waldenburg Mb. and lower part of Brüggl Mb.)	B-5
Fig. B-11:	Thin section BOZ2-1-432.87, Passwang Fm. (Waldenburg Mb. and lower part of Brüggl Mb.)	B-5
Fig. B-12:	Thin section BOZ2-1-429.43, Passwang Fm. (Waldenburg Mb. and lower part of Brüggl Mb.)	B-5
Fig. B-13:	Thin section BOZ2-1-422.67, Passwang Fm. («Humphriesi-Sch.»)	B-6
Fig. B-14:	Thin section BOZ2-1-420.59, Passwang Fm. («Humphriesi-Sch.»)	B-6
Fig. B-15:	Thin section BOZ2-1-336.09, Hauptrogenstein	B-6
Fig. B-16:	Thin section BOZ2-1-334.98, Hauptrogenstein	B-7
Fig. B-17:	Thin section BOZ2-1-333.20, Hauptrogenstein («Movelier Beds» and «Spatkalk»)	B-7
Fig. B-18:	Thin section BOZ2-1-309.57, Hauptrogenstein («Movelier Beds» and «Spatkalk»)	B-7

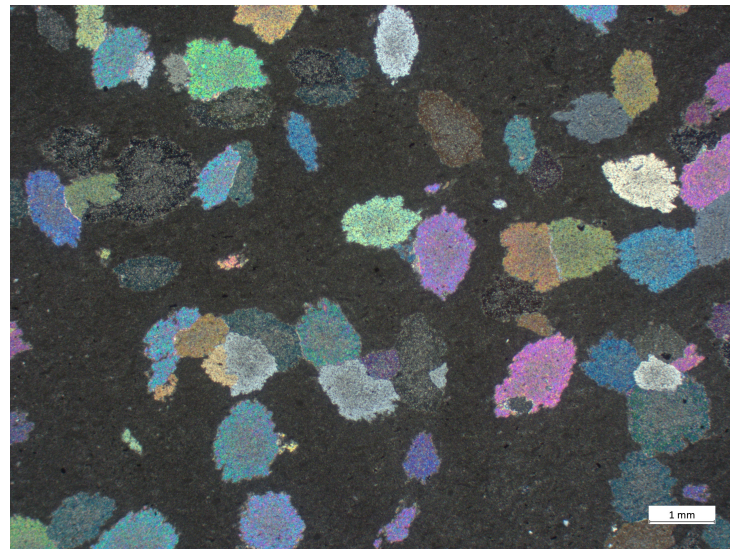
**Fig. B-1:**

Bivalves-biopelsparite and large dolomitic burrow: Numerous thin-shelled pelecypods (bivalves) and pellets with microsparite and sparite cement.

thin section photo

BOZ2-1-798.17

Schinznach Fm.

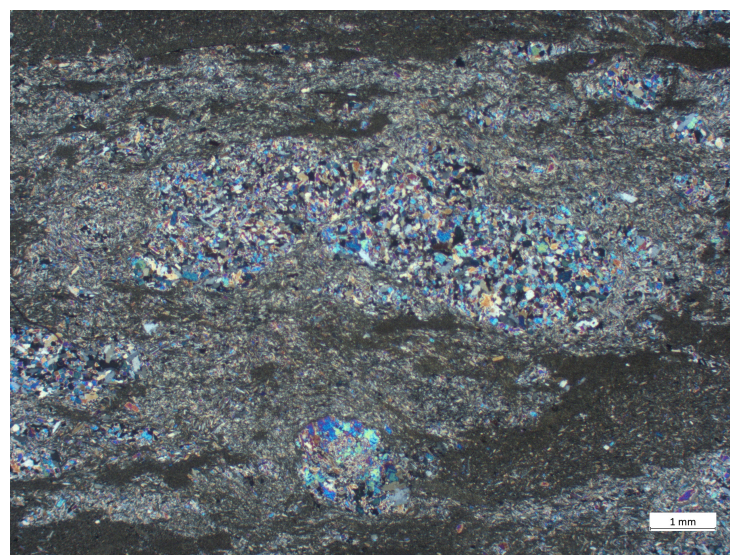
**Fig. B-2:**

Single anhydrite crystals (colourful), up to 1 mm big, grown in a dolomicrite

thin section photo,
taken with crossed nicols

BOZ2-1-748.33

Schinznach Fm.

**Fig. B-3:**

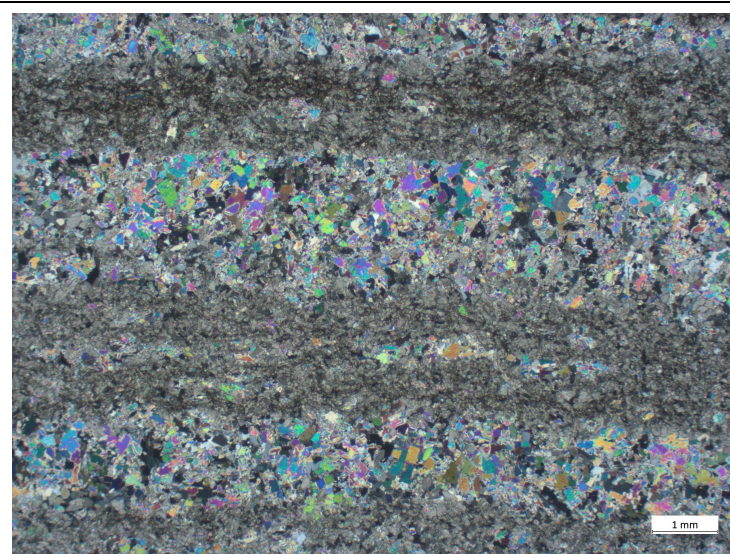
Claystone with anhydrite nodules, composed of blocky and acicular crystals (bluish and reddish colours)

thin section photo,
taken with crossed nicols

BOZ2-1-712.56

Bänkerjoch Fm.

Selected photos of microfacies from Schinznach Fm. and Bänkerjoch Fm.

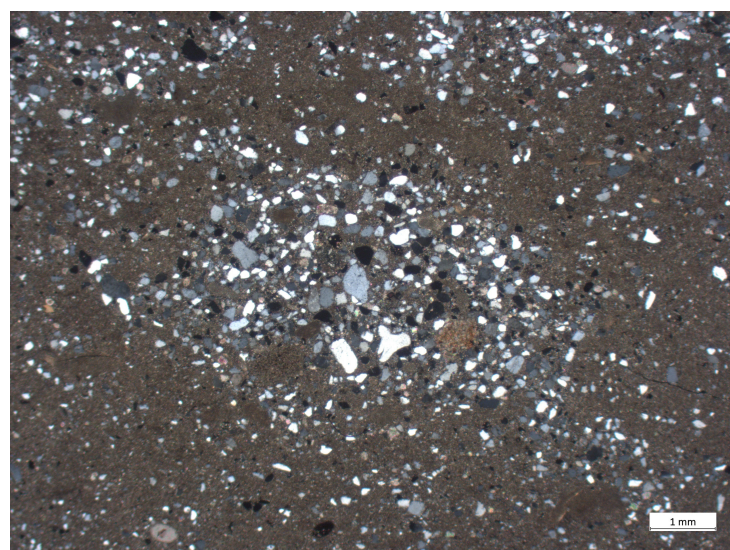
**Fig. B-4:**

Thin-layered alternation of fine-crystalline anhydrite and argillaceous dolostone

thin section photo,
taken with crossed nicols

BOZ2-1-684.75

Bänkerjoch Fm.

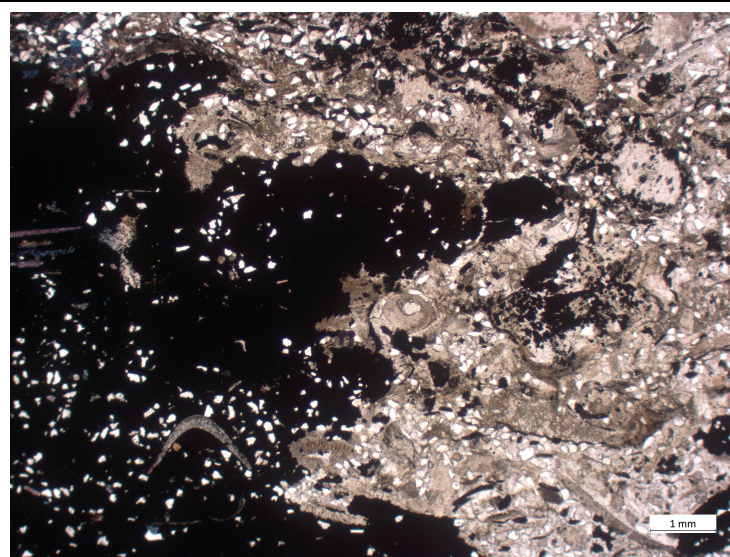
**Fig. B-5:**

Sandy dolostone (argillaceous), composed of quartz grains (grey colours) and rock fragments, sedimented with clayey, dolomitic matrix

thin section photo,
taken with crossed nicols

BOZ2-1-624.43

Klettgau Fm. (Gruhalde Mb.)

**Fig. B-6:**

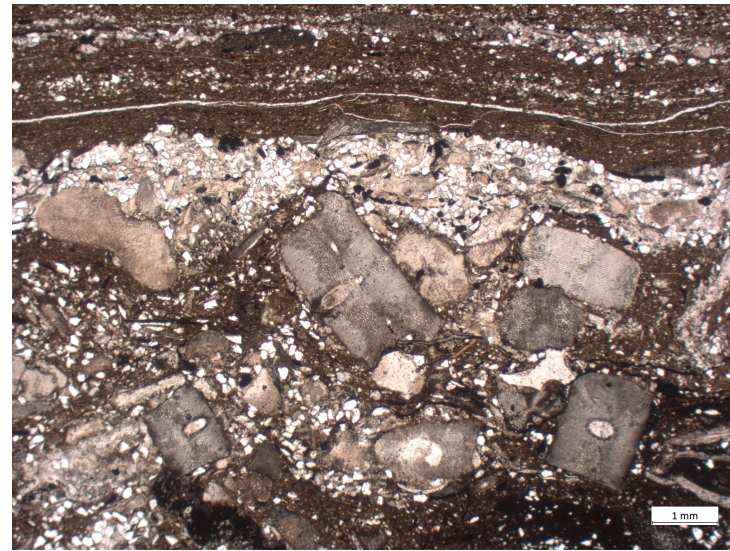
Strongly pyritized, sandy, bioclastic layer of crinoid skeletal elements, bivalves and quartz grains (white)

thin section photo

BOZ2-1-485.52 (lower part)

Opalinus Clay

Selected photos of microfacies from Bänkerjoch Fm., Klettgau Fm. and Opalinus Clay

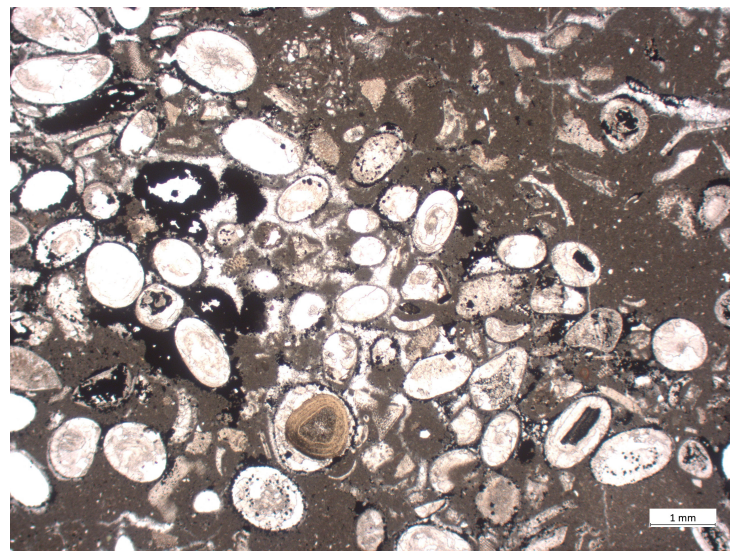
**Fig. B-7:**

Sandy, bioclastic layer of big crinoid skeletal elements, bivalves and quartz grains, sedimented with micrite matrix

thin section photo

BOZ2-1-485.52 (upper part)

Opalinus Clay

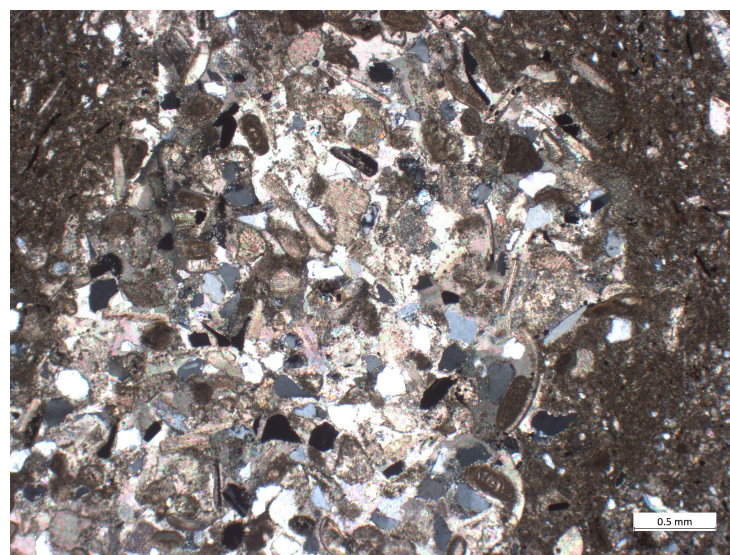
**Fig. B-8:**

Iron-oolites, now calcitic, a few with original chamosite composition, and some pyrite (black); a biotrititic calcareous marl, which follows above the iron-oolite, at top right

thin section photo

BOZ2-1-467.43

Opalinus Clay

**Fig. B-9:**

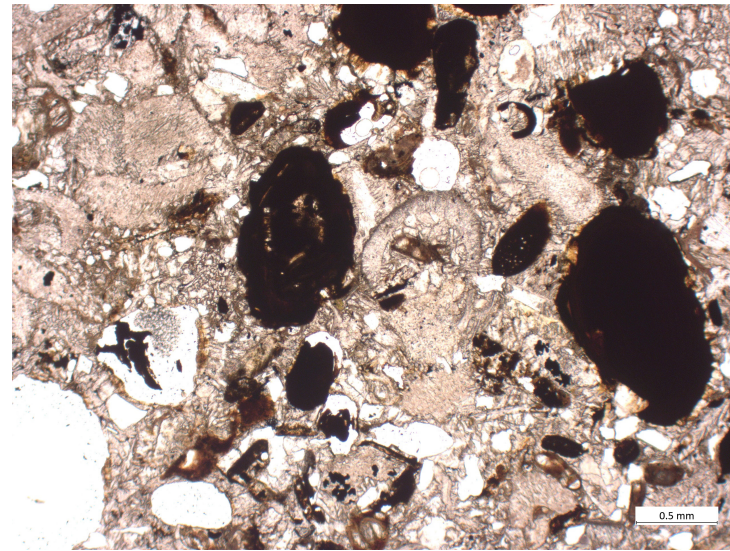
A bioclastic limestone (sandy) lense in a silty claystone subunit: the biogene components and pellets are cemented by clear calcite cement

thin section photo,
taken with crossed nicols

BOZ2-1-451.83

Opalinus Clay

Selected photos of microfacies from Opalinus Clay

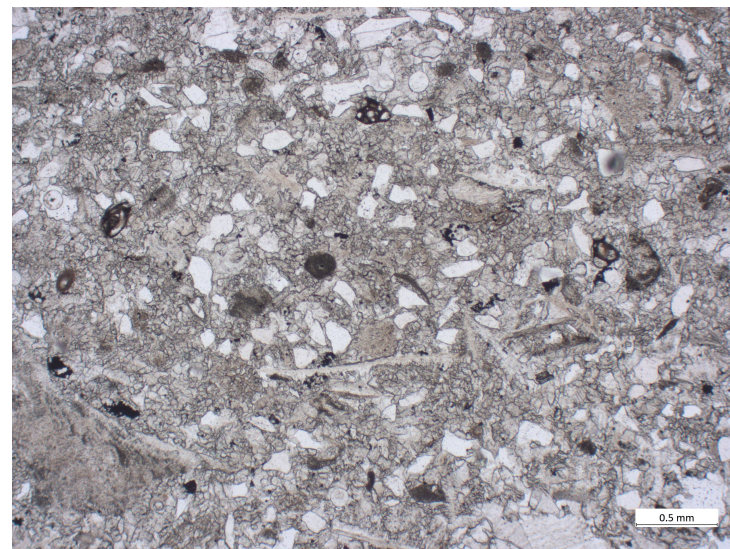
**Fig. B-10:**

bioclastic limestone (sandy)
with few iron-oooids: crinoid
skeletal elements are the
dominant components

thin section photo

BOZ2-1-448.81

Passwang Fm.
(Waldenburg Mb. and lower
part of Brüggli Mb.)

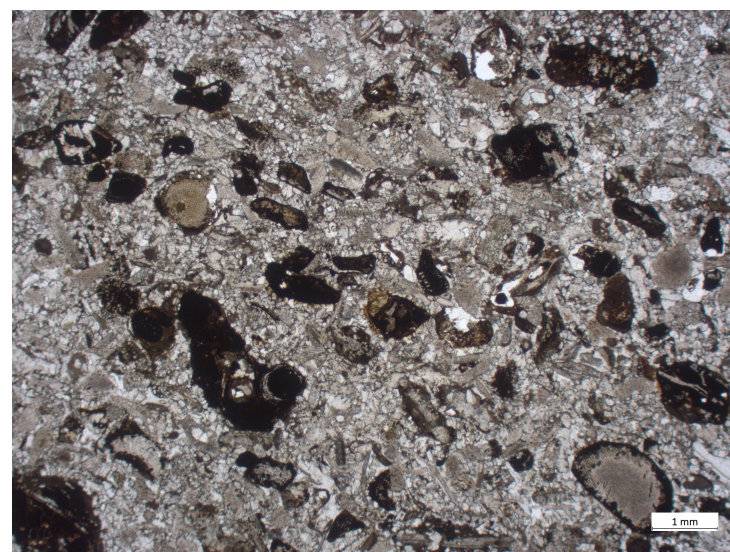
**Fig. B-11:**

Sandy limestone (bioclastic):
quartz sand and biogene
components are surrounded
by "stellate calcite cement"
and microsparite

thin section photo

BOZ2-1-432.87

Passwang Fm.
(Waldenburg and lower part
of Brüggli Mb.)

**Fig. B-12:**

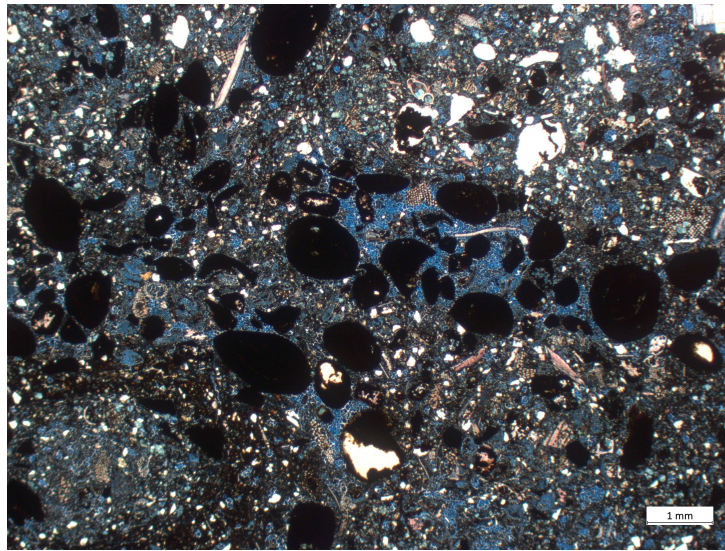
Bioclastic limestone
(limonitic), composed of
limonitic and non-limonitic
echinoderm- and bivalve
biotritus, as well as
limonitic oncoids with calcite
cement and limonitic matrix

thin section photo

BOZ2-1-429.43

Passwang Fm.
(Waldenburg and lower part
of Brüggli Mb.)

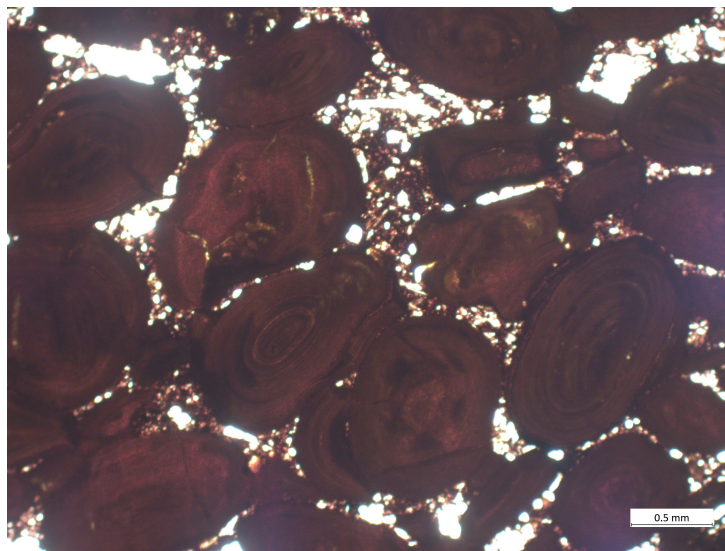
Selected photos of microfacies from Passwang Fm.

**Fig. B-13:**

Bioclastic limestone (iron-oolitic): iron-oolids, limonitic bioclasts and – pellets with limonitic matrix, iron-calcite cement (blue stained) and iron-dolomite (light blue) thin section photo

TS stained for calcite = red, ferroan calcite = blue

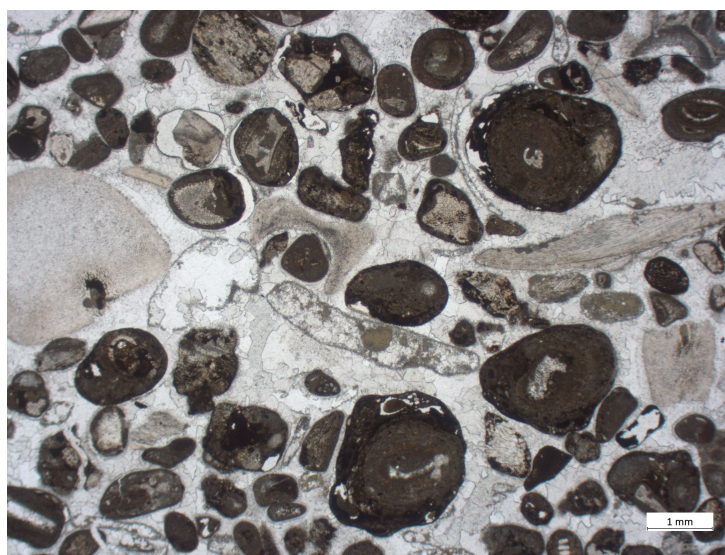
BOZ2-1-422.67
Passwang Fm.
(«Humphriesi-Schichten»)

**Fig. B-14:**

Iron-oolite, calcareous, composed of numerous iron-oolids and iron-oid-aggregates

thin section photo

BOZ2-1-420.59
Passwang Fm.
(«Humphriesi-Schichten»)

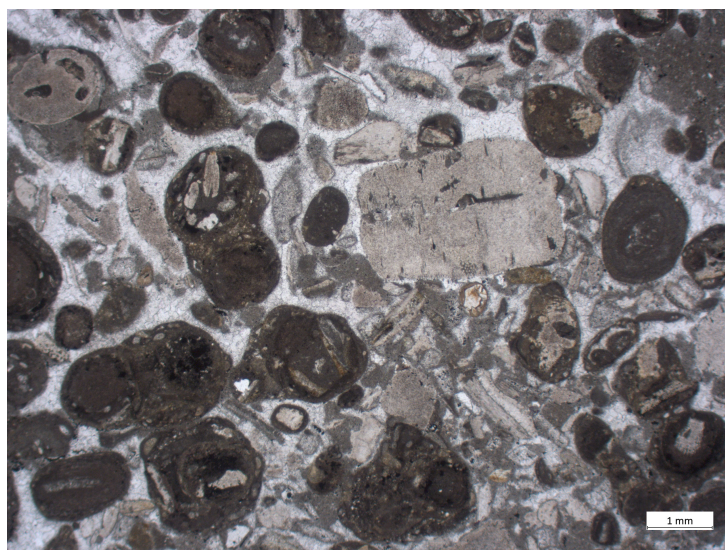
**Fig. B-15:**

Oncolitic limestone with various oncoids: a big one (bottom center and also top right) shows an ooid core and a biogene cortex; present are echinoderms and bivalves too

thin section photo

BOZ2-1-336.09
Hauptrogenstein

Selected photos of microfacies from Passwang Fm. and Hauptrogenstein

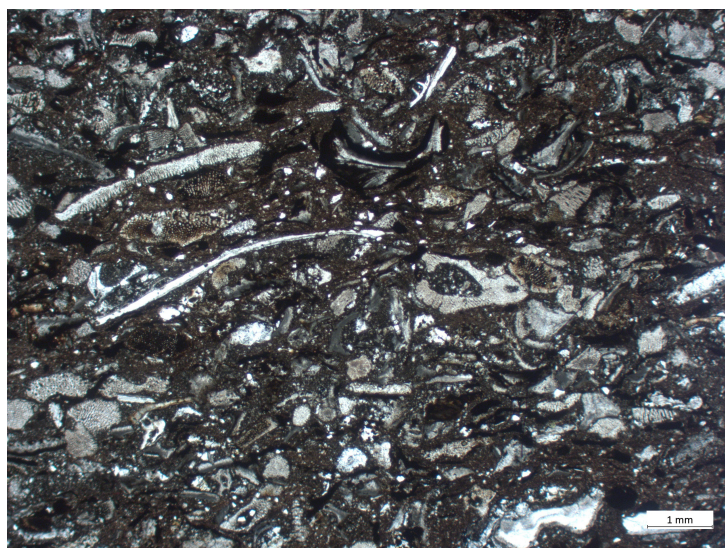
**Fig. B-16:**

Aggregate grains (left side) are frequent components of these oncolitic limestones; they are accompanied of echinoderm elements (center) and bivalves

thin section photo

BOZ2-1-334.98

Hauptrogenstein

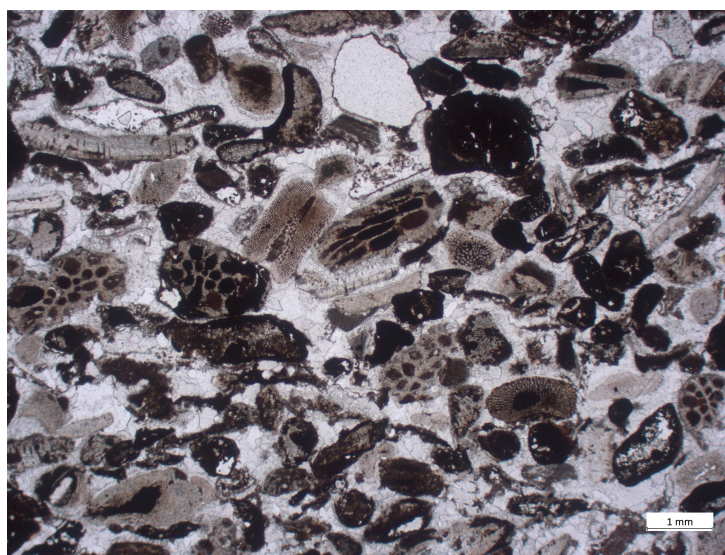
**Fig. B-17:**

Bioclastic limestone (limonitic), composed of limonitic biogene components and limonitic matrix

thin section photo

BOZ2-1-333.20

Hauptrogenstein
(lower part of «Movelier Beds» and «Spatkalk»)

**Fig. B-18:**

Bioclastic limestone (limonitic) with limonitic bryozoans, echinoderms, bivalves and calcite cement

thin section photo

BOZ2-1-309.57

Hauptrogenstein
(upper part of «Movelier Beds» and «Spatkalk»)

Selected photos of microfacies from Hauptrogenstein

Appendix C: Plates of ammonites

Plate I: BOZ2-1 (573.58 – 548.09 m)C-3

Plate II: BOZ2-1 (420.28 – 419.23 m)C-5

Plate I BOZ2-1 (573.58 – 548.09 m)

- Fig. 1: *Leioceras* ex gr. *subglabrum* (Buckman, 1902), depth: 573.58 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 2: *Leioceras* ex gr. *opalinum* (Reinecke, 1818), depth: 563.60 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 3: *Leioceras* ex gr. *opalinum* (Reinecke, 1818), depth: 548.85 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 4: *Discinisca* sp., depth: 548.68 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 5: *Leioceras* ex gr. *opalinum* (Reinecke, 1818), depth: 548.09 m, Opalinus Clay, Opalinum-Zone, Opalinum-Subzone.

All figures are illustrated in individual scales; black bars indicate 1 cm.

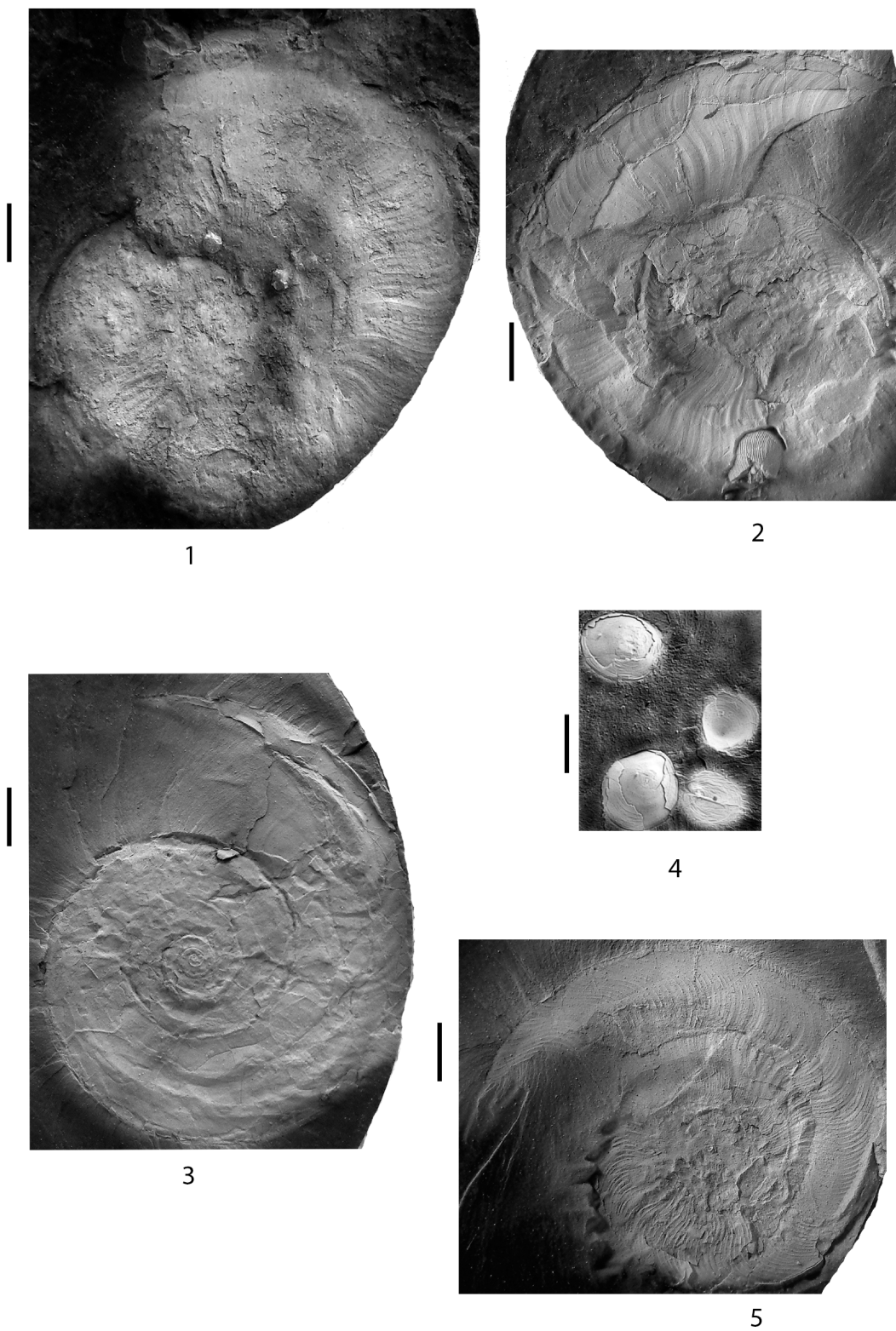


Plate I: BOZ2-1 (573.58 – 548.09 m)

Plate II BOZ2-1 (420.28 – 419.23 m)

Figs. 1a, 1b: *Dorsetensia* sp., depth: 420.28 m, Passwang Fm. («Humphriesi-Schichten»), Humphriesianum Zone, Romani Subzone?. Fig. 1a: lateral view, 1b: cross section.

Figs. 2a – 2d: *Itinsaites* sp. ? (left) and *Belemnopsis* sp.? (right), depth: 419.23 m, Passwang Fm. («Humphriesi-Schichten»), Humphriesianum Zone, Humphriesianum Subzone. *Itinsaites* sp. ? : Fig. 2a: lateral view, 2b: cross section, 2c: ventral view and *Belemnopsis* sp.: Fig. 2a: ventral view, 2d: cross section.

All figures are illustrated in individual scales; black bars indicate 1 cm.

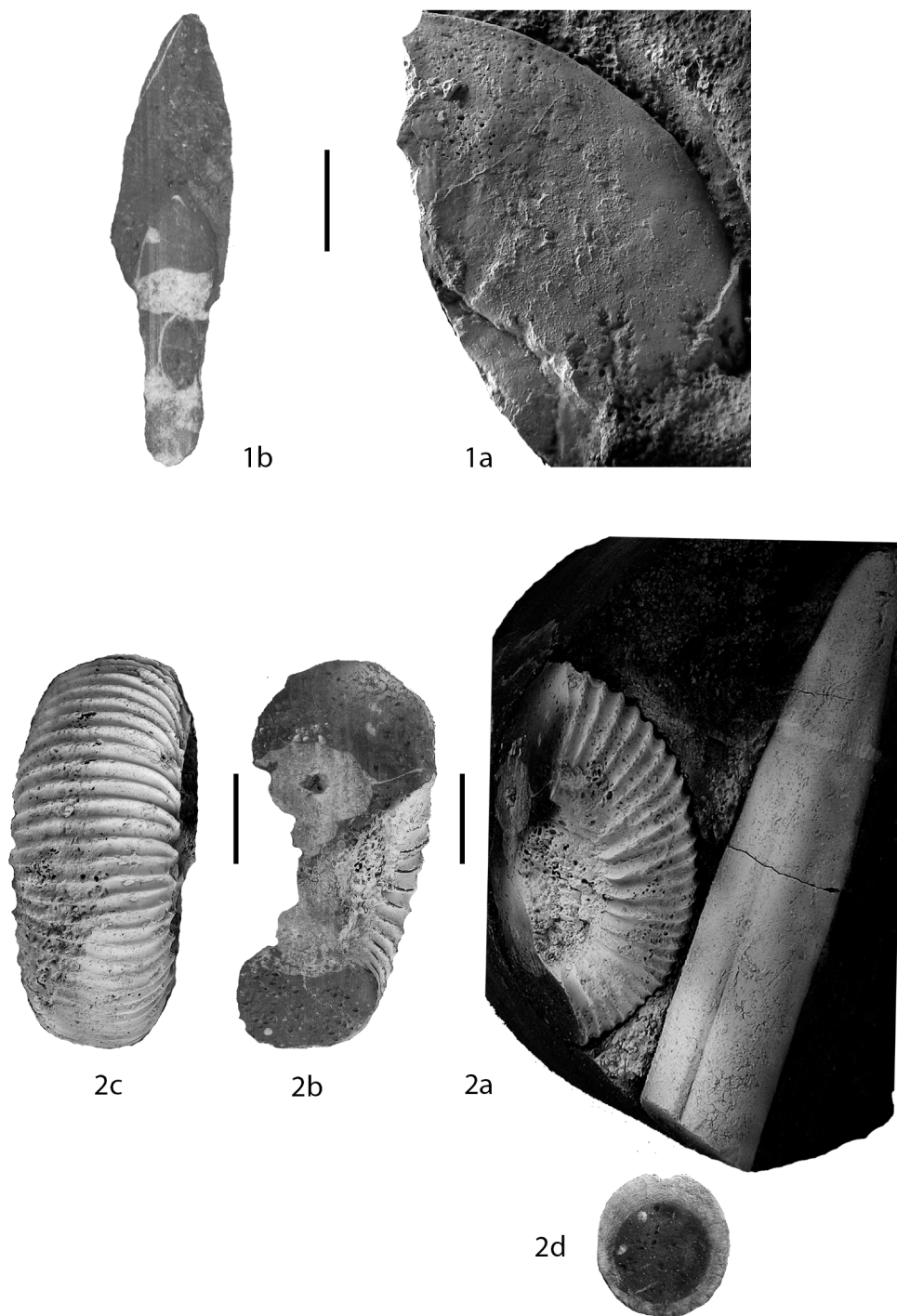


Plate II: BOZ2-1 (420.28 – 419.23 m)

Appendix D: Palynostratigraphy

Appendix D1: Range Chart: Quantitative stratigraphic distribution of Middle Jurassic palynomorphs in the Bözberg-2-1 borehole

Appendix D2: Depth/Age plot: Bözberg-2-1 borehole

Note: The appendices are only included in the digital version of this report (PDF) and can be found under the paper clip symbol.

Appendix E: Chemostratigraphy

Appendix E1:	List of all geochemical samples and results mainly drilled from specific calcareous beds and concretions in the Opalinus Clay and its confining units.	E-2
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Appendix E1: List of all geochemical samples and results mainly drilled from specific calcareous beds in the Opalinus Clay and its confining units

Data are discussed in Section 3.4 and partly illustrated in Fig. 3-4 (part of the data points lie outside the presented scale for the $\delta^{13}\text{C}_{\text{carb}}$): CC: drilled from a calcareous concretion, SN: drilled from a septarian nodule, MF: drilled from macrofossil, TS: drilled directly from thin section sample (see microfacies description in Section 3.1). For definition of "hiatus bed" & "hiatus concretion" see Section 2.1.

Depth [m]	Description of sample		TS	$\delta^{13}\text{C}_{\text{carb}}$ [‰ VPDB]	$\delta^{18}\text{O}_{\text{carb}}$ [‰ VPDB]	Carbonate [wt.-%]
386.25	Calcareous bed	HC		-0.77	-1.50	86.0
403.99	Belemnite	MF		1.04	1.01	100.0
407.67	Calcareous bed	HC	×	1.66	-2.64	73.7
451.50	hardground	HC		1.06	-1.77	74.0
467.50	Septarien nodule?	CC		-3.83	-1.73	79.8
480.03	Calcareous nodule	HC		-12.85	-4.33	67.9
480.17	Calcareous nodule, firmground?	HC		-3.92	-3.95	82.4
480.55	Septarien nodule?	CC		-14.15	-1.73	81.8
489.01	Calcareous sand lense	CC		-3.40	-5.54	63.1
563.74	Calcareous to septarian nodule?	SN?		-20.89	-1.61	80.1
564.20	Calcareous to septarian nodule?	SN?		-22.97	-3.61	79.0
564.42	Calcareous to septarian nodule?	SN?		-27.49	-1.50	79.5
579.50	«Oberer Stein» (Rietheim Mb.)			0.76	-5.77	79.0
579.60	«Oberer Stein» (Rietheim Mb.)			-0.74	-4.33	99.4
580.50	«Homog. Kalkbank» (Rietheim Mb.)			-0.38	-3.40	93.0
581.08	«Unterer Stein» (Rietheim Mb.)		×	-1.23	-3.56	98.9