

Arbeitsbericht NAB 20-09

**TBO Trüllikon-1-1:
Data Report**

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

June 2021

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

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dinoflagellate cysts, 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 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 Trüllikon-1-1 borehole.

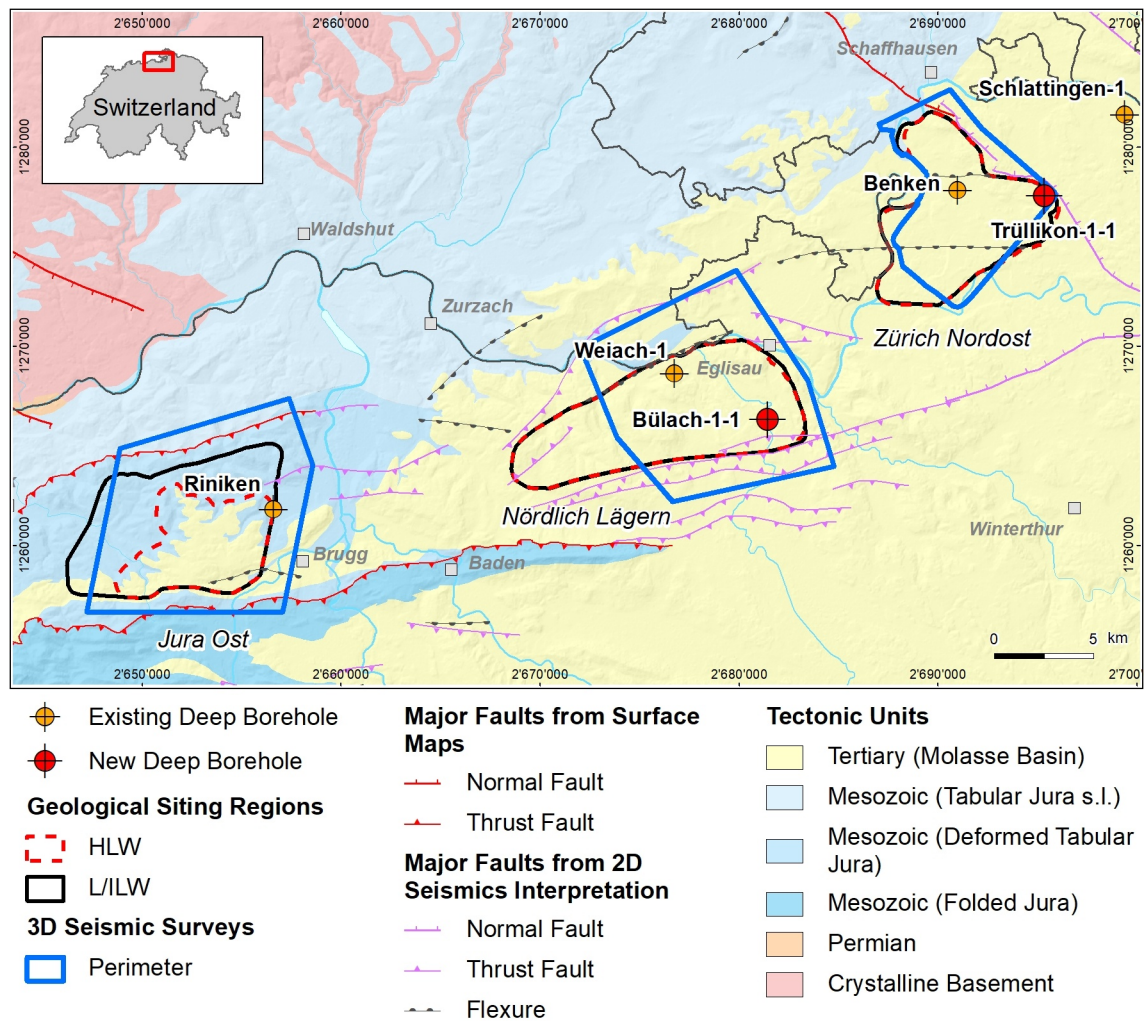


Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Trüllikon-1-1 (TRU1-1) exploratory borehole is the second borehole drilled within the framework of the TBO project. The drill site is located in the eastern part of the Zürich Nordost siting region (Fig. 1-2). The vertical borehole reached a final depth of 1'310 m (MD)¹. The borehole specifications are provided in Tab. 1-1.

Tab. 1-1: General information about the TRU1-1 borehole

Siting region	Zürich Nordost
Municipality	Trüllikon (Canton Zürich / ZH), Switzerland
Drill site	Trüllikon-1 (TRU1)
Borehole	Trüllikon-1-1 (TRU1-1)
Coordinates	LV95: 2'695'372.648 / 1'277'548.076
Elevation	Ground level = top of rig cellar: 475.07 m above sea level (asl)
Borehole depth	1'310.0 m measured depth (MD) below ground level (bgl)
Drilling period	15. August 2019 – 5. April 2020 (spud date to end of rig release)
Drilling company	PR Marriott Drilling Ltd.
Drilling rig	Rig-16 Drillmec HH102
Drilling fluid	Water-based mud with various amounts of different components such as ² : 46 – 712 m: Pure-Bore® 712 – 1'161 m: Potassium silicate 1'161 – 1'310 m: Sodium chloride & polymers

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The main lithostratigraphic boundaries in the TRU1-1 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.

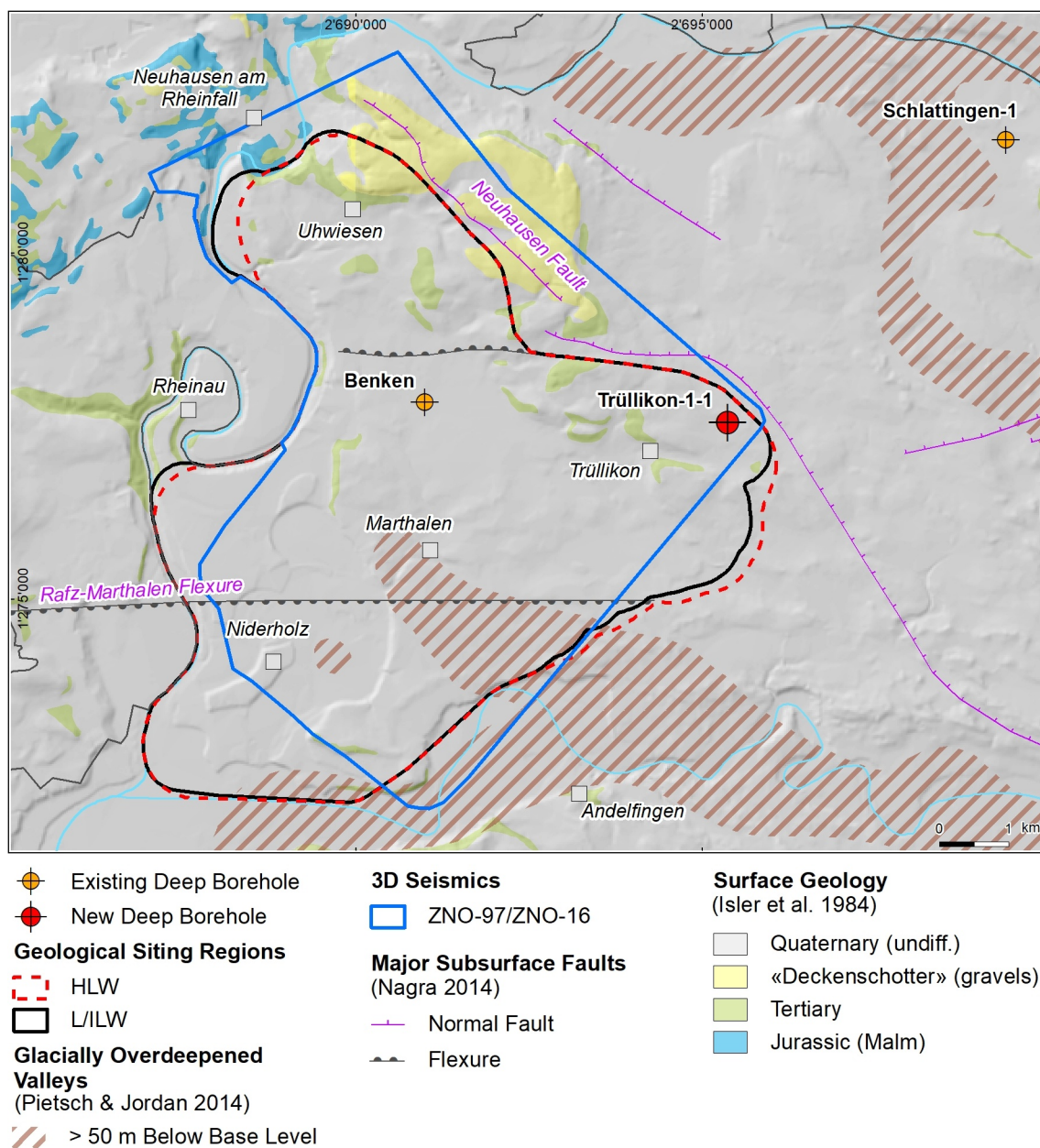
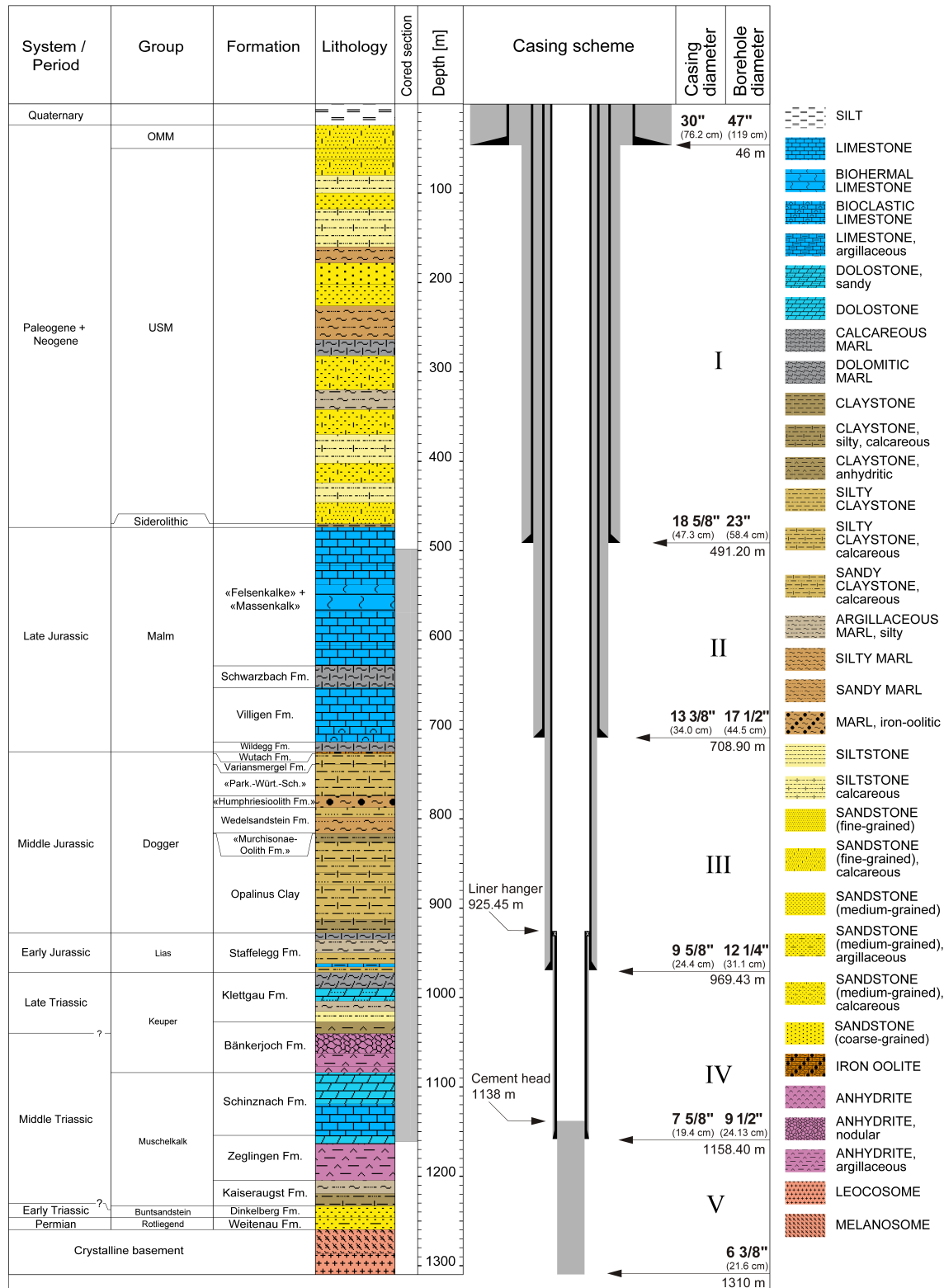


Fig. 1-2: Overview map of the investigation area in the Zürich Nordost siting region with the location of the TRU1-1 borehole in relation to the boreholes Benken and Schlattigen

Fig. 1-3: Lithostratigraphic profile and casing scheme for the TRU1-1 borehole³³ For detailed information see Dossier I and III.

1.3 Documentation structure for the TRU1-1 borehole

NAB 20-09 documents the majority of the investigations carried out in the TRU1-1 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. 1-2).

This documentation aims at early publication of the data collected in the TRU1-1 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. 1-2: List of dossiers included in NAB 20-09

Black indicates the dossier at hand.

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

1.4 Scope and objectives of this dossier

The present data report complements the lithostratigraphic report (Dossier III) on the TRU1-1 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 (05.06.2020) 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 TRU1-1 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 TRÜLLIKON-1-1				
System / Period	Group	Formation	Metres MD	Member / Sub-unit
Quaternary			24	
Paleogene / Neogene	OMM		50	
	USM		470	
	Siderolithic		474	
Jurassic	Late	Malm	«Felsenkalke» + «Massenkalk»	
			Schwarzbach Fm.	
			Villigen Fm.	
			Wildeggen Fm.	
				Hornbuck Mb.
	Middle	Dogger	Wutach Fm.	
			Variansmergel Fm.	
			«Parkinsoni-Württembergica-Sch.»	
			«Humphriesoolith Fm.»	
			Wedelsandstein Fm.	
			«Murchisonae-Oolith Fm.»	
			Opalinus Clay	
				«Sub-unit with silty calcareous beds»
				«Upper silty sub-unit»
				«Mixed clay-silt-carbonate sub-unit»
				«Clay-rich sub-unit»
	Early	Lias	Staffelegg Fm.	
				Gross Wolf Mb.
				Rietheim Mb.
				Breitenmatt Mb. and Rickenbach Mb.
				Grünschoholz Mb.
				Frick Mb.
				Begglingen Mb.
				Schambelen Mb.
				Belchen Mb.
				Gruhalde Mb.
Triassic	Late	Keuper	Klettgau Fm.	
				Seebi Mb.
				Gruhalde Mb.
				Gansingen Mb.
				Ergolz Mb.
				«Claystone with anhydrite nodules»
				«Cyclic sequence»
				«Thin-layered anhydrite and claystone sequence»
	Middle	Muschelkalk	Bänkerjoch Fm.	
				«Banded massive anhydrite»
			Schinznach Fm.	
				Asp Mb.
				Stamberg Mb.
				Liedertswil Mb.
				Leutschenberg Mb. and Kienberg Mb.
				«Dolomitzone»
				«Sulfatzone»
				«Orbicularismergel»
				«Wellenmergel»
				«Wellendolomit»
	Early	Bsst.	Dinkelberg Fm.	
Permian	Rotlieg.	Weitenau Fm.		
		Crystalline basement		
			1'310.0	Final depth

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

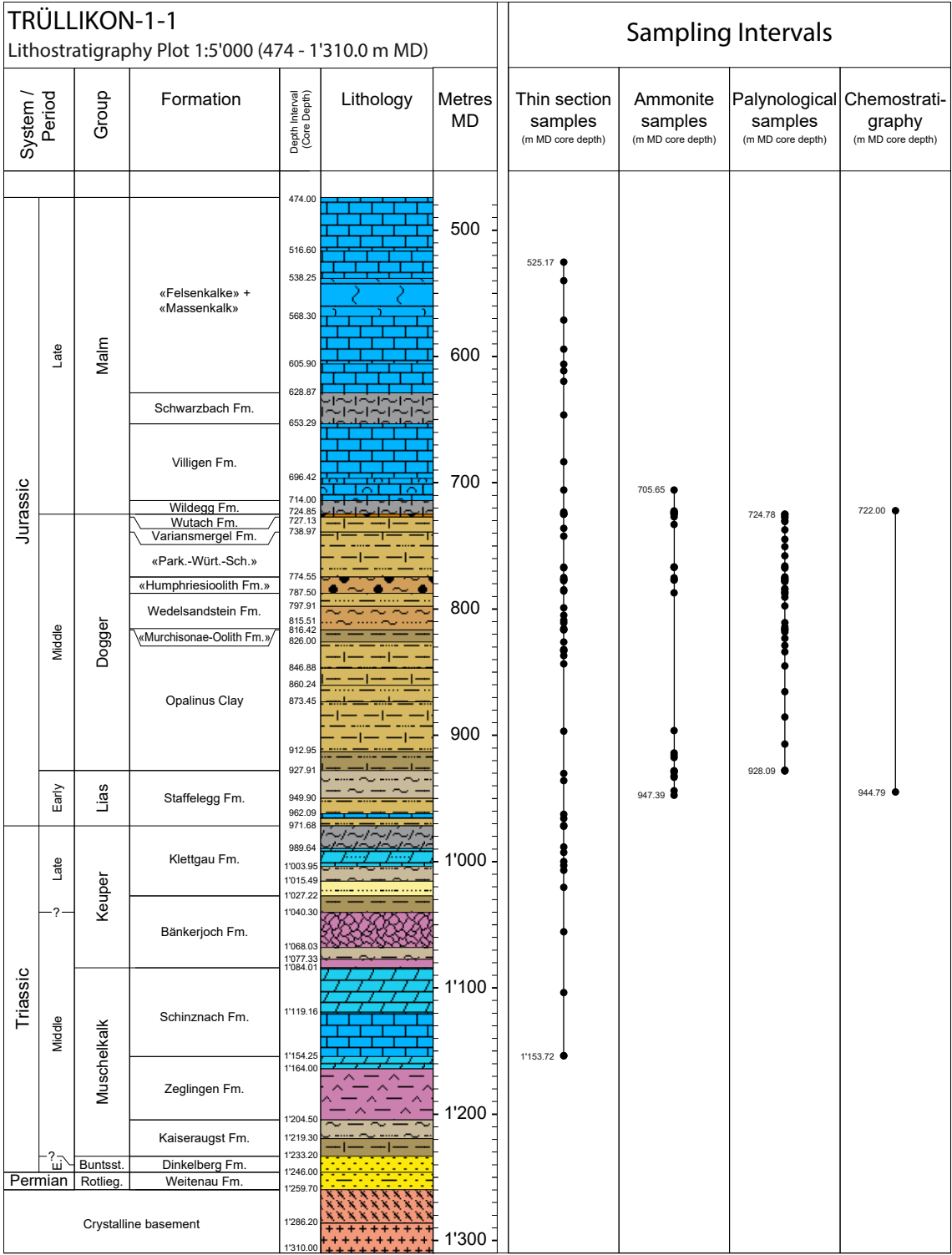


Fig. 1-5: Lithostratigraphy plot (1:5'000) from the Mesozoic succession with the individual sampling intervals for thin sections, macrofossils, palynological analysis and chemostratigraphy

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.

All thin sections from Trüllikon-1-1 have been prepared by the Thin Section Lab (TSL). The thin sections from calcareous lithologies have a standard length of 4 cm. Lithologies sensitive to water such as claystones and argillaceous sediments (swelling of clay minerals) or evaporates (dissolution of evaporitic minerals) were prepared using petroleum. These sensitive thin sections, due to the different preparation, 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

54 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 micrometer 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 21 thin section photographs for microfacies analysis is documented in Appendix B (Figs. B-1 to B-21).

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.

Fe-stromatolites and stromatolitic clasts: Iron-mineralised microbial mats or and 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 show relicts of iron mineral layers.

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 (e.g. TRU1-1-972.00, Fig. B-3 or TRU1-1-896.67, Fig. B-5). The calcite crystals form small "stellates", i.e. a habitus typical for "hiatus beds" (firm-, hard-grounds) (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 detritical gypsum crystals. In some cases, the rhombohedrons consist of iron-dolostone, which are stained blue after the thin section staining (e.g. TRU1-1-1055.52).

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/ micro-sparitic limestone (e.g. TRU1-1-525.17). 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, TRU1-1-1055.52).

Quartz cement: Authigenic quartz rims grown during diagenesis around detrital quartz grains (e.g. TRU1-1-1003.02); also quartz/chalcedony in silicified bivalves.

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 mineralized by iron and manganese oxides or calcium phosphates.

2.2 Ammonite preparation

The TRU1-1 cores were carefully examined for macrofossils at the Würenlingen (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 an abrasive. In one case (depth 776.99 m), some biloxite (white corundum) was used. Residual material from preparing eighth 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 make their fine structure more visible. A selection of ammonites is documented on four plates (Plates I – IV) 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

Sampling

The sampling of the TRU1-1 focused primarily on the Dogger and Lias Groups and therefore primarily on the clay mineral-rich layers of the Opalinus Clay. The sampling resolution was one metre, except for some intervals with denser sampling density (mainly hardgrounds and condensed intervals). All 286 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 ($n = 12$) with results from calcareous beds, calcitic concretions and a macrofossil (belemnite) can be found in Appendix E1 of this report.

Inorganic (carbonate) analyses

The 286 samples were analyzed for stable carbon ($\delta^{13}\text{C}_{\text{carb}}$) and oxygen isotope ($\delta^{18}\text{O}_{\text{carb}}$) of bulk carbonate; 274 continuous samples (roughly in metre resolution) and additional 12 samples from specific calcareous beds in the Opalinus Clay and its upper confining unit (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 $\pm 4.60 \text{ ‰}$. 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. 2019).

Organic analyses

The powders remaining after inorganic analysis from 237 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 $\pm 0.81 \text{ ‰}$, respective $\pm 0.12 \text{ ‰}$ 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 (TRU1-1-1153.72, 1153.62, 1103.66)

The two samples TRU1-1-1153.72 and TRU1-1-1153.62, taken from the border zone of the Zeglingen Formation to Schinznach Formation are both, regarding their mineralogical composition, limestones (calcitic). Therefore, both belong to the Schinznach Formation, independent of the dolomitic stromatolite sequence containing TRU1-1-1153.72, counted as "other biogenes" in Tab. 3-1. This thin section is a calcitic oosparite, partly dolomitised (ooids 38 vol.-%, Tab. 3-1) with some pellets, echinoderms and foraminifera in a partly micritic matrix. Calcite cement (10 vol.-%) and numerous (26 vol.-%) dolomite crystals complete the microfacies. TRU1-1-1153.62 has a similar composition, but more ooids (54 vol.-%, Tab. 3-1), more fossil fragments (total 13 vol.-%) and much less dolomite (5 vol.-%).

The sample TRU1-1-1103.66 is a dolostone (micritic to microsparitic) (63 vol.-%, Tab. 3-1) with 19 vol.-% fossils (bivalves, gastropods), some ooids and oncoids (together 9 vol.-%), as well as 9 vol.-% porosity.

Bänkerjoch Formation (TRU1-1-1055.52)

The sample TRU1-1-1055.52 is one of those sandy looking beds, which are commonly developed in the Bänkerjoch Formation. The thin section contains elongated dolomite rhombohedrons (60 vol.-%, Tab. 3-1) replacing gypsum, which has been deposited as an arenitic gypsum layer without quartz grains (Fig. B-1, Appendix B). Some crystals and nodules of anhydrite (22 vol.-%) are present too.

Klettgau Formation (TRU1-1-1020.30, 1006.80, 1003.02, 999.87, 992.67, 988.32, 972.00)

Most of the analysed beds or lithologies of the Klettgau Formation are sandstones or intraformational breccias:

TRU1-1-1020.30 is a thin bedded, fine-grained sandstone (argillaceous) of the Ergolz Member with 62 vol.-% (Tab. 3-1) quartz grains and rock fragments, which are sedimented with argillaceous matrix (22 vol.-%) or cemented by anhydrite (11 vol.-%) in alternating layers. The detrital grains have grain sizes from 0.03 – 0.35 mm with an average of 0.1 mm.

TRU1-1-1006.80 represents a bed of a lithology, which developed a few times in the red dolomitic marl sequence of the Klettgau Formation – an intraformational breccia, consisting of 83 vol.-% (Tab. 3-1) dolomitic intraclasts, sedimented with a dolomitic, marly matrix (12 vol.-%) and few quartz silt grains (5 vol.-%).

The samples TRU1-1-1003.02 and TRU1-1-999.87 from the Seebi Member are coarse-grained sediments, sandstones and an intraformational breccia (TRU1-1-992.67). The last one consists of dolomicritic intraclasts (73 vol.-%, Tab. 3-1) and dolomitic marl matrix (23 vol.-%) (Fig. B-2). The two sandstones are poorly sorted, with grain sizes up to 3 mm, with quartz-, calcite- and anhydrite cement (TRU1-1-1003.02, Tab. 3-1) and dolomicritic matrix (TRU1-1-999.87). The sample TRU1-1-1003.02 has 10 vol.-% porosity.

The most frequent facies of the Klettgau Formation is a dolomitic marl which has been analysed by TRU1-1-988.32. The sample contains 12 vol.-% quartz-silt in a nodular marly dolomite matrix (85 vol.-%, Tab. 3-1) and small calcite "eyes" (3 vol.-%) (mud cracks or root traces).

The sample TRU1-1-972.00 from the Belchen Member shows a somehow strange microfacies – strange in the context of Klettgau Formation, the continental, alluvial and fluvial formation. TRU1-1-972.00 is a biomicrosparite (fine-sandy) with bivalves (32 vol.-%, Tab. 3-1) (Fig. B-3) and microsparite matrix (33 vol.-%) with quartz grains (15 vol.-%). A special calcite cement, grown within the matrix, seems to be a stellate cement, typical for "hiatus beds" (Wetzel & Allia 2000).

Staffelegg Formation (TRU1-1-971.35, 965.78, 962.44, 935.81, 930.13)

The lowermost analysed bed (TRU1-1-971.35) of the Staffelegg Formation comes from the limestone at the base of the generally silty argillaceous Schambelen Member. The thin section is an oosparite, composed of, up to 1.5 mm, grain-supported, ooids (38 vol.-%, Tab. 3-1), bivalves (13 vol.-%) and few oosparite intraclasts (8 vol.-%), cemented by calcite sparite (33 vol.-%) (Fig B-4).

Sample TRU1-1-965.78 (Beggingen Member), a biomicrite (iron-oolitic), shows a complex microfacies, consisting of several different components: limonitic and calcitic iron-ooids (12 vol.-%, Tab. 3-1), limonitic bioclasts (11 vol.-%) and "normal" biodetritus (35 vol.-% echinoderms, bivalves and others). They are embedded in micrite matrix (10 vol.-%) and siderite (15 vol.-%) as well as calcite sparite and stellate cement. The second analysed bed, TRU1-1-962.44, from the Beggingen Member is a "normal" limestone (biodetritic) of closely packed echinoderm (24 vol.-%, Tab. 3-1) and bivalve detritus (28 vol.-%), with few foraminifera (5 vol.-%), sedimented with micrite matrix (32 vol.-%).

The thin section TRU1-1-935.81, from a limestone bed of the Riethem Member, shows numerous filamentous bivalves (43 vol.-%, Tab. 3-1) in a micritic/microsparitic/sideritic matrix. Micrite, microsparite and the tiny siderite crystals cannot be separated; therefore, they are counted together (48 vol.-%).

Also, TRU1-1-930.13 from a nodular limestone of the Gross Wolf Member is a biomicrite, but with less biodetritus – echinoderms (14 vol.-%, Tab. 3-1) and bivalves (15 vol.-%) – and more micrite matrix (68 vol.-%).

Opalinus Clay (TRU1-1-896.67, 843.33, 836.84, 833.00, 832.49, 831.91, 826.03)

We focussed our microfacies analyses on calcareous beds/layers which interrupt the silty claystones of Opalinus Clay. Some of them are also iron-oolitic, but mainly replaced by calcite.

The one of the lower part, TRU1-1-896.67, a calcareous, marly bed, seems to be a "hiatus bed". It consists of numerous little calcite crystals (65 vol.-%, Tab. 3-1), similar to "stellate cement", grown within an argillaceous matrix (30 vol.-%) (Fig. B-5).

The two thin sections TRU1-1-843.33 and TRU1-1-836.84 are taken from nodular, intraclasts-bearing calcareous hardgrounds: TRU1-1-843.33 has pyrite-rich micrite clasts (21 vol.-%, Tab. 3-1), TRU1-1-836.84 has different, micritic and phosphoritic components (Fig. B-6). Both contain biodetritus (total up to 21 vol.-%, Tab. 3-1) and quartz silt (12, resp. 10 vol.-%, Tab. 3-1). The components are embedded in a micritic calcareous to marly matrix with some calcite "stellate cement" (5, resp. 11 vol.-%, Tab. 3-1).

TRU1-1-833.00 comes from a complex hardground, consisting of few different horizons: in the lower part a pyrite/calcite crust developed on an iron-oid-bearing micrite (now replaced by calcite, marked with an asterix behind the number in Tab 3-1) (Fig. B-7). Above follows a silty, biodetritic micrite layer, which is covered by a stromatolitic crust and an iron-oolite (iron-oids replaced by calcite) (Fig. B-8).

The sample TRU1-1-832.49 has been taken out of a sequence with few mm-thin biodetritic layers in the silty claystones. It contains biodetritus of echinoderms (7 vol.-%, Tab. 3-1) and bivalves (3 vol.-%), quartz silt (10 vol.-%) and pyrite (5 vol.-%) in a calcareous clay matrix. The carbonate content cannot be estimated in this thin section.

Another hardground was analysed by TRU1-1-831.91: it consists of silty, biodetritic micrite intraclasts (45 vol.-%, Tab. 3-1), few iron-stromatolitic flakes, biodetritus (14 vol.-%) and quartz silt (12 vol.-%) in a sideritic (15 vol.-%) clay matrix.

Then, the sample TRU1-1-826.03, which represents a hardground too, contains iron-oolitic intraclasts (11 vol.-%, Tab. 3-1, Fig. B-9) with biodetritus (16 vol.-%), quartz silt (19 vol.-%) and relatively much pyrite (18 vol.-%) in a sideritic clay matrix.

All iron-oids of the Opalinus Clay have lost their original iron-mineralic composition by replacement by calcite or by leaching and cementation by calcite. If such calcitic iron-oids have been noted in the "Fe-oids" column in Tab. 3-1, they are marked with an asterix behind the number.

«Murchisonae-Oolith Formation» (TRU1-1-816.40, 816.28)

The two samples of the «Murchisonae-Oolith Formation» are a limestone (iron-oolitic) (TRU1-1-816.40, 28 vol.-% iron-oids) and an iron-oolite (calcareous) (TRU1-1-816.28, 48 vol.-% iron-oids) (Tab. 3-1). All iron-oids have, as seen in the Opalinus Clay, no longer their original iron minerals – goethite, limonite, chamosite - but a calcite composition (TRU1-1-816.28, Fig. B-10). But not in the same way: the calcitic iron-oids of TRU1-1-816.40 contain more relicts of iron-minerals and micritic calcite, those of TRU1-1-816.28 show more clear calcite crystals. But in detail the composition of the ooids is very complex. Several ooids of TRU1-1-816.40 have now a "cement" rim of pyrite. Some biodetritus (14, resp. 6 vol.-%, Tab. 3-1), probably one coral fragment (TRU1-1-816.28) and some intraclasts complete the components. All are embedded in micritic matrix.

Wedelsandstein Formation (TRU1-1-815.44, 810.82, 808.86, 804.83, 798.92)

The analysed beds of the Wedelsandstein Formation are one iron-oolitic at the base (TRU1-1-815.44) and three calcareous/quartz-rich beds from the lower and one from the upper part of the formation.

All iron-oids of the basal bed are parts of intraclasts (Fig. B-11), so the rock name is not an iron-oolite, but intramicrite and due to the high content of quartz sand (20 vol.-%, Tab. 3-1) intramicrite (sandy). Few of the intraclasts have an iron-stromatolitic crust (Fig. B-11). Again, the iron-oids in the intraclast are replaced by calcite. The biodetritical components derive from echinoderms (9 vol.-%), bivalves (7 vol.-%), sponge spicules (2 vol.-%) and others (2 vol.-%).

The lowermost analysed calcareous/quartz-rich bed (TRU1-1-810.82) is sandier than the others above. The calcareous sandstone consists of 45 vol.-% (Tab. 3-1) quartz sand (mean grain size of 0.07 mm) (Fig. B-12), 17 vol.-% biotrititic components in a micrite matrix (21 vol.-%) with some sparite cement (10 vol.-%) and iron-dolomite rhombohedrons (3 vol.-%).

The three others (TRU1-1-808.86, 804.83 and 798.92) are quite similar: they have less quartz sand, but more biotritus. TRU1-1-798.92, for example, consists of 36 vol.-% (Tab. 3-1) biotritus, 25 vol.-% quartz sand (Tab. 3-1), 30 vol.-% calcite cement and few other grains. The whole thin section looks like a mosaic of equal calcite crystals (Fig. B-13) without big differences between biotritus and cement.

«Humphriesiolith Formation» (TRU1-1-785.68, 784.67, 777.50, 776.49, 776.41, 774.93)

The «Humphriesiolith Formation» is composed of a lower iron-oolitic/limonitic interval (thin section TRU1-1-785.68 and 784.67) and an upper iron-oolitic interval (TRU1-1-777.50, 776.49, 776.41 and 774.93) and in between a marly interval with limestone beds.

The sample TRU1-1-785.68 – a biosparite (limonitic) – mainly consists of limonitic biotritus (echinoderms, bivalves, 48 vol.-%, Tab. 3-1), few other biogens (2 vol.-%) and pellets (7 vol.-%). They are cemented by calcite (21 vol.-%) and limonite (12 vol.-%). In consideration of the limonite within the biotritus and the cement, the analysed sample is more a limonite than a limestone.

TRU1-1-784.67 contains iron-oolids (16 vol.-%, Tab. 3-1), with sizes up to 1.2 mm, but distinctly more biotritus, such as serpulids (15 vol.-%), bivalves (9 vol.-%), echinoderms (7 vol.-%) and others (6 vol.-%). They are embedded in limonitic matrix and stellate cement (24 vol.-%) (Fig. B-14). Therefore, the bed of TRU1-1-784.67 may be a "hiatus bed".

TRU1-1-777.50, taken of the upper iron-oolitic interval, shows numerous thick-walled bivalves (27 vol.-%, Tab. 3-1), echinoderms (8 vol.-%), serpulids (6 vol.-%), other biogens (4 vol.-%) and pellets (7 vol.-%). Calcite cement (14 vol.-%), micrite matrix (10 vol.-%) and iron-dolomite (23 vol.-%) and quartz cement within a shell complete the microfacies.

The three samples TRU1-1-776.49, TRU1-1-776.41 and TRU1-1-774.93 are quite similar, limestones (iron-oolitic) to iron-oolites. They differ in their content of iron-oolids (17, 18 and 27 vol.-%, Tab. 3-1) and their composition and content of biogens: sponge spicules, echinoderms, "normal" and thick-walled bivalves (Tab. 3-1). All iron-oolids are, contrary to those of the older formations, still iron-mineralic (Fig. B-15 and B-16). The iron-oolids of TRU1-1-776.41 show flattened outlines (Fig. B-15). The iron-oolids of TRU1-1-774.93 reach sizes up to 1.5 mm (with mean of 1 mm), those of TRU1-1-776.41 have up to 1 mm (mean 0.6 mm). The components of all three beds are sedimented with micrite matrix.

«Parkinsoni-Württembergica-Schichten» and Variansmergel-Formation (TRU1-1-767.30, 766.72, 742.22, 735.98)

These two units consists mainly of silty, argillaceous beds with biotritus and few limestone beds. In addition, an around 1 m thick iron-oolid bearing marly interval is interstratified nearly 7 m above the base of the «Parkinsoni-Württembergica-Schichten». It represents probably the «Parkinsoni-Oolith» (767.35 – 766.15 m).

We analysed two thin sections of the probable «Parkinsoni-Oolith», TRU1-1-767.30 and TRU1-1-766.72. The lower one has no iron-oids: it consists of quartz silt (25 vol.-%, Tab. 3-1), small biotrititic components: 14 vol.-% echinoderms (Tab. 3-1), 12 vol.-% bivalves and 2 vol.-% others, as well as little brownish "nodules" (counted as intraclasts, 4 vol.-%), but their origin and composition is not clear, and micrite matrix (40 vol.-%). The upper one, TRU1-1 766.72, has iron-oids. It is a calcareous marl (iron-oolitic) which can be addresses as a "hiatus bed": limonitic iron-oids (17 vol.-%, Tab. 3-1), up to 1.2 mm, biotritus (21 vol.-%), quartz fine-sand (6 vol.-%), lying in micrite/marl matrix with stellate cement (21 vol.-%).

The other two thin sections have been taken of calcareous/quartz-rich beds, one of the «Parkinsoni-Württembergica-Schichten» (TRU1-1-742.22) and one of the Variansmergel Formation (TRU1-1-735.98). They look, in the case of the components very similar: biotritus (echinoderms 20 and 14 vol.-%, respectively, Tab. 3-1; bivalves: 17, and 19 vol.-% respectively) and quartz silt (28 vol.-%) or quartz sand (17 vol.-%). But the two beds differ in their cementation: TRU1-1-742.22 has a "stellate" cement (30 vol.-%) (Fig. B-17), TRU1-1-735.98 in contrast "normal" cement (30 vol.-%) around the components, and micrite matrix (16 vol.-%) (Fig. B-18).

Wutach Formation (TRU1-1 724.86)

The one sample, TRU1-1-724.86, of the Wutach Formation consists of 20 vol.-% iron-oids, with sizes of 0.1-1 mm, some biotritus (8 vol.-%), few quartz grains (4 vol.-%) and micrite matrix (64 vol.-%, Tab. 3-1). The iron-oids, which are still iron-mineralic, have small calcite cement rims.

Wildegge Formation (TRU1-1 724.78, 724.25, 723.04)

The Wildegge Formation has at its base lithological highly variable, but thin beds, which lead to some subunits as «Mumienmergel Bed», «Mumienkalk Bed», «Glaukonitsandmergel Bed» *sensu* Gygi (1977, 2000, 2012). So, the thin sections serve to look for "Mumien" (encrusted nodules), glauconite and iron-oids or other iron-mineralisations.

The lowermost sample (TRU1-1-724.78), sampled from the «Glaukonitsandmergel Bed», is a calcareous marl (iron-oolitic), consisting of 0.3 – 1 mm little iron-oids (18 vol.-%, Tab. 3-1), quartz silt (7 vol.-%), biotritus (6 vol.-%) and iron-dolomitic (13 vol.-%) marly matrix, as well as 2 vol.-% glauconite.

The thin-section TRU1-1-724.25 shows a strange phenomenon: an undulating limonite crust (Fig. B-20) and limonite "drops", both with iron-dolomite crystals (carbonated cells?) inside. The limonite crust covers a silty marl with sponge nodules and glauconite grains (Fig. B-19).

TRU1-1-723.04 is a limestone with different nodules: "normal" micritic sponge nodules (18 vol.-%, Tab. 3-1) and nodules, encrusted by encrusting foraminifera (15 vol.-%, counted as oncoids), some biotritus (8 vol.-%), pellets (5 vol.-%) and iron-dolomitic (10 vol.-%), partly marly, micrite matrix (44 vol.-%). Some burrows are also visible.

Villigen Formation (TRU1-1-705.65, 683.33)

The rather monotonous microfacies of the Villigen Formation has been analysed by two thin sections: TRU1-1-705.65 for the nodular, spongy limestones and TRU1-1-683.33 for the massive micrites.

TRU1-1-705.65, representing one facies of the Hornbuck Member at the base of the Villigen Formation, consists of micritic sponge nodules (66 vol.-%, Tab. 3-1), few bivalves (4 vol.-%), serpulids (4 vol.-%), foraminifera (2 vol.-%, other biogens) and micrite matrix (24 vol.-%).

TRU1-1-683.33, on the other hand, is a pure micrite, a mudstone with only some tiny (0.02 mm) dolomite rhombohedrons (10 vol.-%, Tab. 3-1).

Schwarzbach Formation (TRU1-1-646.21)

The one thin section (TRU1-1-646.21) of the Schwarzbach Formation consists of bivalve clasts (8 vol.-%, Tab. 3-1), echinoderm elements (5 vol.-%), pellets (11 vol.-%), foraminifera (2 vol.-%), dolomite (9 vol.-%) and micrite matrix (65 vol.-%). The dolomite crystals are concentrated in burrows and in the upper thin section part.

«Felsenkalke» + «Massenkalk» (TRU1-1-619.58, 611.22, 605.97, 594.04, 571.08, 539.86, 525.17)

Most of the analysed thin sections of the «Felsenkalke» and «Massenkalk» show more or less strong diagenetic alterations: TRU1-1-611.22, 605.97 and 594.07 have up to 85 vol.-% (Tab. 3-1) dolomite, TRU1-1-571.08 and 539.86 are microsparites/dedolomites.

TRU1-1-619.58 is a nodular calcareous marl with some biogenic components (16 vol.-%, Tab. 3-1). The nodules have sizes from 0.2 – 20 mm and irregular shapes. Some of them are sponge nodules (6 vol.-%), most (20 vol.-%) are pellets, originated by bioturbation. They stay in a marly, micritic matrix (56 vol.-%).

The two samples TRU1-1-611.22 and TRU1-1-594.07 are dolostones with a dolomite content of 65 and 85 vol.-% respectively (Tab. 3-1). The first one still shows remains of the primary composition: bivalve and echinoderm biotritus (8 vol.-%), pellets/micritic sponge nodules (5 vol.-%) and micrite matrix (22 vol.-%). The bivalves contain authigenic quartz. TRU1-1-594.07 is a pure dolostone with beautiful rhombohedrons (Fig. B-21) and a porosity of 8 vol.-% (Tab. 3-1) as well as calcite cement (7 vol.-%) within the pores.

TRU1-1-605.97 is a biomicrite (dolomitic), consisting of tiny biogenic components (12 vol.-%, Tab. 3-1), scattered small dolomite rhombohedrons (18 vol.-%) and micrite matrix (70 vol.-%). The two thin section TRU1-1-611.22 and TRU1-1-605.97 were taken, among other things, to verify the glauconitic content of the two calcareous marl beds mentioned in the Dossier III (611.23 – 610.67 m and 606.80 – 605.90 m). However, both thin sections do not contain glauconite grains.

Both samples TRU1-1-571.08 and TRU1-1-539.86 show a pelletoidal, microsparitic structure with some visible rhombohedron edges, some bivalves, sponge nodules, sponge spicules and micrite matrix. But it is difficult to distinguish microsparite grown from neomorphism and microsparite developed from dedolomitisation. Therefore, all these vague structured parts are counted as microsparite (Tab. 3-1). In the case of the pellets (62 vol.-%, TRU1-1-539.86) it is not sure which ones are really components and which ones are relicts of diagenetic alterations.

And at last, TRU1-1-525.17 is a "normal" biomicrite with small biogenic components (16 vol.-%, Tab. 3-1) and micrite matrix (77 vol.-%).

Tab. 3-1: Microfacies analysis from TRU1-1 (1'153.72 – 525.17 m); numbers in vol.-%

Microfacies analysis TRU1-1 (525.17 - 1'153.72 m)	clay matrix, micrite, microsparite	dolomitic matrix	limonitic matrix	components (and biohermal organisms)														cements, diagenesis													
				calcitic biogenes								allochems						calcite cement	"stellate cement" (s) cone-in-cone calcite (c)	(Fe)-dolomite	dedolomite	anhydrite, gypsum	quartz cement	pyrite	limonite, Fe-mineral- ised nodules	siderite	glauconite	mica	porosity		
				echinoderms	bivalves	limonitic echinod. + bivalves	serpulids	corals	sponges, spicules	other biogenes	Fe-stromatolite + stromatolitic clasts	pellets, peloids	ooids	oncoids	Fe-ooids	intraclasts	detrital quartz + silic. rock fragm.													quartz grainsize (mm)	
525.17 m: biomicrite «Felsenkalke» + «Massenkalk»	77			5	4				4	3								4			3										
539.86 m: pelmicrosparite «Felsenkalke» + «Massenkalk»	34										62							4													
571.08 m: biopelmicrite / dedolomite «Felsenkalke» + «Massenkalk»	60				5					18		12						5													
594.07 m: dolostone «Felsenkalke» + «Massenkalk»																		7		85									8		
605.97 m: biomicrite (dolomitic) «Felsenkalke» + «Massenkalk»	70			4	8														18												
611.22 m: dolostone (calcareous) «Felsenkalke» + «Massenkalk»	22			3	5							5							65												
619.58 m: calcareous marl, nodular «Felsenkalke» + «Massenkalk»	56			6	5				6	5		20											2								
646.21 m: biopelmicrite (dolomitic) Schwarzbach Fm.	65			5	8					2		11							9												
683.33 m: micrite (dolomitic) Villigen Fm.	90																		10												
705.65 m: biomicrite, nodular Villigen Fm.	24				4		4		66	2																					
723.04 m: biomicrite nodular/ ?oncomic. Wildeggen Fm.	44			3	5				18			5		15					10												
724.25 m: limestone (iron-stromatolitic) Wildeggen Fm.	50			3	3						20	4					5	0.04		10							5				
724.78 m: calcareous marl (iron-oolitic) Wildeggen Fm.	53			3	3									18		7	0.05		13								2	1			
724.86 m: limestone (iron-oolitic) Wutach Fm.	64			3	5									20		4	0.05	4													
735.98 m: biosparite (sandy) Varisanzmergel Fm.	16			14	19					4						17	0.07	30													
742.22 m: biosparite (silty) / "hiatus b.?" «Parkinsoni-Württemb.-Sch.»				20	17					5						28	0.06		30												
766.72 m: c. marl (iron-ool.) / "hiatus b." «Parkinsoni-Württemb.-Sch.»	35			5	13					3				17		6	0.07		21												
767.30 m: biomicrite (silty) «Parkinsoni-Württemb.-Sch.»	40			14	12					2					4	25	0.06						3								
774.93 m: limestone (iron-oolitic) «Humphriesoolith Fm.»			62	3	9					2				18		4	0.04					2									
776.41 m: limestone (iron-oolitic) «Humphriesoolith Fm.»			42	9	11				9	2				17		3		5				2									
776.49 m: limestone (iron-oolitic) «Humphriesoolith Fm.»			25	13	17				10	3				27					3			2									
777.50 m: biosparite (dolomitic) «Humphriesoolith Fm.»	10			8	27		6			4		7						14	23			1									
784.67 m: limestone (iron-oolitic) «Humphriesoolith Fm.»			13	7	9		15			6				16		8		24				2									
785.68 m: biosparite (limonitic) «Humphriesoolith Fm.»						48				2		7				4		21	6				12								
798.92 m: sandy limestone Wedelsandstein Fm.				14	18		2			2		3				25	0.08	30				1	3				1	1			
804.83 m: sandy limestone Wedelsandstein Fm.	12			12	13					2		4				28	0.07	25					3					1			
808.86 m: sandy limestone Wedelsandstein Fm.	10			11	14		1			2		5				33	0.08	20				2				1	1				
810.82 m: calcareous sandstone Wedelsandstein Fm.	21			7	8					2						45	0.07	10	3			2					2				
815.44 m: intramicrite (sandy) Wedelsandstein Fm.	27			9	7				2	2					28	20	0.07					4					1				
816.28 m: iron-oolite (calcareous) «Murchisonae-Oolith Fm.»	38			3	3									48				5				3									
816.40 m: limestone (iron-oolitic) «Murchisonae-Oolith Fm.»	43			8	6									28	4							11									
826.03 m: hardground Opalinus Clay	22			5	11										11	19	0.05	5					18		8		1				
831.91 m: hardground Opalinus Clay	13			8	6										45	12	0.05								15		1				
832.49 m: calcareous marl (silty) Opalinus Clay	75			7	3											10	0.05					5									
833.00 m: hardground Opalinus Clay	44			9	5					1	3	6			11*		14	0.05					6					1			
836.84 m: hardground Opalinus Clay	31			12	6					3					23	10	0.06		11			4									
843.33 m: hardground Opalinus Clay	40			7	3										21	12	0.05		5			10					2				
896.67 m: "hiatus bed" Opalinus Clay	30															5	0.04		65												
930.13 m: biomicrite Staffellegg Fm. (Gross Wolf Mb.)	68			14	15					3																					
935.81 m: biomicrite Staffellegg Fm. (Rietheim Mb.)	48				43					3												6									
962.44 m: biomicrite Staffellegg Fm. (Begglingen Mb.)	32			24	28					5								8				3									
965.78 m: biomicrite (iron-oolitic) Staffellegg Fm. (Begglingen Mb.)	10			8	14	11				13				12				4	8			5		15							
971.35 m: oosparite Staffellegg Fm. (Schambelen Mb.)					13					2		38			8	3	0.10	33				3									
972.00 m: "hiatus bed", biom. (f.-sandy) Klettgau Fm. (Belchen Mb.)	33				32											15	0.10		17			3									
988.32 m: dolomitic marl Klettgau Fm. (Gruhalde Mb.)		85														12	0.05	3													
992.67 m: intraformational breccia Klettgau Fm. (Seebi Mb.)		23													73				4												
999.87 m: sandstone (dolomitic) Klettgau Fm. (Seebi Mb.)		7													3	74	0.80	16													
1'003.02 m: sandstone Klettgau Fm. (Seebi Mb.)																79	0.60	4	2			5							10		
1'006.80 m: intraformational breccia Klettgau Fm. (Gruhalde Mb.)		12													83	5	0.05														
1'020.30 m: sandstone (argillaceous) Klettgau Fm. (Ergolz Mb.)	22															62	0.10					11					5				
1'055.52 m: dolomitic marl Bankenloch Fm.	18																		60		22										
1'103.66 m: dolostone (mic.to mic.spar.) Schinznach Fm. (Starnberg Mb.)		63			12					7		5	4																9		
1'153.62 m: oomicrite Schinznach Fm. (Leutsch. + Kienb. Mb.)	12			8	5							7	54					6	5			3									
1'153.72 m: oosparite (dolomitic) Schinznach Fm. (Leutsch. + Kienb. Mb.)	10			5						3		8	38					10	26												

3.2 Ammonite stratigraphy

Of the recovered ammonites (list Appendix A2), specimens (depth 787.07 m and 705.67 m) could not be extracted because there was no separation between the rock matrix and the fossil, and the rock matrix did not react to potassium hydroxide. Several ammonites were unfortunately so damaged by drilling or sampling that the genus or species could not be determined.

Typically, the ammonites are distributed differently over the individual time periods drilled by the well. They are relatively common in the Toarcian and Early Aalenian, where ammonite fragments and cross sections are locally very common in the range between 925 and 911 m. In the Late Aalenian and Early Bajocian, ammonites are very rare with the exception of the Humphriesianum Zone. Only in the Late Bajocian could they be found more frequently again. In the Bathonian and Callovian evidence of ammonites is sparse. In addition, the objects could not be well-determined because of their size or preservation. Only in the succession of the Oxfordian stage the ammonites become more numerous, but also difficult to determine. 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 can have an effect on the biostratigraphic classification.

We documented a selection of ammonites with photographs, and these are shown on four plates (Plate I-IV) 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 from a profile section are present, the more precisely we can determine the biostratigraphic classification of that section (Tab. 3-2). Furthermore, it must be considered that not all ammonites have the same index value and that the state of preservation of the objects also plays an important role. In this respect, a certain error must always be expected. This error is in the range of about one ammonite Subzone (SZ) but can be as high as one ammonite Zone (Z) when the available data is insufficient.

Staffelegg Formation

- 947.41 m: *Amaltheus* ex gr. *margaritatus* (de Montfort, 1808). The ammonite is a compressed steinkern and rather poorly preserved. Age: It comes from the Late Pliensbachian, Margaritatus Zone. Lithology: biotrititic limestone (slightly argillaceous) with belemnites, a Rhynchonellida and numerous shell fragments (bivalves?). The ammonite is illustrated on Plate I, Fig. 1 (Appendix C, for all figures in this chapter).
- 943.83 m: *Dactylioceras* (*Orthodactylites*) sp. ammonite fragment in steinkern preservation. The genus *Dactylioceras* is restricted to the Early Toarcian. Age: Tenuicostatum Zone? Lithology: grey mica-bearing marl with pyritized burrow fillings, a belemnite, bivalves and shell fragments. The ammonite fragment is illustrated on Plate I, Fig. 2.
- 933.17 m: *Haugia?* sp. Truncated ammonite steinkern. Age: the genus occurs in Late Toarcian, in the Variabilis Zone. Lithology: light grey biotrititic limestone with numerous burrows with diameters up to 3 mm. In the rock there are further partly pyritized ammonite cross sections. The ammonite is illustrated on Plate I, Figs. 3a and 3b.

- 932.14 m: *Pseudogrammoceras* ex gr. *fallaciosum* (Bayle, 1878). Truncated ammonite. Age: the species is very common in the Thouarsense Zone, Fallaciosum Subzone. Lithology: light grey, splintery, strongly bioturbated limestone with ammonites and burrows up to 4 mm diameter. The ammonite is illustrated on Plate I, Fig. 4.
- 929.18 m: *Pleydellia* sp. several fragments and one internal whorl. Age: Aalensis Zone, probably Aalensis Subzone. Lithology: dark grey, biotrititic calcareous marl (echinoderms, shell fragments). Three ammonite fragments are illustrated on Plate I, Figs. 5a to 5c.
- 928.10 m: *Pleydellia* sp. A poorly preserved, deformed steinkern and several fragments. Age: due to ribbing, Aalensis Zone, possibly Torulosum Subzone. Lithology: dark grey biotrititic claystone. The ammonite is illustrated on Plate I, Fig. 6.
- 928.03 m: *Pleydellia* ex gr. *buckmani* (Maubeuge, 1947). Two flattened, somewhat indistinct imprints. Age: Aalensis Zone, Torulosum Subzone. Lithology: grey biotrititic marl. The ammonite is illustrated on Plate I, Fig. 7.

Opalinus Clay

- 917.53 m: *Leioceras opalinum* (Reinecke, 1818). Flattened truncated specimen with recrystallized calcitic shell preservation. The shell was regenerated after an injury in the body chamber area. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark grey claystone. The ammonite is illustrated on Plate II, Fig. 1.
- 915.74 m: *Leioceras opalinum* (Reinecke, 1818) Microconch. Flattened specimen with recrystallized calcitic shell preservation and partially preserved apophysis. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark grey claystone. The ammonite is illustrated on Plate II, Fig. 2.
- 913.89 m: *Leioceras opalinum* (Reinecke, 1818). Incomplete, compacted truncated specimen with recrystallized calcitic shell preservation. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark grey claystone with shell fragments (ammonites?) and pyrite concretion. The ammonite is illustrated on Plate II, Fig. 3.
- 896.19 m: *Leioceras opalinum* (Reinecke, 1818). Flattened truncated specimen with recrystallized calcitic shell preservation. Age: occurs in the Opalinum Zone, Opalinum Subzone. Lithology: dark grey silty claystone. The ammonite is not illustrated.

«Humphriesiolith Formation»

- 787.07 m: Ammonite indet. The ammonite could not be extracted because there was no separation between the rock matrix and the fossil. No age determination is possible. The ammonite is not illustrated.
- 776.99 m: *Chondroceras* ex gr. *gervillii* (Sowerby, 1818). Several specimens. Age: Humphriesianum Zone, Humphriesianum Subzone, Gervillii cycloides faunal horizon. Lithology: biotrititic limestone. Other fossils are bivalves (genus *Entolium*), echinid spines and an asterozoan ossicle (marginalia). The ammonites are illustrated on Plate II, Figs. 4 and 5.

- 776.74 m: *Stephanoceras* sp. Steinkern with compacted body chamber. Age: Humphriesianum Zone, Humphriesianum Subzone. Lithology: very fine-grained dark grey-brown iron-oolite. Diameter of the iron-oolids about 0.1 mm. Other fossils are a few bivalve fragments. The ammonite is illustrated on Plate II, Figs. 6a and 6b.
- 775.17 m: Truncated ammonite in shell preservation. Age: due to the form of the venter, the ammonite probably originates from the Late Bajocian. Lithology: grey-brown, limestone (iron-oolitic, slightly argillaceous). The iron-oolids are goethitic/limonitic and reach diameters up to about 1.1 mm. Other fossils are bivalves. The ammonite is not illustrated.

«Parkinsoni-Württembergica-Schichten»

- 766.92 m: *Parkinsonia* ex gr. *subarietis-rarecostata*. Ammonite with recrystallized shell preservation. Age: Parkinsoni Zone, Acris Subzone. Lithology: dark grey-brown limestone (iron-oolitic, argillaceous). The iron ooids are cloud-like distributed in the rock. Diameter of the iron-oolids up to about 0.6 mm. The shape of the iron ooids is round to oval in cross-section. Other fossils are belemnites, ammonites, oysters and bivalves. The ammonite is illustrated on Plate III, Figs. 1a and 1b.
- 766.76 m: *Parkinsonia* ex gr. *subarietis-rarecostata*. Two steinkerne of truncated ammonites with shell preservation in the area of the phragmocone. Age: Parkinsoni Zone, Acris Subzone. Lithology: dark, grey-brown marl (iron-oolitic). Diameter of the iron-oolids up to about 0.8 mm. The shape of the iron-oolids is round to oval in cross-section. There are also broken specimens. As a further fossil an echinid spine could be found in cross section. The ammonites are illustrated on Plate III, Figs. 2a to 3b.
- 766.53 m: *Parkinsonia*? sp. Macroconch. Flattened steinkern. Age: Parkinsoni Zone? Lithology: dark brown marl (iron-oolitic). The iron-oolids are distributed like clouds in the rock. Diameter of the iron-oolids up to about 0.6 mm. The shape of the iron-oolids is round to oval in cross-section. There are also broken specimens. Further fossils are a belemnite fragment, an oyster, and a small ammonite. The ammonite is illustrated on Plate III, Fig. 4.

Variansmergel Formation

- 732.94 m: *Morphoceras* sp. Steinkern in pyritic preservation. Age: Early Bathonian. Lithology: mica-bearing grey marl. Other fossils are small oysters ("*Ostrea*" *knorri*) and another bivalve. The ammonite is illustrated on Plate III, Fig. 5.

Wutach Formation

- 726.89 m: Ammonite. Truncated specimen with partial shell preservation. Age: Late Bathonian to Early Callovian. Lithology: limestone (iron-oolitic, argillaceous). The iron-oolids measure up to one mm in diameter. The iron-oolids are dark and up to 0.5 mm in size. They are of goethitic to limonitic composition. The inner part is often replaced by calcite. The ammonite is not illustrated.
- 725.08 m: Perisphinctidae indet. Truncated phragmocon of a macroconch. The ammonite is not determinable on genus or species level. Age: probably Bathonian or Callovian. Lithology: beige to grey limestone (iron-oolitic, argillaceous). The ammonite is not illustrated.

Wildegge Formation

- 724.30 m: *Kranaosphinctes?* sp. Truncated specimen with partial preservation of the shell in an intraclast ("mummy"). Age: Plicatilis Zone? Lithology: dark grey limestone with light clasts (reworked burrows?) and partly limonite encrusted intraclasts. Glauconite bearing (matrix and clasts) and some biotritus (echinoderms). The ammonite is not illustrated.
- 724.15 m: Oppelidae indet. Truncated specimen in steinkern preservation. Age: the fragment is too small for dating. Lithology: hard, light-coloured, bioturbated limestone with some glauconite and biotritus (echinoderms). The ammonite is not illustrated.
- 723.48 m: *Perisphinctes* sp. Microconch. Flattened steinkern. Age: probably Transversarium Zone. Lithology: dark grey marl with few intraclasts and numerous burrows. The ammonite is not illustrated.
- 723.10 m: Perisphinctidae indet. Truncated phragmocone. Age: Oxfordian. Lithology: grey limestone with dark grey intraclasts and burrows. Other fossils are crinoid skeletal elements. The ammonite is not illustrated.
- 723.07 m: *Perisphinctes* sp. Truncated phragmocone. Age: Transversarium Zone. Lithology: grey limestone with dark grey intraclasts and burrows. Other fossils are crinoid skeletal elements. The ammonite is illustrated on Plate IV, Fig. 1.
- 722.21 m: *Dichotomosphinctes?* sp. Truncated incomplete steinkern. Age: Transversarium Zone, Rotoides Subzone or Bifurcatus Zone, Stenocycloides Subzone. Lithology: dark grey marl with few bioclasts (echinoderms). The ammonite is illustrated on Plate IV, Fig. 2.
- 705.67 m: Perisphinctidae? indet. Truncated small ammonite steinkern. The ammonite could not be extracted because there was no separation between the rock matrix and the fossil, and the rock matrix did not react to potassium hydroxide. No age determination is possible. The ammonite is not illustrated.

Tab. 3-2: Ammonite determination from TRU1-1

Depth [m]	Identification	Ammonite Zone (Subzone) or Age
705.67	Perisphinctidae indet.	no
722.21	<i>Dichotomosphinctes?</i> sp.	Transversarium Zone (Rotoides SZ) or Bifurcatus Zone (Stenocycloides SZ)
723.07	<i>Perisphinctes</i> sp.	Transversarium Zone
723.10	Perisphinctidae indet.	Oxfordian
723.48	<i>Perisphinctes</i> sp. Microconch	probably Transversarium Zone
724.15	Oppelidae indet.	no
724.30	<i>Kranaosphinctes?</i> sp.	Plicatilis Zone?
725.08	Perisphinctidae indet.	Bathonian or Callovian?
726.89	Ammonite	Late Bathonian to Early Callovian
732.94	<i>Morphoceras</i> sp.	Early Bathonian
766.53	<i>Parkinsonia?</i> sp. Macroconch	Parkinsoni Zone?
766.76	<i>Parkinsonia</i> ex gr. <i>subarietis-rarecostata</i>	Parkinsoni Zone (Acris Subzone)
766.92	<i>Parkinsonia</i> ex gr. <i>subarietis-rarecostata</i>	Parkinsoni Zone (Acris Subzone)
775.17	Ammonite	Late Bajocian
776.74	<i>Stephanoceras</i> sp.	Humphriesianum Zone (Humphriesianum SZ)
776.99	<i>Chondroceras</i> ex gr. <i>gervillii</i> (Sowerby, 1818)	Humphriesianum Zone (Humphriesianum SZ, Gervillii Horizon)
787.07	Ammonite, indet.	no
896.19	<i>Leioceras opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum SZ)
913.89	<i>Leioceras opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum SZ)
915.74	<i>Leioceras opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum SZ)
917.53	<i>Leioceras opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum SZ)
928.03	<i>Pleydellia</i> ex gr. <i>buckmani</i> (Maubeuge, 1947)	Aalensis Zone (Torulosum SZ)
928.10	<i>Pleydellia</i> sp.	Aalensis Zone (Torulosum SZ?)
929.18	<i>Pleydellia</i> sp.	Aalensis Zone (probably Aalensis SZ)
932.14	<i>Pseudogrammoceras</i> ex gr. <i>fallaciosum</i> (Bayle, 1878)	Thouarsense Zone (Fallaciosum Subzone)
933.17	<i>Haugia?</i> sp.	Variabilis Zone
943.83	<i>Dactylioceras</i> (<i>Orthodactylites</i>) sp.	Tenuicostatum Zone?
947.41	<i>Amaltheus</i> ex gr. <i>margaritatus</i> (de Montfort, 1808)	Margaritatus Zone

System	Stage	Zone	Subzone
Jurassic	Late	Oxfordian	
	Middle	Callovian	
	Early	Bathonian	
	Late	Bajocian	
Jurassic	Early	Toarcian	
	Late	Pliensbachian	
	Early	Sinemurian	
Jurassic	Late	Hettangian	
	Early	Hettangian	

TRU1-1

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 TRU1-1

3.3 Palynostratigraphy

The studied samples mostly yielded a good palynological residue with rich and diverse palynofloras. Preservation is good. The palynomorph assemblages are composed of mainly dinoflagellate cysts, pollen and spores. Minor components are prasinophytes, acritarchs, fungal remains, foraminiferal test linings and green algae (e.g. *Botryococcus*). A total of 146 dinoflagellate cyst taxa, 25 other aquatic palynomorphs and 47 pollen and spore taxa are recorded.

Some reworked sporomorphs (*Densosporites* spp., *Ricciisporites tuberculatus*) 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 44 studied samples from core Trüllikon-1-1 are dated to span the interval from the Aalenian/Toarcian boundary to the Callovian. Eight palynological samples were taken from ammonite samples (marked in grey in Appendix A4). The biostratigraphic results of the analyses of palynoflora and the ammonites match well. There are 19 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 interval 928.09 – 927.54 m (3 samples): Late Toarcian, Aalensis Zone to Early Aalenian, Opalinum Zone, Opalinum Subzone

The palynoflora of the three samples in this interval is characterised by very high abundances of one species, *Evansia?* cf. *granochagrinata*. This species dominates the palynoflora reaching 39 %, 77 % or 85 % respectively, of all palynomorphs counted. Other dinoflagellate cysts present, though in low numbers, belong to the family Phallocystaceae (*Andreodinium* aff. *elongatum*, *Andreodinium* sp. 2, *Dodekovia bullula*, *Dodekovia knertensis*, *D. pseudochytroideis*, *Moesiodinium raileanui* (questionable), *Reutlingia cardobarbata*, *R. nasuta*, *Susadinium scrofoides*) and to the family Valvaeodiniaceae (*Valvaeodinium* spp., *V. cavum*, *V. sphaerechinatum*, *V. vermipellitum*). There are species of *Nannoceratopsis* (*Nannoceratopsis* spp., *N. gracilis* s.l., *N. triangulata*), species of *Scriniocassis* (*Scriniocassis limbicavatus*, *S. priscus*, *S. weberi*), as well as *Kallosphaeridium praussii*, *Hystrichodinium?* sp., *Mancodinium semitabulatum*, *Wallodinium laganum* and *Wittnaudinium minutum*. *Nannoceratopsis triangulata* and *Wallodinium laganum* were not recorded in the bottommost sample.

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

Composition of the dinoflagellate cyst assemblages is typical for the interval straddling the Toarcian/Aalenian boundary. *Evansia?* cf. *granochagrinata* and *Wallodinium laganum* have their FADs (First Appearance Datums) in the Late Toarcian, probably Levesquei Zone. *Kallosphaeridium praussii* and *Nannoceratopsis triangulata* first appear in the latest Toarcian or close to the Toarcian/Aalenian boundary. The very high abundance or dominance of *Evansia?* cf. *granochagrinata* is typical for an age of the samples straddling the Toarcian/Aalenian boundary, Aalensis Zone/Opalinum Subzone. This characteristic bioevent at the Early to Middle Jurassic boundary defines the palynostratigraphical unit A of Feist-Burkhardt & Pross (2010).

Sample interval 906.87 – 823.12 m (7 samples): Early Aalenian, Opalinum Zone, Opalinum Subzone

Composition of the dinoflagellate cyst assemblages is similar to the interval below. *Evansia?* cf. *granochagrinata* is still common to abundant, but abundance decreases. Diversity of Phallocystaceae and Valvaodiniaceae increases with the occurrence of further species such as *Dodekovia* spp., *Ovalicysta hiata*, *Parvocysta bjaerkei*, *Phallocysta? frommernensis* (common) and *Reutlingia fausta*. The species *Nannoceratopsis dictyambonis*, *N. gracilis* s.s., *N. plegas plegas* and *N. tricerias* have their first occurrence in this interval.

The interval is defined by the first occurrence of *Phallocysta? frommernensis* to the last occurrence of *Wallodinium laganum*. The species *Phallocysta? frommernensis* and *Scriniocassis weberi* have their last occurrence near the top of this interval.

According to Feist-Burkhardt & Pross (2010) there are four marker species for the Early Aalenian Opalinuston Formation (German stratigraphy): *Kallosphaeridium praussii*, *Phallocysta? frommernensis*, *Nannoceratopsis triangulata* and *Wallodinium laganum*. All four marker species occur in this interval. The acme of *Phallocysta? frommernensis* defines the palynostratigraphical unit B of Feist-Burkhardt & Pross (2010) of the Opalinuston Formation.

The sample interval is therefore dated as Early Aalenian Opalinum Zone, Opalinum Subzone and corresponds to palynostratigraphical unit B of Feist-Burkhardt & Pross (2010).

The occurrence of *Luehndea spinosa* in the uppermost two samples (828.71 m and 823.12 m) indicates reworking of Early Jurassic Late Pliensbachian to earliest Toarcian sediments in the source area.

Sample interval 818.03 – 816.44 m (2 samples): Early Aalenian, Opalinum Zone, ? Bifidatum Subzone

Composition of the dinoflagellate cyst assemblages is still similar to that of the interval below, but differs in showing the common to abundant occurrence of questionable *Batiacasphaera* sp. A. The species *Nannoceratopsis triangulata* has its last occurrence at the top of the interval.

The interval is defined by the first occurrence of questionable *Batiacasphaera* sp. A to the last occurrence of *Nannoceratopsis triangulata* and the first occurrence of *Evansia? spongogranulata* in the interval above.

Batiacasphaera spp. has its FAD in the upper part of Opalinum Zone. *Batiacasphaera* sp. A is known to be abundant in the Bifidatum Subzone (ex «Comptum» Subzone, Dietze et al. 2021) of Opalinum Zone. *Nannoceratopsis triangulata* has its LAD (Last Appearance Datum) in the Opalinum Zone. *Evansia? spongogranulata* has its FAD in the Murchisonae Zone.

The interval is dated Opalinum Zone, probably Bifidatum Subzone (ex «Comptum» Subzone).

Sample interval 816.03 – 815.67 m (2 samples): Middle Aalenian, Murchisonae Zone to lower Bradfordensis Zone

The interval is characterised by the first occurrence of *Evansia? spongogranulata* and the common occurrence of *Nannoceratopsis plegas* with its subspecies *N. plegas brevicornis*, *N. plegas dictyornata* and *N. plegas plegas*. The species *Scriniocassis limbicavatus* and *S. priscus* have their last occurrences at the top of the interval. Representatives of the genus *Dissiliodinium* are not yet present but have their first occurrence in the interval above.

Evansia? spongogranulata has its FAD in Murchisonae Zone. *Scriniocassis limbicavatus* and *S. priscus* have their LADs in Bradfordensis Zone. *Dissiliodinium* spp. have an FAD in the upper part of Bradfordensis Zone.

The sample is dated Murchisonae to lower Bradfordensis Zone.

The occurrence of *Luehndea spinosa* in the uppermost sample (815.67 m) indicates reworking of Early Jurassic Late Pliensbachian to earliest Toarcian sediments in the source area.

Sample 814.17 m (1 sample): Early Bajocian, Ovale Zone

The dinoflagellate cyst assemblage in this sample differs a lot from the interval below. Representatives of the genus *Dissiliodinium* are abundant. The following species have their first occurrence: *Dissiliodinium* aff. *giganteum*, *D. giganteum* (abundant), *D. lichenoides*, *Evansia? eschachensis*, *Gongylodinium erymnoteichon* (abundant) and *Reutlingia gochtii*.

The interval is defined as from the first occurrence of *Dissiliodinium giganteum* to the first occurrence of *Cavatodissiliodinium hansgochtii* in the interval above.

Dissiliodinium giganteum has an FAD in the Ovale Zone. *Evansia? eschachensis* has an LAD in Ovale Zone. *Cavatodissiliodinium hansgochtii* has an FAD in Laeviuscula Zone.

The sample is dated Ovale Zone.

Sample 810.65 m (1 sample): Early Bajocian, Ovale to Laeviuscula Zone

In addition to species known from below, this sample shows the first occurrence of *Cavatodissiliodinium hansgochtii* (common) and of *Durotrigia daveyi*. The species *Evansia? eschachensis* last occurs in this sample. *Batiacasphaera laevigata* has its first occurrence in the interval above.

The interval is defined by the first occurrence of *Cavatodissiliodinium hansgochtii* to the last occurrence of *Evansia? eschachensis*.

The LAD of *Evansia? eschachensis* is in Ovale Zone. The FAD of *Cavatodissiliodinium hansgochtii* and *Batiacasphaera laevigata* is in Laeviuscula Zone.

The sample is dated Ovale to Laeviuscula Zone.

Sample interval 797.44 – 784.01 m (6 samples): Early Bajocian, Laeviuscula Zone

Dinoflagellate cyst assemblages are similar to the interval below with i.a. *Batiacasphaera* spp., *Cavatodissiliodinium hansgochtii*, *Dissiliodinium* spp., *Dissiliodinium giganteum*, *Durotrigia daveyi* and *Gongylodinium erymnoteichon*. In some samples these species may be common to abundant. The species *Batiacasphaera laevigata* has its first occurrence at the base of the interval.

The interval is defined as from the first occurrence of *Batiacasphaera laevigata* to the first occurrence of *Kallosphaeridium hypornatum* in the interval above.

The FAD of *Batiacasphaera laevigata* is Laeviuscula Zone. The FAD of *Kallosphaeridium hypornatum* is Sauzei Zone.

The interval is dated Laeviuscula Zone.

Sample interval 783.78 – 778.21 m (2 samples): Early Bajocian, Sauzei Zone

Assemblages in this interval still resemble those from below. *Kallosphaeridium hypornatum* has its first occurrence at the base of the interval. Last occurrences in the interval are *Cavatodissiliodinium hansgochtii*, *Dissiliodinium giganteum*, *Evansia? spongogranulata* and *Mancodinium semitabulatum*. The last three occur up to the top of the interval.

The interval is defined as from the first occurrence of *Kallosphaeridium hypornatum* to the last occurrence of *Dissiliodinium giganteum* and *Evansia? spongogranulata* and the first occurrence of *Acanthaulax crispa* and others in the interval above.

The FAD of *Kallosphaeridium hypornatum* is in Sauzei Zone. The LADs of *Dissiliodinium giganteum* and *Evansia? spongogranulata* are in Sauzei Zone. The FAD of *Acanthaulax crispa*, is in Humphriesianum Zone.

The interval is dated Sauzei Zone.

Sample interval 777.82 – 776.73 m (3 samples): Early Bajocian, Humphriesianum Zone

The sample is characterised by numerous first occurrences: *Acanthaulax crispa*, questionable *Atopodinium* sp. 1, *Cavatodissiliodinium* sp. 1, sp. 2, sp. 3, *Durotrigia filapicata*, questionable "*Hypolytodium*" sp., questionable *Phallocysta thomasii*, *Valensiella/Ellipsoidictyum* spp. and *Wanaea* sp. 1. The species "*Hypolytodium*" sp. and *Phallocysta thomasii* are recorded with questionable specimens only. They last occur in the topmost sample of the interval.

The interval is defined as from the first occurrence of *Acanthaulax crispa* and others to the last occurrence of questionable "*Hypolytodium*" sp. and *Phallocysta thomasii*.

All species mentioned have FADs within Humphriesianum Zone. The ranges of "*Hypolytodium*" sp. and *Phallocysta thomasii* are considered to be restricted to the Romani and Humphriesianum Subzones of the Humphriesianum Zone.

The sample is dated Humphriesianum Zone.

Sample 775.65 m (1 sample): Early Bajocian, Humphriesianum Zone, Blagdeni Subzone

Samples of this interval are similar to before but lack "*Hypolytodium*" sp. and *Phallocysta thomasii*. In addition, there are the first occurrences of unquestionable *Atopodinium* sp. 1, *Rhynchodiniopsis? regalis* and *Rhynchodiniopsis? sp. 1*.

"*Hypolytodium*" sp. and *Phallocysta thomasii* are considered to have LADs of Humphriesianum Subzone of Humphriesianum Zone. *Rhynchodiniopsis? regalis* has its FAD in Blagdeni Subzone of Humphriesianum Zone.

The sample is dated Blagdeni Subzone of Humphriesianum Zone.

Sample 775.16 m (1 sample): Early Bajocian, Humphriesianum Zone, Blagdeni Subzone to Late Bajocian, Niortense Zone

The assemblage is characterised by numerous first occurrences: *Atopodinium polygonale*, *Endoscrinium* spp., *Gongylodinium hocneratum*, *Gonyaulacysta pectinigera*, *Korystocysta gochtii*, *Meiourogonyaualax valensii*, *Nannoceratopsis spiculata*, *Rosswangia simplex*, *Valvaeodinium spinosum*. The species *Durotrigia daveyi* is common in this sample and also in the next higher sample in the interval above. Last occurring in this interval is also unquestionable *Nannoceratopsis gracilis* s.l.

The FADs of the first occurring species are Humphriesianum Zone (*Meiourogonyaualax valensii*, *Nannoceratopsis spiculata*) and Niortense Zone (*Atopodinium polygonale*, *Gonyaulacysta pectinigera*, *Korystocysta gochtii*, *Rosswangia simplex*, *Valvaeodinium spinosum*) and higher within Niortense Zone (consistent *Gongylodinium hocneratum*). The LAD of *Nannoceratopsis gracilis* s.l. is Niortense Zone.

The top of consistent *Durotrigia daveyi* is considered to be Humphriesianum Zone, but the species may reach up to Garantiana Zone.

The dinoflagellate cyst taxa present indicate an age of Niortense Zone. The concurrent common occurrence of *Durotrigia daveyi*, though, may indicate a slightly older age of latest Humphriesianum Zone (Blagdeni Subzone).

Sample interval 774.47 – 767.51 m (2 samples): Late Bajocian, Niortense to Garantiana Zone

The assemblages show again numerous first occurrences, i.a. *Carpathodinium predae*, *Ctenidodinium continuum*, *Ctenidodinium sellwoodii* group and *Endoscrinium asymmetricum*. The species *Durotrigia daveyi* is common in the bottom sample of the interval and is recorded higher up only with a few questionable specimens.

The FADs of *Carpathodinium predae* and *Ctenidodinium continuum* are Niortense Zone, that of *Endoscrinium asymmetricum* is higher in Niortense Zone, that of *Ctenidodinium sellwoodii* group is Garantiana Zone. The top of consistent *Durotrigia daveyi* is considered to be top Humphriesianum Zone, but the species may reach up to Garantiana Zone.

The sample interval is interpreted as Niortense to Garantiana Zone in age.

Sample 766.75 m (1 sample): Late Bajocian, Garantiana to Parkinsoni Zone

The assemblage in this sample is similar to below. *Durotrigia daveyi* has its last occurrence in this sample with a few questionable specimens. *Chytroeisphaeridia chytroeides* occurs the first time.

The sample interval is defined by the last occurrence of questionable *Durotrigia daveyi* to the first occurrence of *Gonyaulacysta eisenackii* and *Orobodinium automobile* in the interval above.

The LAD of *Durotrigia daveyi* is Garantiana Zone. The FADs of *Gonyaulacysta eisenackii* and *Orobodinium automobile* are Parkinsoni Zone.

The sample is dated Garantiana to Parkinsoni Zone.

Sample 765.81 m (1 sample): Late Bajocian, Parkinsoni Zone

The sample is characterised by the first occurrences of *Gonyaulacysta eisenackii* and *Orobodinium automobile* and the last occurrence of *Acanthaulax crispa*.

The FADs of *Gonyaulacysta eisenackii* and *Orobodinium automobile* are Parkinsoni Zone. The LAD of *Acanthaulax crispa* is in Parkinsoni Zone.

The sample is dated Parkinsoni Zone.

Sample interval 757.75 – 737.20 m (4 samples): Early Bathonian, Zigzag Zone

The assemblages are characterised by the abundant and diverse occurrence of species of the genus *Ctenidodinium*, with *Ctenidodinium* spp., *Ct. combazii*, *Ct. continuum*, *Ct. cornigerum*, *Ct. ornatum* and *Ct. sellwoodii* group. Important taxa first occurring at the base of the interval are *Cleistosphaeridium* sp. 1, *Ctenidodinium combazii*, *Lithodinia* spp., questionable *Sirmiodiniopsis* sp. and *Tubotuberella dangeardii*. The species *Meiourogonyaualax valensii* last occurs at the top of the interval.

The FAD of *Ctenidodinium combazii* is within the uppermost part of Parkinsoni Zone, those of *Lithodinia* spp. and *Tubotuberella dangeardii* are in Zigzag Zone. The LAD of *Meiourogonyaualax valensii* is in Zigzag Zone.

The high diversity and abundance of *Ctenidodinium* species and the presence of *Ctenidodinium combazii* are typical for the Bathonian and earliest Callovian.

The sample is dated Zigzag Zone.

Sample 730.62 m (1 sample): Early Bathonian, Zigzag Zone, Tenuiplicatus Subzone to Middle Bathonian, Morrisi Zone

The assemblage of the sample is similar to those from below. In addition, there are i.a. *Eodinia* spp. and the first occurrence of chorate dinoflagellate cysts close to *Cleistosphaeridium ehrenbergii* s.l., recorded here within *Cleistosphaeridium* spp.

The interval is defined as from the first occurrence of *Cleistosphaeridium* spp. to the first occurrences of questionable *Atopodinium prostaticum* and questionable *Pareodinia prolongata* in the interval above.

The FAD of *Cleistosphaeridium ehrenbergii* s.l. is in Tenuicostatum Subzone of Zigzag Zone. The FADs of *Atopodinium prostaticum* and *Pareodinia prolongata* are Hodsoni Zone.

The sample is interpreted Tenuiplicatus Subzone of Zigzag Zone to Morrisi Zone.

Sample interval 729.84 – 727.32 m (2 samples): Late Bathonian, Hodsoni Zone

The assemblages are similar to below. In addition, there are the first occurrences of questionable *Atopodinium prostaticum* and questionable *Pareodinia prolongata*. *Ctenidodinium minimum* shows an acme. Last occurring at the top of the interval are i.a. *Carpathodinium predae*, *Gongylodinium hocneratum*, *Gonyaulacysta pectinigera* and *Rhynchodiniopsis? regalis*.

The interval is defined as from the first occurrence of questionable *Atopodinium prostaticum* and questionable *Pareodinia prolongata* to the last occurrence of *Rhynchodiniopsis? regalis*.

The FADs of *Atopodinium prostaticum* and *Pareodinia prolongata* and the LAD of *Rhynchodiniopsis? regalis* are in Hodsoni Zone.

The interval is dated Hodsoni Zone.

Sample 726.88 m (1 sample): Late Bathonian, Hodsoni to Discus Zone

The assemblages are similar to below with abundant and diverse species of *Ctenidodinium*, unquestionable *Atopodinium prostaticum*, *Nannoceratopsis pellucida* and *Pareodinia prolongata*. Last occurring in this sample are *Atopodinium polygonale*, *Ctenidodinium combazii*, *Gongylodinium erymnoteichon* and *Valvaeodinium spinosum*.

The FADs of *Atopodinium prostaticum* and *Pareodinia prolongata* are Hodsoni Zone. The LAD of *Valvaeodinium spinosum* is Discus Zone. The LAD of *Gongylodinium erymnoteichon* was previously considered to be in Hodsoni Zone, but the species has recently been observed to occur up to the Discus Zone (SFB, pers. obs. 2020). The LAD of *Ctenidodinium combazii* is Herveyi Zone.

The sample interval is dated Hodsoni to Discus Zone.

Sample interval 725.11 – 724.78 m (3 samples): Early Callovian, Koenigi Zone to Middle Callovian Jason Zone

Composition of the dinoflagellate cyst assemblages in this interval is different to below. Chorate dinoflagellate cysts are common. There are numerous first occurrences at the base of the interval, i.a. *Adnatosphaeridium caulleryi*, complex skolochorate dinocysts indet., *Korystocysta pachyderma*, *Lithodinia caytonensis*, *Mendicodinium groenlandicum*, *Rhynchodiniopsis cladophora*, *Rigaudella filamentosa*, *Sentusidinium rioultii*, *Sentusidinium? varispinosum*, *Sirmiodinium grossii*, *Stephanelytron scarburghense* (mainly specimens with two small coronae), and in the next sample higher up *Compositosphaeridium polonicum* and *Rigaudella aemula*. Last occurring in this interval are i.a. *Aldorfia aldorfensis*, *Korystocysta gochtii*, *Nannoceratopsis spiculata*, *Sentusidinium? varispinosum*, *Stephanelytron scarburghense* and *Valvaeodinium vermicylindratum*.

There are species with FADs in Herveyi Zone (*Lithodinia caytonensis*, *Rhynchodiniopsis cladophora*, *Sentusidinium? varispinosum*, *Sirmiodinium grossii*, *Stephanelytron scarburghense*), in Koenigi Zone (*Korystocysta pachyderma*, *Mendicodinium groenlandicum*), and in Jason Zone (*Compositosphaeridium polonicum*). There are species with their LADs in Calloviense Zone (*Aldorfia aldorfensis*, *Sentusidinium? varispinosum*, *Valvaeodinium vermicylindratum*) and in Jason Zone (*Nannoceratopsis spiculata*, *Korystocysta gochtii*).

The sample interval is interpreted Koenigi to Jason Zone.

Tab. 3-3: List of analysed palynology samples from TRU1-1

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

Depth [m]	Age	Zone & Subzone
724.78	Middle – Early Callovian	Jason - Koenigi Zone
724.86	Middle – Early Callovian	Jason - Koenigi Zone
725.11	Middle – Early Callovian	Jason - Koenigi Zone
726.88	Late Bathonian	Discus - Hodsoni Zone
727.32	Late Bathonian	Hodsoni Zone
729.84	Late Bathonian	Hodsoni Zone
730.62	Middle – Early Bathonian	Morrisi - Zigzag Z (Tenuiplicatus SZ)
737.20	Early Bathonian	Zigzag Zone
744.66	Early Bathonian	Zigzag Zone
750.52	Early Bathonian	Zigzag Zone
757.75	Early Bathonian	Zigzag Zone
765.81	Late Bajocian	Parkinsoni Zone
766.75	Late Bajocian	Parkinsoni - Garantiana Zone
767.51	Late Bajocian	Garantiana - Niortense Zone
774.47	Late Bajocian	Garantiana - Niortense Zone
775.16	Late – Early Bajocian	Niortense Zone - Humphriesianum Zone (Blagdeni SZ)
775.65	Early Bajocian	Humphriesianum Zone (Blagdeni SZ)
776.73	Early Bajocian	Humphriesianum Zone
776.95	Early Bajocian	Humphriesianum Zone
777.82	Early Bajocian	Humphriesianum Zone
778.21	Early Bajocian	Sauzei Zone
783.78	Early Bajocian	Sauzei Zone
784.01	Early Bajocian	Laeviuscula Zone
785.93	Early Bajocian	Laeviuscula Zone
787.06	Early Bajocian	Laeviuscula Zone
787.62	Early Bajocian	Laeviuscula Zone
790.56	Early Bajocian	Laeviuscula Zone
797.44	Early Bajocian	Laeviuscula Zone
810.65	Early Bajocian	Laeviuscula - Ovale Zone
814.17	Early Bajocian	Ovale Zone
815.67	Middle Aalenian	lower Bradfordensis - Murchisonae Zone
816.03	Middle Aalenian	lower Bradfordensis - Murchisonae Zone
816.44	Early Aalenian	Opalinum Zone (?Bifidatum SZ; ex «Comptum» SZ)
818.03	Early Aalenian	Opalinum Zone (?Bifidatum SZ; ex «Comptum» SZ)
823.12	Early Aalenian	Opalinum Zone (Opalinum SZ)
828.71	Early Aalenian	Opalinum Zone (Opalinum SZ)
833.80	Early Aalenian	Opalinum Zone (Opalinum SZ)
844.96	Early Aalenian	Opalinum Zone (Opalinum SZ)
865.37	Early Aalenian	Opalinum Zone (Opalinum SZ)
885.41	Early Aalenian	Opalinum Zone (Opalinum SZ)
906.87	Early Aalenian	Opalinum Zone (Opalinum SZ)
927.54	E. Aalenian - L. Toarcian	Opalinum Zone (Opalinum SZ) - Aalensis Zone
928.03	E. Aalenian - L. Toarcian	Opalinum Zone (Opalinum SZ) - Aalensis Zone
928.09	E. Aalenian - L. Toarcian	Opalinum Zone (Opalinum SZ) - Aalensis Zone

3.4 Chemostratigraphy

The sampling of the TRU1-1 cores focused primarily on 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. Figs. 3-8 and 3-9 illustrate the fully analysed interval from the middle part of the Staffelegg Formation up to the base of the Wildegge Formation (944.79 – 722.00 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, Dry Clay values in wt.-% with vertical axis in m MD log depth (*cf.* Dossier X), XRD measurements (calcite: blue, dolomite/ankerite: green, siderite: red; *cf.* Dossier VIII) and C(org) measurements in blue (*cf.* Dossier VIII). In addition, formation boundaries were highlighted with black lines and other formal or informal subintervals with grey lines. Following stratigraphic abbreviations were used in Figs. 3-2 to 3-9: G = Grünschholz Member; B + R = Breitenmatt Member and Rickenbach Member; OPA = Opalinus Clay; Rieth. = Rietheim Member; G. Wolf = Gross Wolf Member; «M.O.» = «Murchisonae-Oolith Formation»; «Hum.» = «Humphriesioolith Formation»; Bi. = Birnenstorf Member; Ef. = Effingen Member.

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, because in most intervals such a small amount of carbonate is present. 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.

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 in the Opalinus Clay and its confining units. Some of the hardground samples were drilled directly from the remaining thin section blocks to correlate the bulk geochemical data with the microfacies analysis. All these data are distinguished in different colours on the following Fig. 3-4 (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).

In contrast to the carbonate measurements, 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 a longer succession, as is to be expected in the middle part of Opalinus Clay, only every second sample was analysed.

Lias Group

Starting from the bottom up (Fig. 3-2), the oldest sediments measured belong to the Early Jurassic (maybe Late Pliensbachian to Early Toarcian). The lowermost measurement (944.79 m) is coming from the uppermost combined Breitenmatt Member and Rickenbach Member. The following measurements between 944.67 m and 927.95 m represent the upper two members of the Staffelegg Formation. They show overall larger variations in their individual measurements, which can be explained by the higher sampling resolution in the Lias Group (some intervals in the Rietheim Member with 5 to 10 cm spacing during the negative carbon isotope event, see discussion in next paragraphs) as well as by the nodular calcareous lithology (Gross Wolf Member).

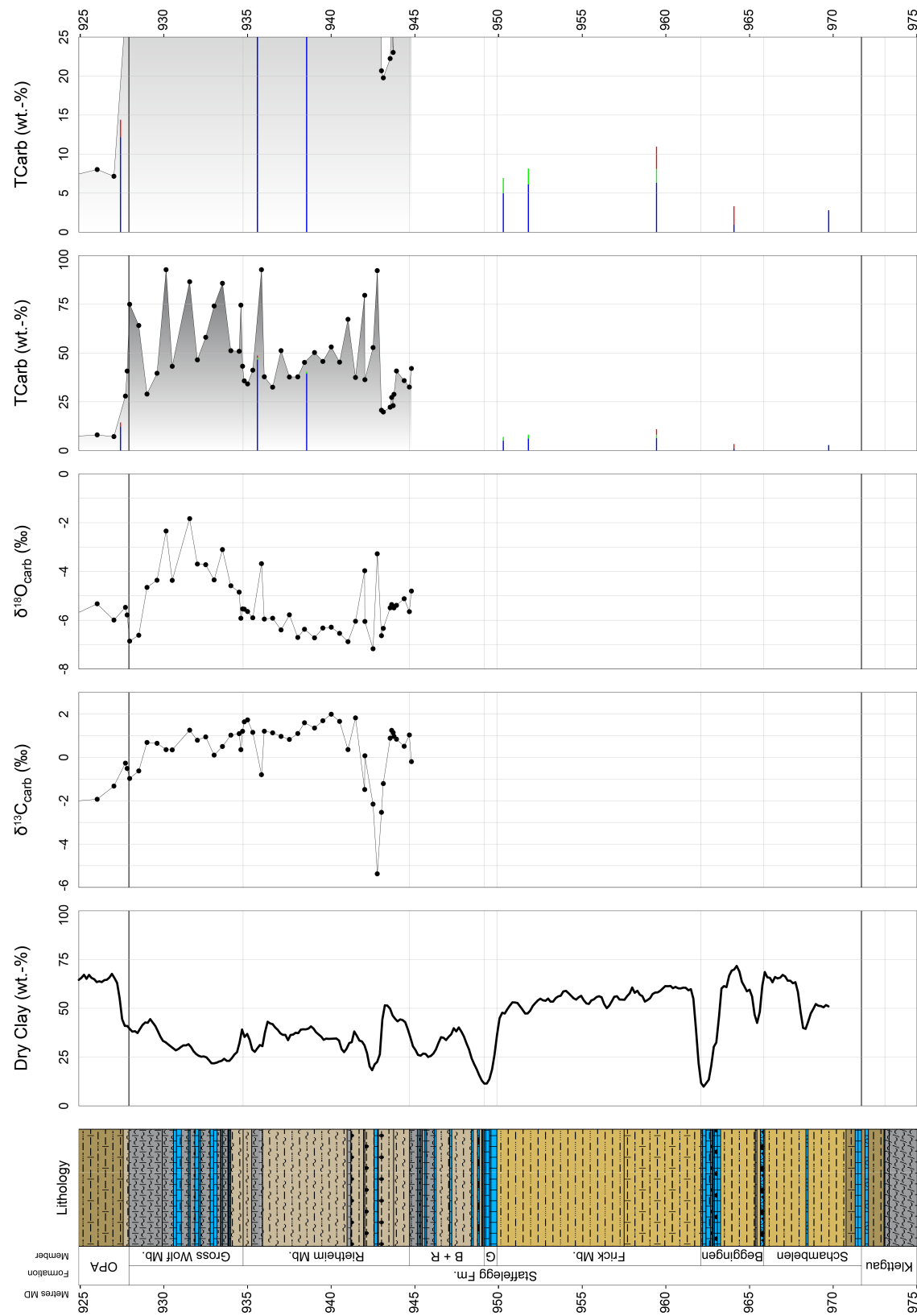


Fig. 3-2: Bulk rock (carbonate) isotopic data from mainly the Lias Group
Geochemical data from 944.79 – 926.01 m, additional explanations and references see text at the beginning of the Section 3.4.

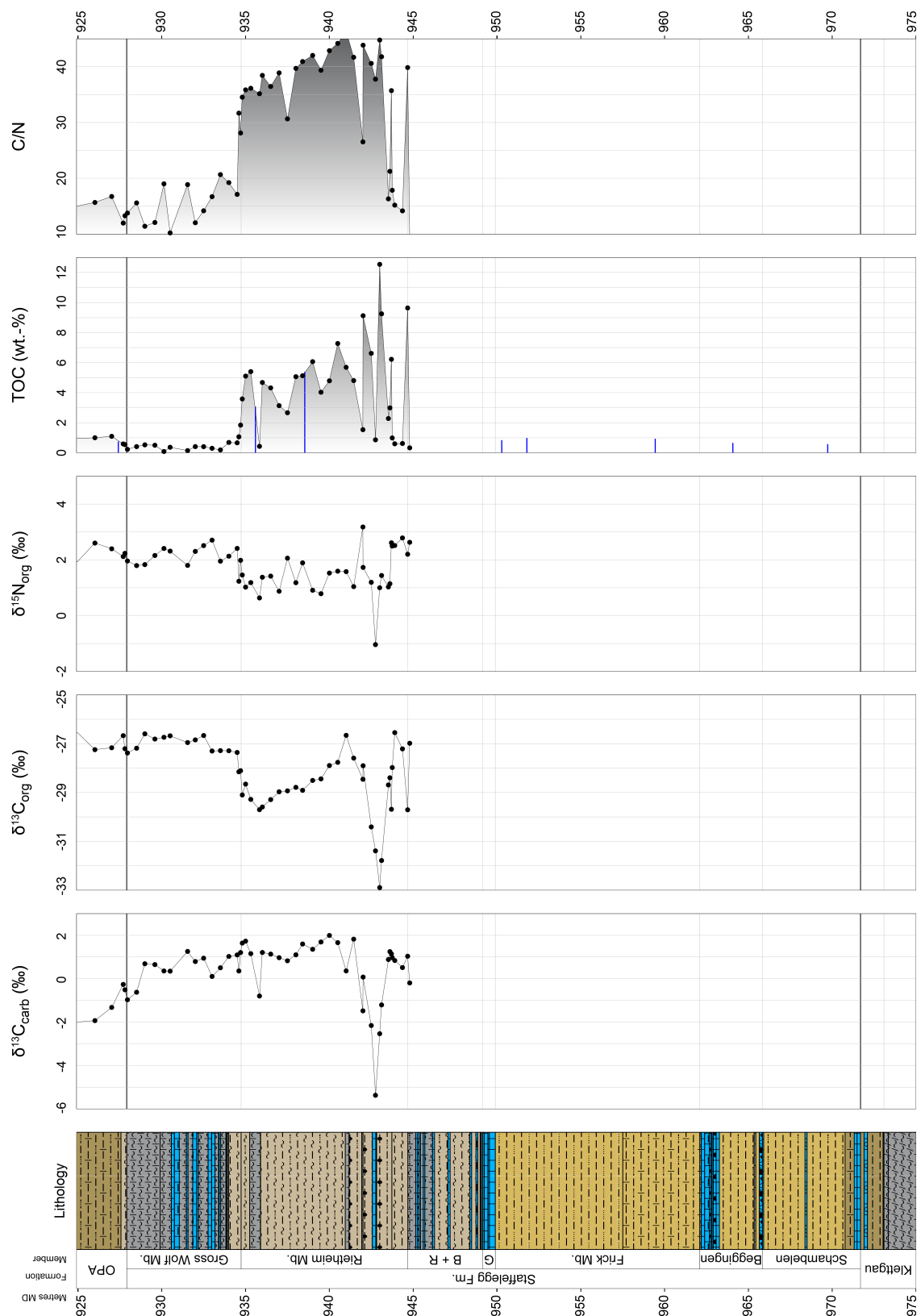


Fig. 3-3: Organic isotopic data from mainly the Lias Group

Geochemical data from 944.79 – 926.01 m, additional explanations and references see text at the beginning of the Section 3.4.

Although the calculated carbonate content is only a semi-quantitative method, the values presented here correspond to the XRD values measured at the University of Bern (*cf.* Dossier VIII). The XRD data are illustrated in the following Fig. 3-2 to provide a visual comparison between the new data presented here and those from the Dossier VIII. As discussed in Wohlwend et al. (2019) based on measurements from the BDB-1 borehole at the Mont Terri Rock Laboratory, the values calculated here follow the calcite wt.-% with an additional mixed signal from the other carbonates since, during the reaction time of 60 min at 72 °C, a complete reaction does not take place for all carbonates.

The semi-quantitative carbonate content (TCarb) values represent the lithological variations in the Rietheim Member and the hanging Gross Wolf Member. In the Rietheim Member the TCarb values show a decreasing trend from almost 40 wt.-% to values around 20 wt.-% just below the «Unterer Stein» (942.82 – 942.48 m). From here upwards the TCarb are around 40 to 50 wt.-% with a second, but less pronounced decreasing trend to the top of the member. The interval is clearly interrupted by higher values measured from the four calcareous interbeds. The three lower beds («Unterer Stein»: 942.82 – 942.48 m, «Homogene Kalkbänke»: 942.01 – 941.93 m and «Oberer Stein»: 940.95 – 941.17 m, nomenclature *sensu* Kuhn & Etter 1994) show a stepwise lower TCarb content with the highest value of 92.3 wt.-% measured from the lowest one to values of 79.6 wt.-% from the middle to 67.3 wt.-% from the upper bed. The «Unterer Stein» could be subdivided into a thicker lower bed from 942.82 to 942.56 m and a clearly marlier upper part from 942.56 to 942.48 m. The uppermost calcareous bed (935.90 – 935.25 m), with a value up to 92.7 wt.-%, represents probably the «Monotisbank» *sensu* Kuhn & Etter 1994.

The $\delta^{13}\text{C}_{\text{carb}}$ values document a slight increasing trend (from close to 0 to 1.2 ‰) in the lowest metre of the Rietheim Member followed by a prominent negative excursion with the most negative value (-5.4 ‰) measured from the sample from the «Unterer Stein». The negative trend is subsequently followed by a rapid increase to positive values close to 2.0 ‰. The values stabilise thereafter in the Gross Wolf Member and decrease to around 0.5 to 1 ‰ towards the top of the Gross Wolf Member. Only the uppermost two samples (928.50 and 927.95 m) show distinct more negative values (-0.6 and -1.0 ‰). The discussed negative excursion represents one of the major Mesozoic negative carbon-isotope excursions (CIE) – the Toarcian-Oceanic Anoxic Event (T-OAE). When looking in detail, the data points, which belong to the 4 calcareous beds (see discussion above) show more negative values than the rest or "background" sediment. The calcareous beds are clearly diagenetic altered and therefore the most negative value from the «Unterer Stein» does not represent the most negative part of the T-OAE (e.g. Röhl & Schmid-Röhl 2005, Montero-Serrano et al. 2015). This can be seen in the $\delta^{13}\text{C}_{\text{org}}$ values (Fig. 3-3) where the most negative one, with a value of -32.9 ‰, was measured just below the bed (at 943.00 m). The following rapid positive shift is also clearly documented in the organic matter, where the most positive value (-26.7 ‰) was measured from the sample of the «Oberer Stein». The $\delta^{13}\text{C}_{\text{org}}$ curve shows great similarity with the data documented from the Aubach section in the Wutach area (Hougaard et al. 2021). The following $\delta^{13}\text{C}_{\text{org}}$ trend to more negative values ends with a very prominent shift or jump at the Rietheim / Gross Wolf Member boundary. This "shift" in the isotopic signal of the organic signal correlates nicely with the semi-quantitative organic carbon content (TOC) content as well as with the C/N ratio. The $\delta^{13}\text{C}_{\text{org}}$ signal is influenced by different sources of the organic matter during the time of the Rietheim to Gross Wolf Member and therefore represents also nicely the lithological boundary between the bituminous – Type I-II kerogene (e.g. Suan et al. 2015, Hougaard et al. 2021) – Rietheim Member and the overlying more calcareous Gross Wolf Member.

As already mentioned above the Rietheim Member is very bituminous. The member itself was defined at the base of the lowermost cm-thick seam of bituminous shale which can be found between 944.68 and 944.65 m (*cf.* Dossier III). This thin bed, with a semi-quantitative TOC

content of 9.6 wt.-% clearly stands out when comparing the samples below and above (Fig. 3-3). Together with the negative CIE of the T-OAE, very high values occur, with maximum values around 12.6 wt.-% contemporaneous with the most negative $\delta^{13}\text{C}_{\text{org}}$ value at 943.00 m. The very bituminous interval, starting around one metre above the base of the Rietheim Member up to the «Homogene Kalkbänke» has an average TOC content of around 6 – 8 wt.-%, which is higher than the content in the upper part with values around 3 – 5 wt.-%. The TOC content of the lower two calcareous beds («Unterer Stein» and «Homogene Kalkbänke») clearly interrupt the high amount with values just around 1 wt.-%. Although the calculated TOC is only a semi-quantitative method, the values presented here correspond well with the two C(org) values measured at the University of Bern from the upper part of the Rietheim Member (*cf.* Dossier VIII). 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 around 0.5 wt.-%.

The C/N ratios somehow show the same trends as the TOC, with the highest ratios measured contemporaneous with the negative CIE of the T-OAE in the Rietheim Member (35 – 46). The overlying Gross Wolf Member shows again a striking different C/N ratio, which is much lower (between 10 and 20) than the ratios from the underlying Rietheim Member. Such high C/N numbers – measured in the Rietheim Member – are very 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 this very unusual C/N ratios in which they determined from sediment trap studies that suboxic microbial degradation via denitrification preferentially utilizes 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.

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, «Murchisonae-Oolith Formation» and the transition into the lower part of the Wedelsandstein 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 compared to those from the underlying Staffelegg Formation (Fig. 3-4) are rather low and very stable. From the base of the Opalinus Clay to around 892 m the average TCarb is around 9 wt.-%. In the above following succession, also including the «Upper silty sub-unit» (860.24 – 846.88 m), the TCarb fluctuates around the average value of 13 wt.-%. But not only the average values but also the variability increases from the lower to the upper succession. It seems that the change in TCarb content goes hand in hand with the macroscopically observed increase in quartz silt content and probably also with an increase in grain size of the siliciclastic input from the «Mixed clay-silt-carbonate sub-unit» (912.95 – 860.24 m) and «Upper silty sub-unit». The uppermost informal sub-unit («Sub-unit with silty calcareous beds», 846.88 – 816.42 m) shows again similar average values around 9 wt.-% as the lowest interval, but with more variability. In the uppermost 10 m a clear trend to almost carbonate free claystone (values around 3 wt.-%) is documented. In the thin «Murchisonae-Oolith Formation» and in the lower part of the hanging Wedelsandstein Formation the TCarb increases and reflects especially in the Wedelsandstein the very alternating succession between sandy/silty-argillaceous sediments and calcareous interbeds.

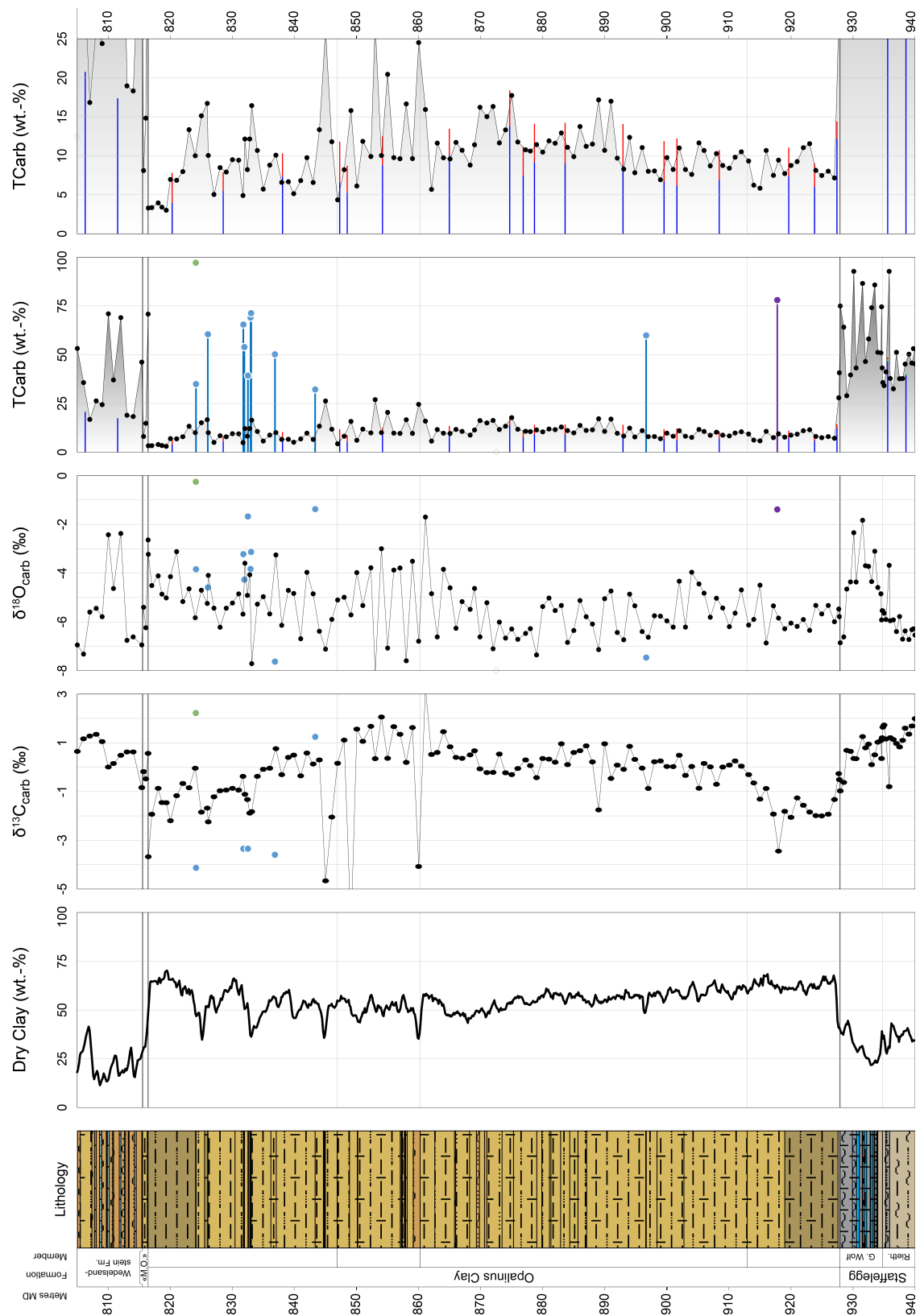


Fig. 3-4: Bulk rock (carbonate) isotopic data from the l. Dogger Group – mainly Opalinus Clay
 Geochemical data from 940.00 – 805.00 m, additional explanations and references see text
 at the beginning of the Section 3.4.

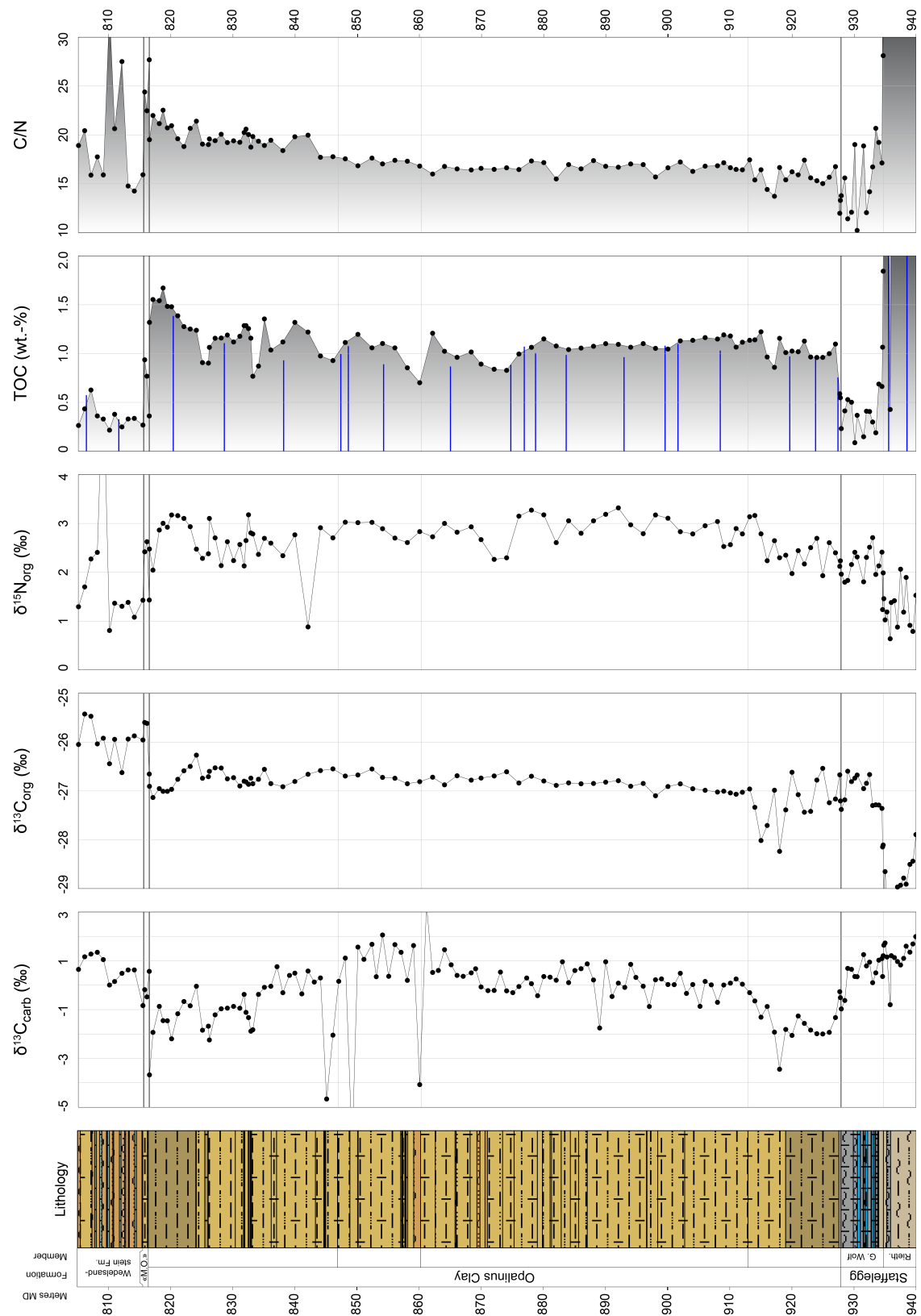


Fig. 3-5: Organic isotopic data from the lower Dogger Group – mainly Opalinus Clay
 Geochemical data from 940.00 – 805.00 m, additional explanations and references see text at the beginning of the Section 3.4.

The above-mentioned Opalinus Clay interval comprises several calcareous beds (see Appendix E1 for data). They are illustrated in Fig. 3-4 by thicker light blue lines ending with blue dots marking the T_{carb} values. Some of them are classified as measurements from "hiatus beds", "hiatus concretions" or calcareous concretions. One of these calcareous beds (896.69 – 896.59 m), a "hiatus bed", can be found in the lower part of the «Mixed clay-silt-carbonate sub-unit». The others – mainly "hiatus beds" or just "hiatus concretions" – are located in the uppermost «Sub-unit with silty calcareous beds». Most of them comprise semi-quantitative carbonate contents that are typical for calcareous marl. Some of the strongly bored calcareous intraclasts show an outer calcareous growth structure (rim) or are "grown" together so that they can be designated as "hiatus concretions" by the definition of Voigt (1968). This is the case for example for the bored intraclasts between 826.05 and 826.00 m.

The $\delta^{13}\text{C}_{\text{carb}}$ data show two, possibly three, negative excursions or intervals (Fig. 3-4): a lower one in the lowermost «Clay-rich sub-unit» (927.91 – 912.95 m) and an upper one in the uppermost «Sub-unit with silty calcareous beds», which could additionally be split into two negative shifting trends separated by the uppermost calcareous bed (824.14 – 824.06 m). The succession in between from 912.95 m to around 837 m shows a trend towards more positive values fluctuating around 0 ‰ with a few measurements in and just under the «Upper silty sub-unit» reaching $\delta^{13}\text{C}_{\text{carb}}$ values of 1.5 to 2 ‰ and one with 3.3 ‰ in and just under the «Upper silty sub-unit». Noticeable are the two "major" negative excursions. The lower negative excursion is represented by clearly decreasing and increasing trends, and reaches the most negative values (-3.4 ‰ at 917.99 m) just below the lower calcareous concretions mentioned above at 917.80 m. The upper negative excursion reaches a lower minimum (-1.8 ‰ at 833.10 m) just beneath a thicker firm- to hardground from 833.03 – 832.78 m. A second minimum is documented slightly higher, reaching values to -2.2 ‰ between 826.09 m and 824.99 m. Also, this one is directly below a firm- to hardground, which is slightly less visible in the cores between (824.14 – 824.06 m). This calcareous bed could also be used to split the upper negative excursion into, the above mentioned, two times negative shifting trends. The $\delta^{13}\text{C}_{\text{carb}}$ value just above at 824.00 m is almost 2 ‰ more positive than the one directly underlying the bed. From 824.00 m to the top of Opalinus Clay at 816.42 m, the values show a decreasing trend with the most negative value (-3.7 ‰) two centimetres beneath the top (sample at 816.44 m).

The $\delta^{13}\text{C}_{\text{carb}}$ data from the calcareous beds or intraclasts document possibly an early diagenetic signal (e.g. Wetzel & Allia 2000). The calcareous concretions or "hiatus concretions" are the only macroscopic features with very negative $\delta^{13}\text{C}_{\text{carb}}$ values (-25 to -26 ‰, Appendix E1). Very fine authigenic calcite was probably precipitated in the very fine original porosity of the Opalinus Clay, which led to the more negative $\delta^{13}\text{C}_{\text{carb}}$ values in the lower and upper negative excursions (see also Wohlwend et al. 2016.). Also remarkable is the scatter of the bulk measurements (in metre resolution) in and just under the «Upper silty sub-unit» (~ 867 – 851 m). The higher scatter is even better visible in the large variability of the $\delta^{18}\text{O}_{\text{carb}}$ data from the same interval. The succession comprises silt lenses, some of them up to several centimetre thick. It was therefore not always possible to sample only the clay mineral-rich sediment. The high variability in the C- and O-isotope data can be explained by varying amounts of silt, which probably comprises very little diagenetic calcite pore fillings in the primary porosity of these lenses.

The $\delta^{13}\text{C}_{\text{carb}}$ data from the «Murchisonae-Oolith Formation» show again more positive values (around -0.5 ‰) compared to the ones just beneath in the uppermost Opalinus Clay. The positive trend can also be seen into the lower part of the Wedelsandstein Formation with values between +0.6 to 0 ‰ in the interval from the base of Wedelsandstein Formation to 810.00 m and values around +1.3 ‰ in the interval above 809.00 m.

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 relatively stable in the central part («Mixed clay-silt-carbonate sub-unit» and «Upper silty sub-unit» to lower part of the «Sub-unit with silty calcareous beds»). The organic carbon isotopes indicate variations only at the base of the Opalinus Clay («Clay-rich sub-unit») and at the top (upper part of the «Sub-unit with silty calcareous beds»). At the base, three to four individual negative trends or peaks can be recognised (926.01 m: -27.2 ‰; 922.00 m: -27.4 ‰; 917.99 m: -28.2 ‰; 915.00 m: -28.0 ‰). The upper two negative trends or peaks may be combined to one larger peak or even excursion with a short positive interval. The amplitude of the three to four variations increases upwards and reaches the maximum in the third with 1.2 ‰ between the most negative and the most positive ones. The values above these variations stabilise around -27.0 ‰. In the «Mixed clay-silt-carbonate sub-unit» and «Upper silty sub-unit», there is an overall trend towards +0.5 ‰ heavier values visible, reaching values around -26.5 ‰ at 852.30 m and 846.00 m. The upper part of the Opalinus Clay («Sub-unit with silty calcareous beds») shows slight variations with first 0.5 ‰ more negative before the $\delta^{13}\text{C}_{\text{org}}$ values increase to an overall positive peak in the Opalinus Clay at 824.00 m with -26.3 ‰. This more positive $\delta^{13}\text{C}_{\text{org}}$ "peak" is measured in the sample just above the uppermost calcareous beds, similar to the positive shift in the $\delta^{13}\text{C}_{\text{carb}}$ data.

At the lithological upper boundary of the Opalinus Clay and even more pronounced afterwards from the two measurements (816.03 m and 815.67 m), sampled from the silty claystone from the «Murchisonae-Oolite Formation», the $\delta^{13}\text{C}_{\text{org}}$ data document a clear positive shift to values around -25.6 ‰. These positive values lead over into the lower part of the Wedelsandstein Formation.

The C/N ratio shows a minor variation in the «Clay-rich sub-unit» and afterwards a stable interval in «Mixed clay-silt-carbonate sub-unit» with a ratio around 17. In the upper two sub-units the C/N ratio increases to around 22 at the top of the Opalinus Clay. The «Murchisonae-Oolite Formation» although very thin documents slightly higher ratios up to 28 before they decrease to low values in the lowermost 2 m of the Wedelsandstein Formation.

Upper part of the Dogger Group

The following described interval – the upper Dogger Group («Murchisonae-Oolite Formation», Wedelsandstein Formation, «Humphriesoolite Formation», «Parkinsoni-Württembergica-Schichten», Variansmergel Formation, Wutach Formation and base of Wildegg Formation) – covers in time the whole Middle Aalenian to Middle Oxfordian substages (Figs. 3-8 and 3-9).

The semi-quantitative TCarb (Fig. 3-6) represents the alternation of silty claystones, argillaceous to calcareous marls and limestones in the upper part of the Dogger Group. However, the TCarb contents are somehow underestimated because of the sampling strategy of not sampling every single limestone bed (focus on the clay mineral-rich sediments – background sedimentation). Nevertheless, the carbonate content curve reflects the inverse wet clay content curve (*cf.* Dossier X). The Wedelsandstein Formation can be divided into two subintervals, representing two different lithologies. The lower one, from the base to around 798 m (lithological boundary in the profile at 797.91 m), includes several calcareous and marly beds in an argillaceous background sediment with a TCarb content around or slightly beyond 25 wt.-%. Calcareous, marly and argillaceous is here merely mentioned in relation to the measured TCarb content, without considering the siliciclastic part. The Wedelsandstein Formation also contains a high siliciclastic content, which will shift the terms (or patterns) in direction of the quartz & feldspar corner of the ternary diagram of Füchtbauer (1988), see also Naef et al (2019) for the slightly modified version of Füchtbauer.

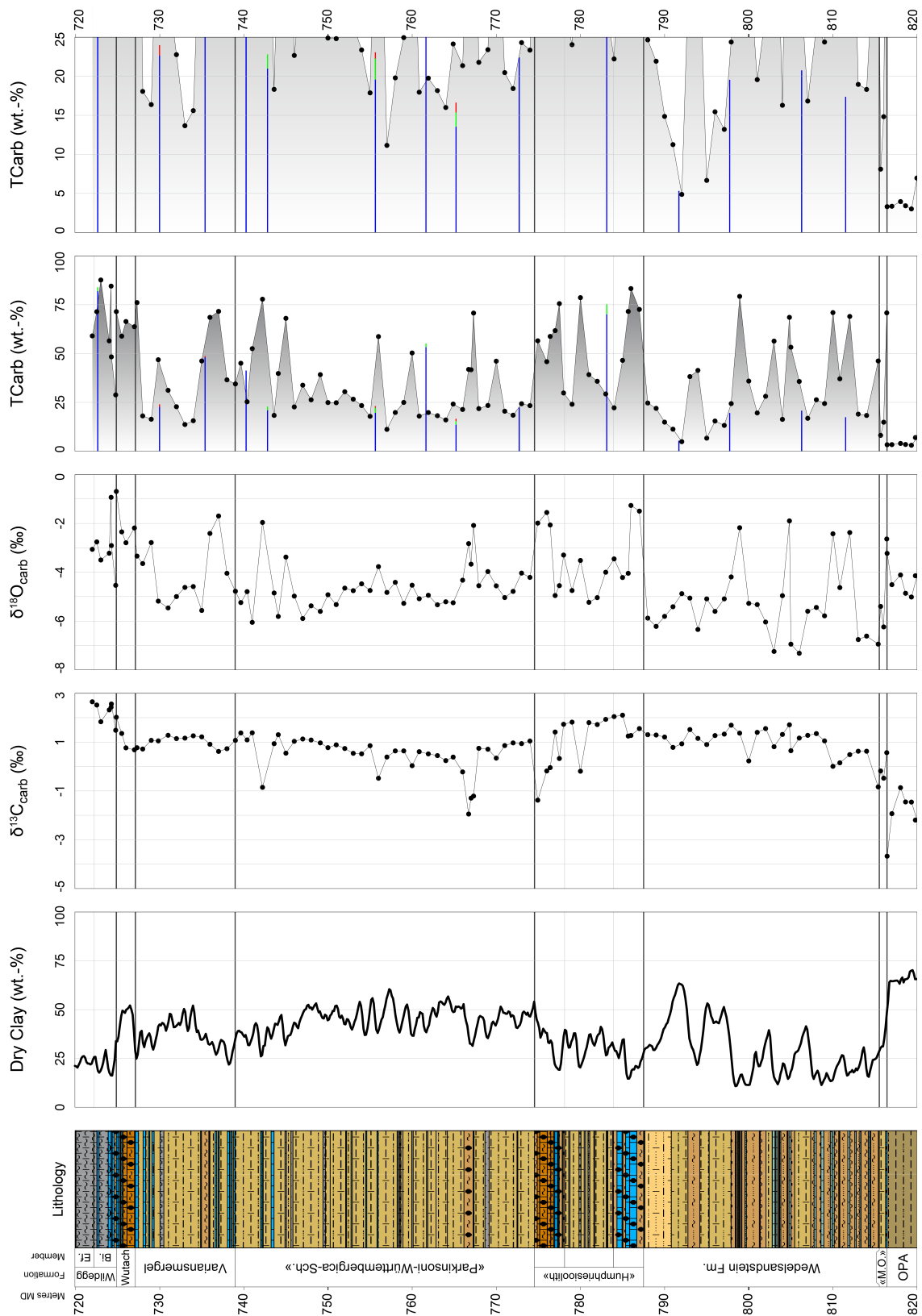


Fig. 3-6: Bulk rock (carbonate) isotopic data from the upper part of the Dogger Group
 Geochemical data from 820.00 – 722.00 m, additional explanations and references see text at the beginning of the Section 3.4.

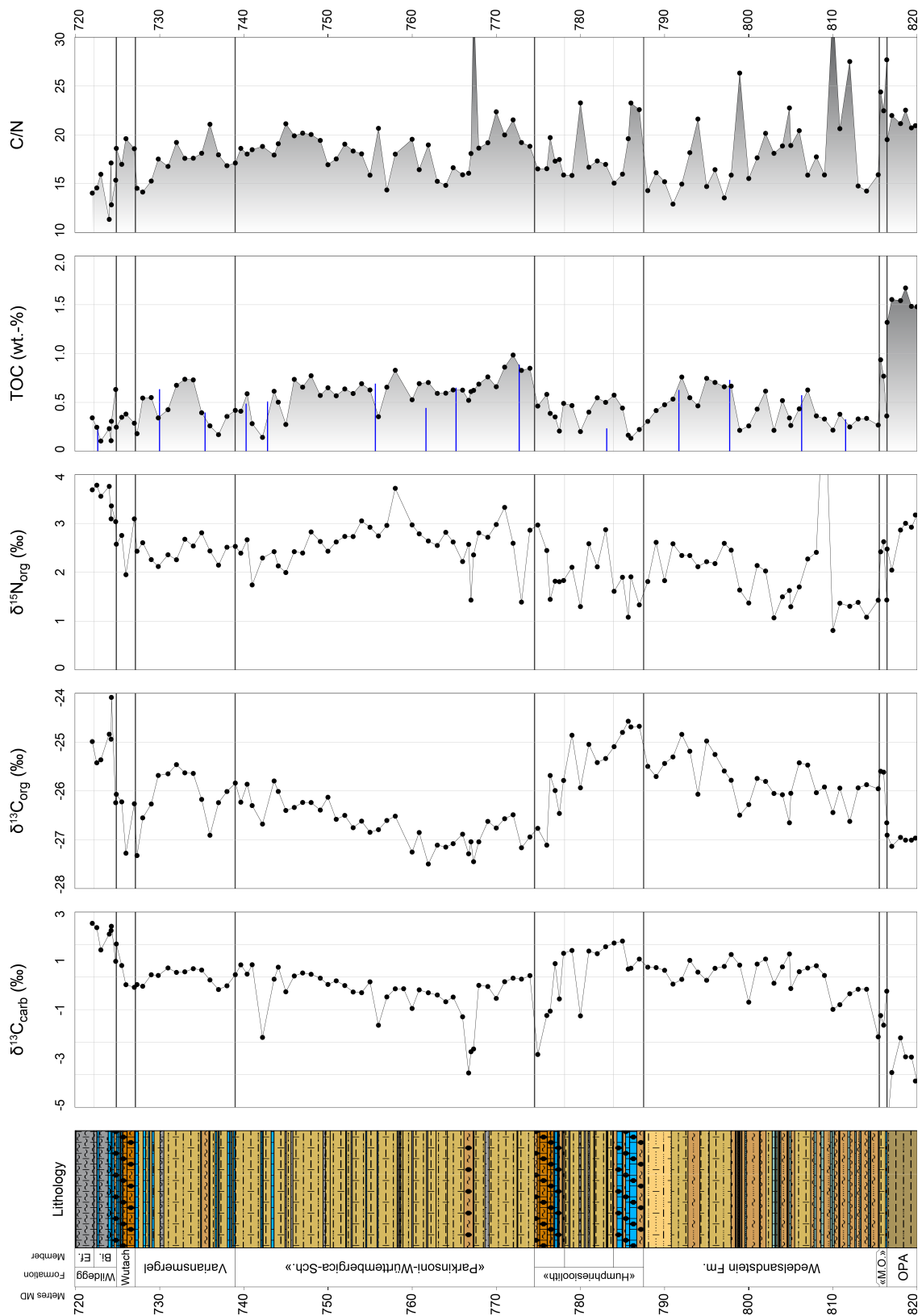


Fig. 3-7: Organic isotopic data from the upper part of the Dogger Group

Geochemical data from 820.00 – 722.00 m, additional explanations and references see text at the beginning of the Section 3.4.

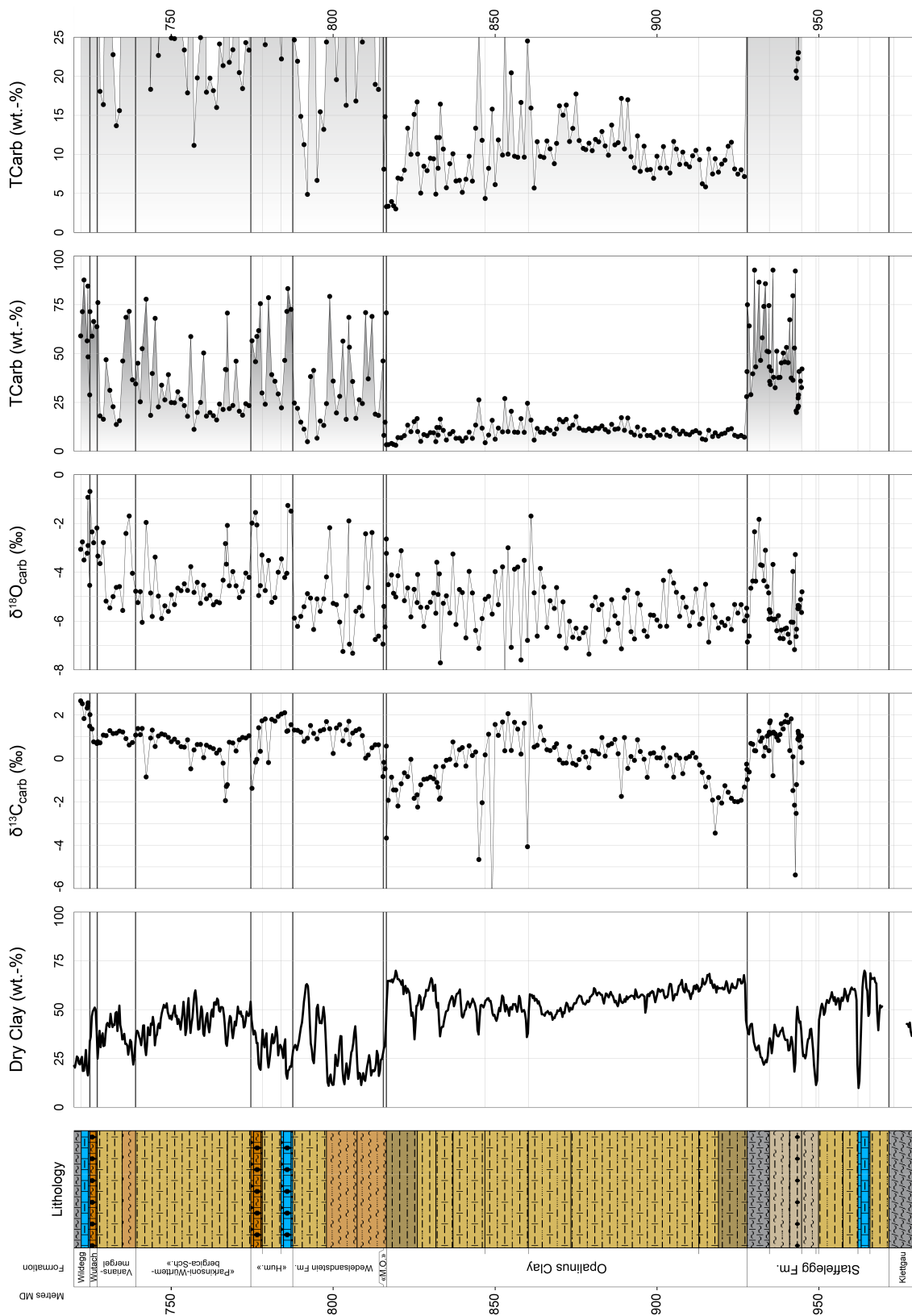


Fig. 3-8: Whole bulk rock (carbonate) isotopic data from TRU1-1

Geochemical data from 944.79 to 722.00 m; additional explanations and references see text at the beginning of the Section 3.4.

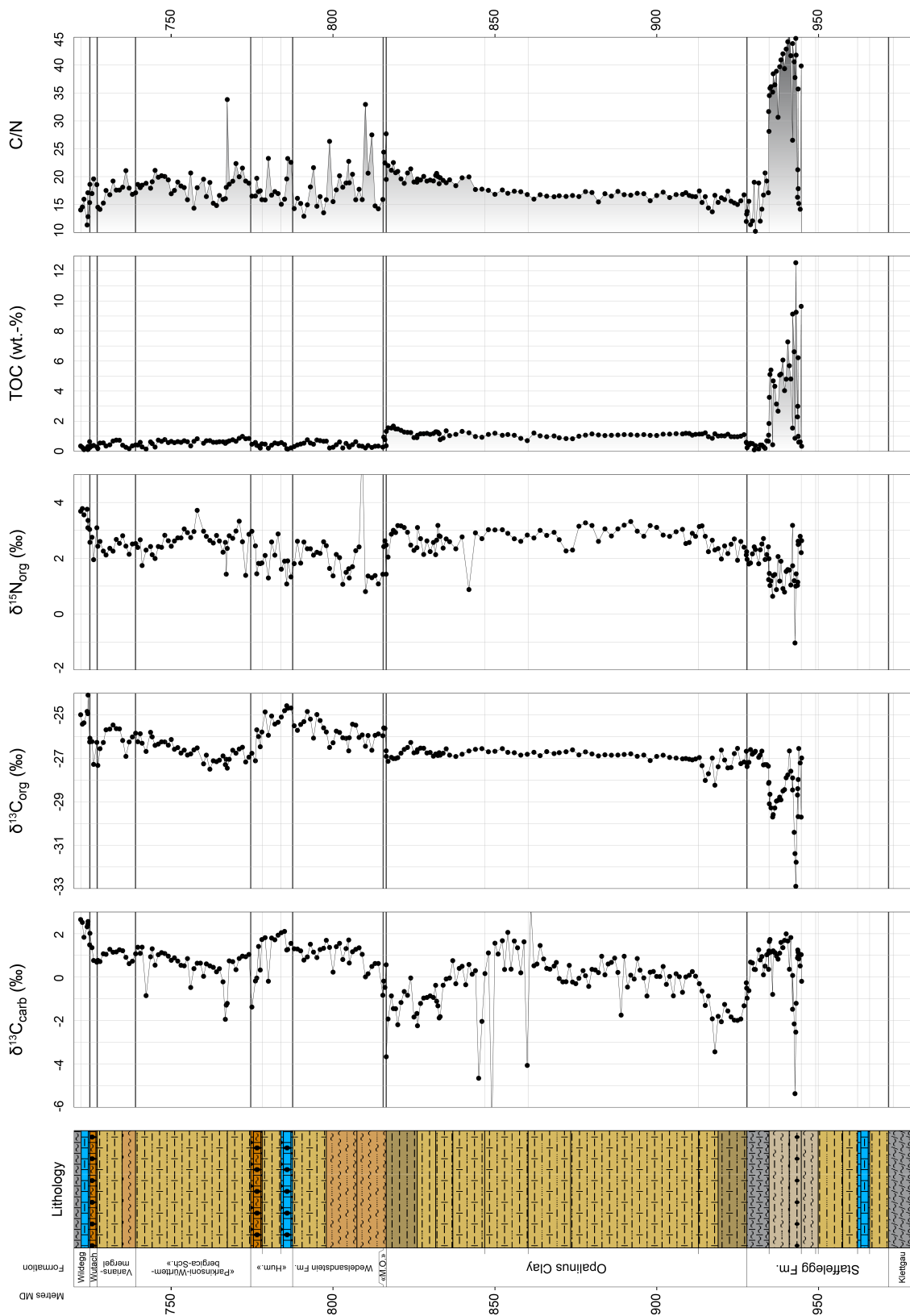


Fig. 3-9: Whole organic isotopic data from TRU1-1

Geochemical data from 944.79 to 722.00 m; additional explanations and references see text at the beginning of the Section 3.4.

The upper subinterval to the top of the formation certainly contains less carbonate, interrupted by two higher values at (793.96 m and 793.00 m). The argillaceous to clayey succession is then interrupted by a distinct more calcareous interval – the «Humphriesioolith Formation» (Fig. 3-6). The lower and upper boundary is clearly represented by a shift in the carbonate content, which therefore goes hand in hand with the occurrence of iron-oolids, defining this formation. Upward the succession only changes again noticeably with the Wutach Formation and Wildegg Formation, both representing a calcareous marl or limestone with variable content of iron-oolids in the Wutach Formation and at the very base of the Wildegg Formation.

Although the $\delta^{18}\text{O}_{\text{carb}}$ data were not discussed extensively until now, the oxygen isotopes show a very high linear correlation with the TCarb content. The higher the content, the more positive the $\delta^{18}\text{O}_{\text{carb}}$, or vice versa the less carbonate, the more negative. This relation nicely shows the diagenetic overprint of the sedimentary succession and therefore, how challenging the interpretation of the $\delta^{18}\text{O}_{\text{carb}}$ data is in such low carbonate sedimentary successions.

As already mentioned above, the $\delta^{13}\text{C}_{\text{carb}}$ data show an overall positive trend from the uppermost Opalinus Clay up section. The C-isotope stabilises between +1.3 and +1.5 ‰ from 809.00 m through the upper Wedelsandstein Formation into the «Humphriesioolith Formation». The most positive value of 2.1 ‰ is reached at 785.00 m in the lower iron-oolitic succession. A similar trend to more positive values was also documented in the time equivalent (Laeviuscula Zone) succession from the Passwang Formation and Hauptrogenstein at Mont Terri (Wohlwend et al. 2019). From 785.00 m upward the $\delta^{13}\text{C}_{\text{carb}}$ data show a decreasing trend which turns slightly above the iron-oolitic beds (at 764.00 m) – which may be correlated with the «Parkinsoni-Oolith» (767.35 – 766.15 m, cf. Dossier III) – in the «Parkinsoni-Württembergica-Schichten». The upper iron-oolitic succession of the «Humphriesioolith Formation» as well as the presumed Parkinsoni-Oolith» are both represented by negative shifts in the $\delta^{13}\text{C}_{\text{carb}}$ data. The $\delta^{13}\text{C}_{\text{carb}}$ values in the «Parkinsoni-Württembergica-Schichten» and Variansmergel Formation vary between 0.2 and 1.4 ‰ and are rather stable until the Wutach Formation. The striking positive shift of almost two per mille to values around +2.6 ‰ at 724.23 m is typical for the Callovian/Oxfordian boundary and was already documented by Rais et al. (2007) in other locations and in the Weiach borehole as well as in the Bülach-1 borehole (Wohlwend et al. 2021). The most positive $\delta^{13}\text{C}_{\text{carb}}$ values were documented by Rais et al. (2007) in the Middle Oxfordian (Transversarium Zone).

The $\delta^{13}\text{C}_{\text{org}}$ data (Fig. 3-7) show a similar increasing trend through the Wedelsandstein Formation as discussed above. The values start from around -26.0 ‰ at the base of the formation and reaching the most positive values of -24.6 ‰ at 785.68 m. The C-isotopes from the organic matter show also from the «Humphriesioolith Formation» to the Variansmergel Formation similar trends: A decreasing trend from the lower iron-oolitic succession of the «Humphriesioolith Formation» with a turnaround at 764.00 m (-27.2 ‰) to more positive values in the Variansmergel Formation. Slightly different or just more pronounced, the $\delta^{13}\text{C}_{\text{org}}$ data of the Wutach Formation show as negative values as in the lowermost «Parkinsoni-Württembergica-Schichten». The following striking positive shift to a peak value of -24.1 ‰ at 724.27 m documents the Callovian/Oxfordian boundary.

The semi-quantitative TOC content is usually around 0.5 wt.-% with a slightly higher content in the lowermost «Parkinsoni-Württembergica-Schichten». C/N ratio varies throughout the upper part of the Dogger Group between 15 and 20 with higher peak values measured from individual calcareous beds.

4 Definition of specific lithostratigraphic boundaries

The boundaries between stratigraphic units, as also shown in the stratigraphic logs of the lithostratigraphy report (Dossier III), were mostly defined based on lithological criteria. According to the guidelines on the stratigraphic nomenclature by Remane et al. (2005), the definition of lithostratigraphic 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 Deep 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 (05.06.2020) and were used for the log descriptions and drawings. In the following paragraphs, the underlying considerations are explained to provide 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 (927.91 – 816.42 m)

The *lower boundary* of the Opalinus Clay is set at 927.91 m at the uppermost surface of a fossiliferous calcareous marl from the underlying Staffelegg Formation (*cf.* Dossier III). The striking decrease in carbonate content (TCarb) from 75 wt.-%, measured from the uppermost sample (927.95 m) of the Gross Wolf Member, to values around 7–9 wt.-% in the basinal Opalinus Clay occurs within the lowermost 0.90 m (Fig. 3-2). Only the lowermost two samples (927.80 and 927.70 m), directly overlying the boundary, show slightly higher contents with values around 27.9 and 40.8 wt.-%. The lithological change between the Gross Wolf Member and the Opalinus Clay is also visible in the clear increase in TOC from values below 0.5 wt.-% to values around 1 wt.-% in the Opalinus Clay (Fig. 3-3).

The *upper boundary* of the Opalinus Clay is set at 816.42 m at the base of the overlying limestone (iron-oolitic) bed (816.42 – 816.26 m) (*cf.* Dossier III). Placing the boundary at this level was not based on lithological reasons alone. Although, the carbonate content (TCarb) and also the TOC document a change in the lithology to less TOC-rich and more calcareous in the hanging part (Figs. 3-4 and 3-5). The silty claystone (calcareous) from 816.26 m to 815.51 m, which directly overlay the hardground, cannot clearly be distinguished from the uppermost interval from the Opalinus Clay. However, it is probably slightly siltier and slightly more calcareous. The boundary was also placed at this level by comparison with the newly established stratigraphy in the Benken borehole (Bläsi et al. 2013). There the palynological sample, taken directly from the hardground, has given already an age from the Bradfordensis Zone. A similar date (lower Bradfordensis – Murchisonae Zone) yielded the palynological sample at 816.03 m in the TRU1-1 core, taken above a similar looking hardground. Therefore, the silty claystone (calcareous) as well as the hardground are almost certainly the same. The positive chemostratigraphic shift (*cf.* Wohlwend et al. 2021) or even jump with an amplitude of around +1 ‰ in the $\delta^{13}\text{C}_{\text{org}}$ values to average values above -26.0 ‰ occurs in that interval ($\delta^{13}\text{C}_{\text{org}}$ values around -27.0 ‰ in the uppermost Opalinus Clay to values around -26.0 ‰ to -25.6 ‰ above; Fig. 3-5).

«Murchisonae-Oolith Formation» (816.42 – 815.51 m)

The *lower boundary* of the «Murchisonae-Oolith Formation» is set at 816.42 m at the base of the limestone (iron-oolitic) bed (816.42 – 816.26 m) (*cf.* Dossier III). The iron-oolitic hardground consist of several calcareous (maybe slightly sideritic) concretions, which are also encrusted and

bored. At the top, or even slightly overlying, a very heavily bored calcareous concretion delimitates the hardground. Detailed discussion about the boundary can be found above at the upper boundary of the Opalinus Clay.

The *upper boundary* of the «Murchisonae-Oolith Formation» is set at 815.51 m at the base of the iron-oolid-bearing calcareous marl which is believed to correspond to the «Sowerbyi-Oolith» of the overlying Wedelsandstein Formation (*cf.* Dossier III). Placing the boundary at this level was mainly supported by comparison with the newly established stratigraphy in the Benken borehole (Bläsi et al. 2013). In both boreholes similar bored iron-oolitic intraclasts are present in the discussed overlying bed. In the TRU1-1 core a few of these intraclasts have an iron-stromatolitic crust (Fig. B-11). The boundary to the hanging Wedelsandstein Formation, is per definition located at the subface of the «Sowerbyi-Oolith» (deposited during the Discites Zone) (German Stratigraphic Scheme; Bloos et al. 2005). In the TRU1-1 core not as many palynological samples were taken around this boundary compared to Benken. The two samples, to narrow the age, were taken at 815.67 m and at 814.17 m. The lower sample, taken below the bed, yields a lower Bradfordensis to Murchisonae Zone age, the upper – above the bed – already an Early Bajocian, Ovale Zone. Therefore, a close chronostratigraphic and lithological correlation with Benken seems to be proven. On these lithological and biostratigraphical reasons the assumption, that the overlying reworked hardground (815.51 – 815.40 m) corresponds with the «Sowerbyi-Oolith» seems to be comprehensible.

Wedelsandstein Formation (815.51 – 787.50 m)

The *lower boundary* of the Wedelsandstein Formation is set at 815.51 m at the base of the iron-oolid-bearing calcareous marl which is believed to correspond to the «Sowerbyi-Oolith» of the Wedelsandstein Formation (*cf.* Dossier III). Detailed discussion about the boundary and the basal «Sowerbyi-Oolith» can be found above at the upper boundary of the «Murchisonae-Oolith Formation».

The *upper boundary* of the Wedelsandstein Formation is set at 787.50 m at the base of the overlying dark reddish-brown marl (iron-oolitic) and limestone (iron-oolitic) of the «Humphriesioolith Formation» (*cf.* Dossier III). Belowe, argillaceous sandstone and a thin sandy limestone bed (787.66 – 787.50 m) occur, both free of iron-oolids. The occurrence of iron-oolitic or limonitic sediments in the hanging succession were used as lithological criteria to define the upper boundary to the overlying «Humphriesioolith Formation» (Bläsi et al. 2013). The resulting age of the purely lithological defined upper boundary lays in the Laeviuscula Zone.

«Humphriesioolith Formation» (787.50 – 774.55 m)

The *lower boundary* of the «Humphriesioolith Formation» is set at 787.50 m at the base of the dark reddish-brown iron-oolite and therefore with the onset of iron-oolids (*cf.* Dossier III). A short discussion about the lower boundary and their age can be found above at the upper boundary of the Wedelsandstein Formation.

The *upper boundary* of the «Humphriesioolith Formation» is set at 774.55 m at the uppermost occurrence of iron-oolids (*cf.* Dossier III). The occurrence of iron-oolitic or limonitic sediments in the succession were used as lithological criteria to define the upper (as well as lower) boundary of the «Humphriesioolith Formation» (Bläsi et al. 2013). The resulting age of the purely lithological defined upper boundary lays in the Garantiana to Niortense Zone.

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 (05.06.2020). Therefore, the present report complements the lithostratigraphic report of Dossier III for the deep borehole Trüllikon-1-1. 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).

6 References

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Appendix A: List of all samples

Appendix A1:	List of all thin sections from TRU1-1 (1'153.72 – 525.17 m)	A-2
Appendix A2:	List of all sampled macrofossils from TRU1-1 (947.39 – 705.65 m)	A-3
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Appendix A1: List of all thin sections from TRU1-1 (1'153.72 – 525.17 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
525.15	525.19	525.17	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-525.17-TS
539.84	539.88	539.86	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-539.86-TS
571.06	571.10	571.08	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-571.08-TS
594.05	594.09	594.07	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-594.07-TS
605.95	605.99	605.97	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-605.97-TS
611.20	611.24	611.22	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-611.22-TS
619.56	619.60	619.58	«Felsenkalke» + «Massenkalk»	14.01.2020	TRU1-1-619.58-TS
646.19	646.23	646.21	Schwarzbach Fm.	14.01.2020	TRU1-1-646.21-TS
683.31	683.35	683.33	Villigen Fm.	14.01.2020	TRU1-1-683.33-TS
705.63	705.67	705.65	Villigen Fm.	14.01.2020	TRU1-1-705.65-TS
723.02	723.06	723.04	Wildegge Fm.	12.03.2020	TRU1-1-723.04-TS
724.23	724.27	724.25	Wildegge Fm.	12.03.2020	TRU1-1-724.25-TS
724.76	724.80	724.78	Wildegge Fm.	12.03.2020	TRU1-1-724.78-TS
724.84	724.88	724.86	Wutach Fm.	12.03.2020	TRU1-1-724.86-TS
735.96	736.00	735.98	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-735.98-TS
742.20	742.24	742.22	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-742.22-TS
766.70	766.74	766.72	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-766.72-TS
767.28	767.32	767.30	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-767.30-TS
774.91	774.95	774.93	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-774.93-TS
776.39	776.43	776.41	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-776.41-TS
776.47	776.51	776.49	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-776.49-TS
777.48	777.52	777.50	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-777.50-TS
784.65	784.69	784.67	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-784.67-TS
785.66	785.70	785.68	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-785.68-TS
798.90	798.94	798.92	Wedelsandstein Fm.	12.03.2020	TRU1-1-798.92-TS
804.81	804.85	804.83	Wedelsandstein Fm.	12.03.2020	TRU1-1-804.83-TS
808.84	808.88	808.86	Wedelsandstein Fm.	12.03.2020	TRU1-1-808.86-TS
810.80	810.84	810.82	Wedelsandstein Fm.	12.03.2020	TRU1-1-810.82-TS
815.42	815.46	815.44	Wedelsandstein Fm.	07.04.2020	TRU1-1-815.44-TS
816.26	816.30	816.28	«Murchisonae-Oolith Fm.»	07.04.2020	TRU1-1-816.28-TS
816.39	816.42	816.40	«Murchisonae-Oolith Fm.»	07.04.2020	TRU1-1-816.40-TS
826.01	826.05	826.03	Opalinus Clay	07.04.2020	TRU1-1-826.03-TS
831.89	831.93	831.91	Opalinus Clay	07.04.2020	TRU1-1-831.91-TS
832.47	832.51	832.49	Opalinus Clay	07.04.2020	TRU1-1-832.49-TS
832.98	833.02	833.00	Opalinus Clay	07.04.2020	TRU1-1-833.00-TS
836.82	836.86	836.84	Opalinus Clay	07.04.2020	TRU1-1-836.84-TS
843.31	843.35	843.33	Opalinus Clay	07.04.2020	TRU1-1-843.33-TS
896.65	896.69	896.67	Opalinus Clay	07.04.2020	TRU1-1-896.67-TS
930.11	930.15	930.13	Staffellegg Fm.	07.04.2020	TRU1-1-930.13-TS
935.79	935.83	935.81	Staffellegg Fm.	07.04.2020	TRU1-1-935.81-TS
962.42	962.46	962.44	Staffellegg Fm.	07.04.2020	TRU1-1-962.44-TS
965.76	965.80	965.78	Staffellegg Fm.	07.04.2020	TRU1-1-965.78-TS
971.33	971.37	971.35	Staffellegg Fm.	07.04.2020	TRU1-1-971.35-TS
971.98	972.02	972.00	Klettgau Fm.	07.04.2020	TRU1-1-972.00-TS
988.30	988.34	988.32	Klettgau Fm.	21.04.2020	TRU1-1-988.32-TS
992.65	992.69	992.67	Klettgau Fm.	21.04.2020	TRU1-1-992.67-TS
999.85	999.89	999.87	Klettgau Fm.	21.04.2020	TRU1-1-999.87-TS
1'003.00	1'003.04	1'003.02	Klettgau Fm.	21.04.2020	TRU1-1-1003.02-TS
1'006.78	1'006.82	1'006.80	Klettgau Fm.	21.04.2020	TRU1-1-1006.80-TS
1'020.28	1'020.32	1'020.30	Klettgau Fm.	21.04.2020	TRU1-1-1020.30-TS
1'055.50	1'055.54	1'055.52	Bänkerjoch Fm.	21.04.2020	TRU1-1-1055.52-TS
1'103.64	1'103.68	1'103.66	Schinznach Fm.	21.04.2020	TRU1-1-1103.66-TS
1'153.60	1'153.64	1'153.62	Schinznach Fm.	21.04.2020	TRU1-1-1153.62-TS
1'153.70	1'153.74	1'153.72	Schinznach Fm.	21.04.2020	TRU1-1-1153.72-TS

Appendix A2: List of all sampled macrofossils from TRU1-1 (947.39 – 705.65 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
705.63	705.67	705.67	Villigen Fm	14.01.2020	TRU1-1-705.67-BS(MF)
722.175	722.24	722.21	Wildegge Fm.	24.02.2020	TRU1-1-722.21-BS(MF)
723.055	723.085	723.07	Wildegge Fm.	24.02.2020	TRU1-1-723.07-BS(MF)
723.085	723.12	723.10	Wildegge Fm.	24.02.2020	TRU1-1-723.10-BS(MF)
723.48	723.50	723.48	Wildegge Fm.	24.02.2020	TRU1-1-723.48-BS(MF)
724.14	724.16	724.15	Wildegge Fm.	24.02.2020	TRU1-1-724.15-BS(MF)
724.275	724.33	724.30	Wildegge Fm.	24.02.2020	TRU1-1-724.30-BS(MF)
725.04	725.115	725.08	Wutach Fm.	24.02.2020	TRU1-1-725.08-BS(MF)
726.87	726.90	726.89	Wutach Fm.	24.02.2020	TRU1-1-726.89-BS(MF)
732.93	732.95	732.94	«Parkinsoni-Württembergica-S.»	24.02.2020	TRU1-1-732.94-BS(MF)
766.52	766.575	766.55	«Parkinsoni-Württembergica-S.»	24.02.2020	TRU1-1-766.55-BS(MF)
766.74	766.785	766.76	«Parkinsoni-Württembergica-S.»	24.02.2020	TRU1-1-766.76-BS(MF)
766.895	766.945	766.92	«Parkinsoni-Württembergica-S.»	24.02.2020	TRU1-1-766.92-BS(MF)
775.15	775.18	775.17	«Humphriesoolith Fm.»	24.02.2020	TRU1-1-775.17-BS(MF)
776.72	776.76	776.74	«Humphriesoolith Fm.»	24.02.2020	TRU1-1-776.74-BS(MF)
776.94	777.04	776.99	«Humphriesoolith Fm.»	24.02.2020	TRU1-1-776.99-BS(MF)
787.05	787.08	787.07	«Humphriesoolith Fm.»	24.02.2020	TRU1-1-787.07-BS(MF)
896.18	896.20	896.19	Opalinus Clay	24.02.2020	TRU1-1-896.19-BS(MF)
913.865	913.905	913.89	Opalinus Clay	24.02.2020	TRU1-1-913.89-BS(MF)
915.72	915.765	915.74	Opalinus Clay	24.02.2020	TRU1-1-915.74-BS(MF)
917.51	917.54	917.53	Opalinus Clay	24.02.2020	TRU1-1-917.53-BS(MF)
928.03	928.045	928.04	Staffelegg Fm.	24.02.2020	TRU1-1-928.04-BS(MF)
928.08	928.12	928.10	Staffelegg Fm.	24.02.2020	TRU1-1-928.10-BS(MF)
929.16	929.19	929.18	Staffelegg Fm.	24.02.2020	TRU1-1-929.18-BS(MF)
932.11	932.16	932.14	Staffelegg Fm.	24.02.2020	TRU1-1-932.14-BS(MF)
933.14	933.20	933.17	Staffelegg Fm.	24.02.2020	TRU1-1-933.17-BS(MF)
943.81	943.845	943.83	Staffelegg Fm.	24.02.2020	TRU1-1-943.83-BS(MF)
947.365	947.41	947.41	Staffelegg Fm.	24.02.2020	TRU1-1-947.39-BS(MF)

Appendix A3: List of other provisionally determined conspicuous macrofossils from TRU1-1 (973.03 – 708.36 m)

Top [m]	Bottom [m]	Fossil	Determination (provisional)
708.36		See urchin (spine)	<i>Rhabdocidaris</i> sp.
711.51		Ammonite	<i>Glochiceras</i>
720.75		Bivalve	<i>Eopecten</i> sp.
731.06		Bivalve	<i>Goniomya</i>
732.94	732.95		indet.
736.87		Bivalve	<i>Pinna</i>
748.86		Ammonite	<i>Oecotraustes?</i> incomplete
755.16	775.18		indet.
778.78	778.84	Belemnite	<i>Megateuthis?</i>
787.57		Bivalve	<i>Ctenostreon</i>
802.11		Wood	
840.07		Belemnite	indet.
843.33		Crinoids	<i>Chariocrinus württembergicus</i>
879.56		Ammonite	<i>Leioceras</i>
911.43		Aptychus	<i>Leioceras</i>
913.48		Ammonites	<i>Leioceras</i>
914.27		Ammonite	<i>Leioceras</i>
914.34		Ammonite	<i>Leioceras</i>
914.41		Ammonite	<i>Leioceras</i>
914.925		Ammonite	<i>Leioceras</i>
914.98		Ammonite	<i>Leioceras</i>
915.18		Ammonite	?
915.25		Ammonite	?
917.55	916.18	Ammonites	<i>Leioceras</i>
918.45	918.96	Ammonites	<i>Leioceras</i>
921.00		Ammonite	<i>Leioceras</i>
924.185		Ammonite	<i>Leioceras</i>
924.79		Ammonite	<i>Leioceras</i>
927.61		Ammonite	<i>Leioceras?</i>
930.40	930.42	Ammonites	?
931.56		Ammonite	?
932.27		Bivalve	<i>Pseudomytiloides dubius</i>
932.96		Ammonite	<i>Pseudogrammoceras?</i>
934.40		Bivalve	<i>Pseudomytiloides dubius</i>
934.78	935.31	Bivalves	<i>Bositra buchi</i>
935.94		Ammonite	<i>Dactylioceras</i> sp.
936.02		Ammonite	<i>Dactylioceras commune</i>
936.22		Ammonite & bivalve	<i>Dactylioceras</i> sp., <i>Pseudomytiloides dubius</i>
936.53		Ammonite	<i>Dactylioceras</i> sp.
941.95		Ammonite	<i>Harpoceras</i>
943.28		Ammonite	?
948.13	948.18	Crinoids	<i>Chladocrinus</i>
973.03		Bivalve	<i>Modiolus</i>

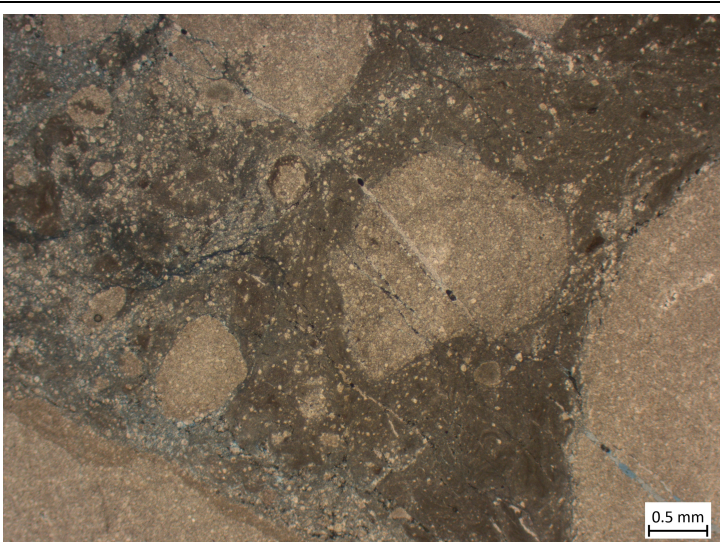
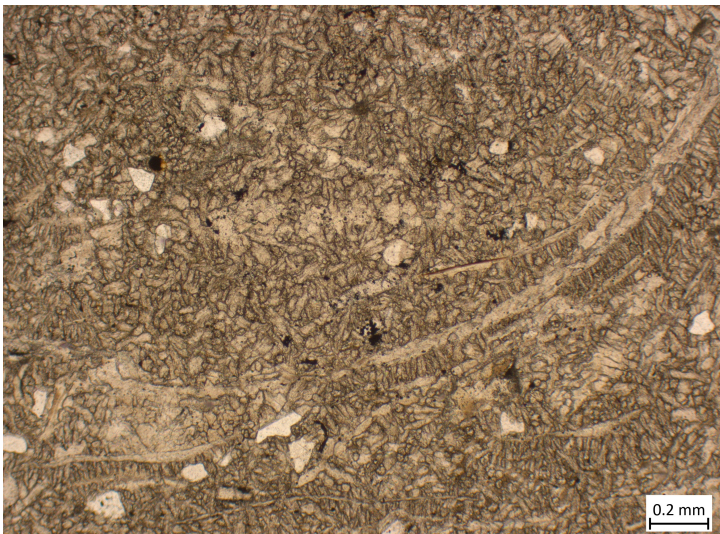
Appendix A4: List of all palynological sample from TRU1-1 (928.09 –724.78 m)

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

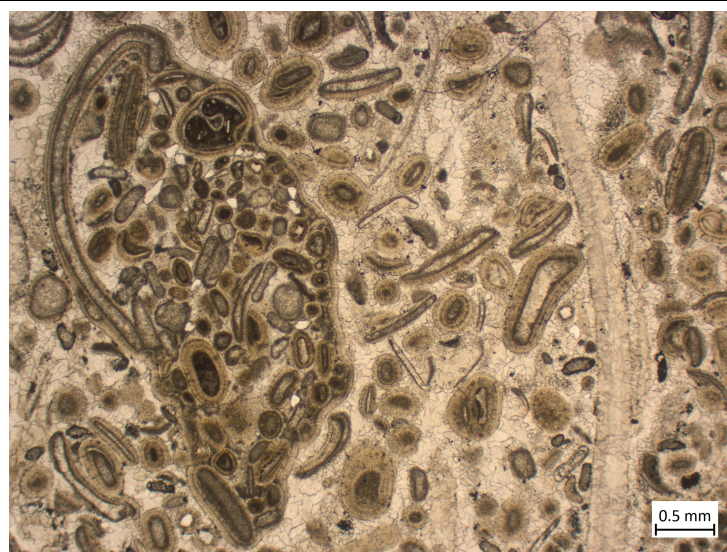
Top [m]	Bottom [m]	Avg. Depth [m]	Formation	Retrieval date [dd.mm.yyyy]	Sample ID
724.76	724.80	724.78	Wildegge Fm.	12.03.2020	TRU1-1-724.78-BS(Pa)
724.84	724.88	724.86	Wutach Fm.	12.03.2020	TRU1-1-724.86-BS(Pa)
725.10	725.115	725.11	Wutach Fm.	30.03.2020	TRU1-1-725.11-BS(Pa)
726.87	726.88	726.88	Wutach Fm.	30.03.2020	TRU1-1-726.88-BS(Pa)
727.31	727.32	727.32	Variansmergel Fm.	12.03.2020	TRU1-1-727.32-BS(Pa)
729.82	729.85	729.84	Variansmergel Fm.	12.03.2020	TRU1-1-729.84-BS(Pa)
730.61	730.63	730.62	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-730.62-BS(Pa)
737.18	737.21	737.20	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-737.20-BS(Pa)
744.64	744.67	744.66	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-744.66-BS(Pa)
750.50	750.53	750.52	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-750.52-BS(Pa)
757.74	757.75	757.75	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-757.75-BS(Pa)
765.79	765.82	765.81	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-765.81-BS(Pa)
766.74	766.75	766.75	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-766.75-BS(Pa)
767.50	767.52	767.51	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-767.51-BS(Pa)
774.45	774.48	774.47	«Parkinsoni-Württembergica-S.»	12.03.2020	TRU1-1-774.47-BS(Pa)
775.15	775.16	775.16	«Humphriesioolith Fm.»	01.04.2020	TRU1-1-775.16-BS(Pa)
775.63	775.66	775.65	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-775.65-BS(Pa)
776.72	776.73	776.73	«Humphriesioolith Fm.»	01.04.2020	TRU1-1-776.73-BS(Pa)
776.94	776.95	776.95	«Humphriesioolith Fm.»	01.04.2020	TRU1-1-776.95-BS(Pa)
777.80	777.83	777.82	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-777.82-BS(Pa)
778.19	778.22	778.21	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-778.21-BS(Pa)
783.76	783.79	783.78	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-783.78-BS(Pa)
784.00	784.02	784.01	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-784.01-BS(Pa)
785.92	785.94	785.93	«Humphriesioolith Fm.»	12.03.2020	TRU1-1-785.93-BS(Pa)
787.05	787.06	787.06	«Humphriesioolith Fm.»	01.04.2020	TRU1-1-787.06-BS(Pa)
787.60	787.63	787.62	Wedelsandstein Fm.	12.03.2020	TRU1-1-787.62-BS(Pa)
790.54	790.57	790.56	Wedelsandstein Fm.	12.03.2020	TRU1-1-790.56-BS(Pa)
797.43	797.45	797.44	Wedelsandstein Fm.	12.03.2020	TRU1-1-797.44-BS(Pa)
810.63	810.66	810.65	Wedelsandstein Fm.	12.03.2020	TRU1-1-810.65-BS(Pa)
814.15	814.18	814.17	Wedelsandstein Fm.	12.03.2020	TRU1-1-814.17-BS(Pa)
815.65	815.68	815.67	«Murchisonae-Oolith Fm.»	12.03.2020	TRU1-1-815.67-BS(Pa)
816.02	816.04	816.03	«Murchisonae-Oolith Fm.»	12.03.2020	TRU1-1-816.03-BS(Pa)
816.42	816.45	816.44	Opalinus Clay	12.03.2020	TRU1-1-816.44-BS(Pa)
818.01	818.04	818.03	Opalinus Clay	12.03.2020	TRU1-1-818.03-BS(Pa)
823.11	823.13	823.12	Opalinus Clay	07.04.2020	TRU1-1-823.12-BS(Pa)
828.70	828.72	828.71	Opalinus Clay	07.04.2020	TRU1-1-828.71-BS(Pa)
833.79	833.81	833.80	Opalinus Clay	07.04.2020	TRU1-1-833.80-BS(Pa)
844.95	844.97	844.96	Opalinus Clay	07.04.2020	TRU1-1-844.96-BS(Pa)
865.36	865.38	865.37	Opalinus Clay	07.04.2020	TRU1-1-865.37-BS(Pa)
885.40	885.42	885.41	Opalinus Clay	07.04.2020	TRU1-1-885.41-BS(Pa)
906.86	906.88	906.87	Opalinus Clay	07.04.2020	TRU1-1-906.87-BS(Pa)
927.53	927.55	927.54	Opalinus Clay	07.04.2020	TRU1-1-927.54-BS(Pa)
928.03	928.04	928.03	Staffellegg Fm.	30.03.2020	TRU1-1-928.03-BS(Pa)
928.08	928.09	928.09	Staffellegg Fm.	30.03.2020	TRU1-1-928.09-BS(Pa)

Appendix B: Photos microfacies

Fig. B-1:	Thin section TRU1-1-1055.52, Bänkerjoch Fm.	B-2
Fig. B-2:	Thin section TRU1-1-992.67, Klettgau Fm. (Seebi Mb.)	B-2
Fig. B-3:	Thin section TRU1-1-972.00, Klettgau Fm. (Belchen Mb.)	B-2
Fig. B-4:	Thin section TRU1-1-971.35, Staffelegg Fm. (Schambelen Mb.)	B-3
Fig. B-5:	Thin section TRU1-1-896.67, Opalinus Clay	B-3
Fig. B-6:	Thin section TRU1-1-836.84, Opalinus Clay	B-3
Fig. B-7:	Thin section TRU1-1-833.00, Opalinus Clay	B-4
Fig. B-8:	Thin section TRU1-1-833.00, Opalinus Clay	B-4
Fig. B-9:	Thin section TRU1-1-826.03, Opalinus Clay	B-4
Fig. B-10:	Thin section TRU1-1-816.28, «Murchisonae-Oolith Fm.»	B-5
Fig. B-11:	Thin section TRU1-1-815.44, Wedelsandstein Fm.	B-5
Fig. B-12:	Thin section TRU1-1-810.82, Wedelsandstein Fm.	B-5
Fig. B-13:	Thin section TRU1-1-798.92, Wedelsandstein Fm.	B-6
Fig. B-14:	Thin section TRU1-1-784.67, «Humphriesioolith Fm.»	B-6
Fig. B-15:	Thin section TRU1-1-776.41, «Humphriesioolith Fm.»	B-6
Fig. B-16:	Thin section TRU1-1-774.93, «Humphriesioolith Fm.»	B-7
Fig. B-17:	Thin section TRU1-1-742.44, «Parkinsoni-Württembergica-Sch.»	B-7
Fig. B-18:	Thin section TRU1-1-735.98, Variansmergel Fm.	B-7
Fig. B-19:	Thin section TRU1-1-724.25, Wildegg Fm. (Birmenstorf Mb.)	B-8
Fig. B-20:	Thin section TRU1-1-724.25, Wildegg Fm. (Birmenstorf Mb.)	B-8
Fig. B-21:	Thin section TRU1-1-594.07, «Felsenkalke» + «Massenkalk»	B-8

	Fig. B-1: Dolomite rhombohedrons, forming a bed of dolostone (argillaceous): dolomite crystals pseudomorph replacing gypsum crystals Thin section (TS) photo TRU1-1-1055.52 Bänkerjoch Fm.
	Fig. B-2: Intraformational breccia: dolostone intraclasts, sedimented in a dolomitic marl matrix Thin section photo TRU1-1-992.67 Klettgau Fm. (Seebi Mb.)
	Fig. B-3: "Hiatus bed": biomicrosparite: biogene components (e.g. bivalves) embedded in a "stellate cement" typical for "hiatus beds" – little calcite crystals, grown in a micrite matrix – and not in open pore space Thin section photo TRU1-1-972.00 Klettgau Fm. (Belchen Mb.)

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

**Fig. B-4:**

Oosparite:
ooids, an oosparitic intraclast
and bivalves, cemented by
calcite sparite

Thin section photo

TRU1-1-971.35

Staffelegg Fm.
(Schambelen Mb.)

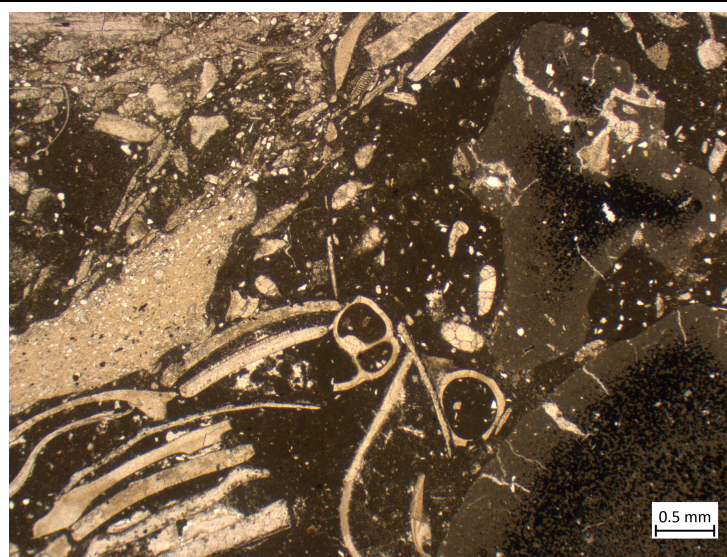
**Fig. B-5:**

"Hiatus bed":
"stellate cement", grown in
an argillaceous matrix, with a
few silt-sized quartz grains
(white) and pyrite (black)

Thin section photo

TRU1-1-896.67

Opalinus Clay

**Fig. B-6:**

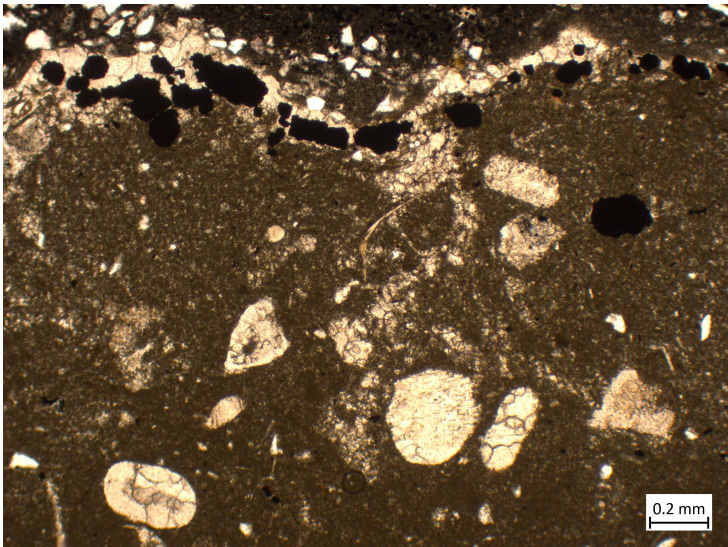
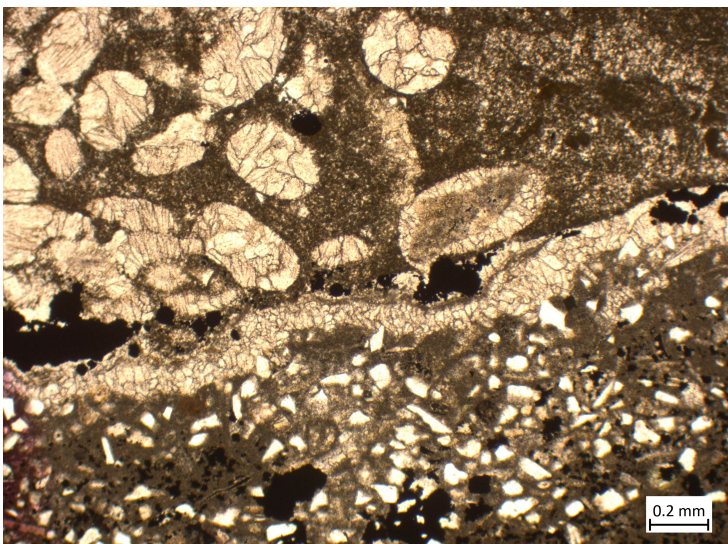
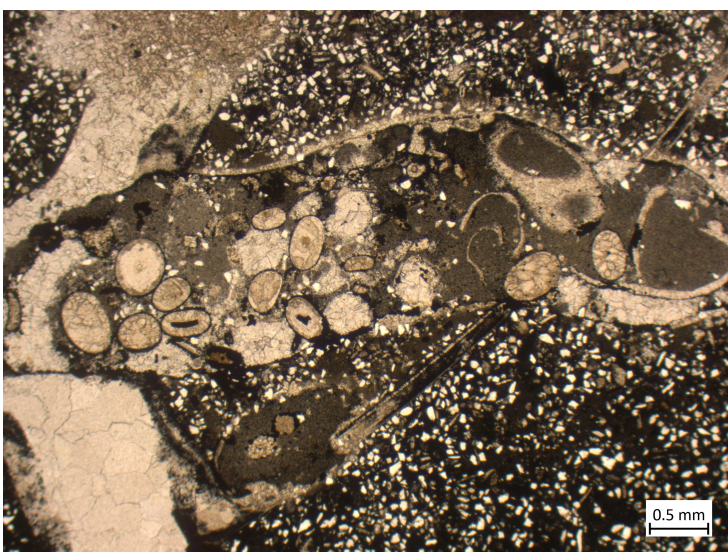
Hardground:
intramicrite, consisting of
phosphoritic and micritic
intraclasts in a micrite matrix
with numerous bivalve and
echinoderm detritus

Thin section photo

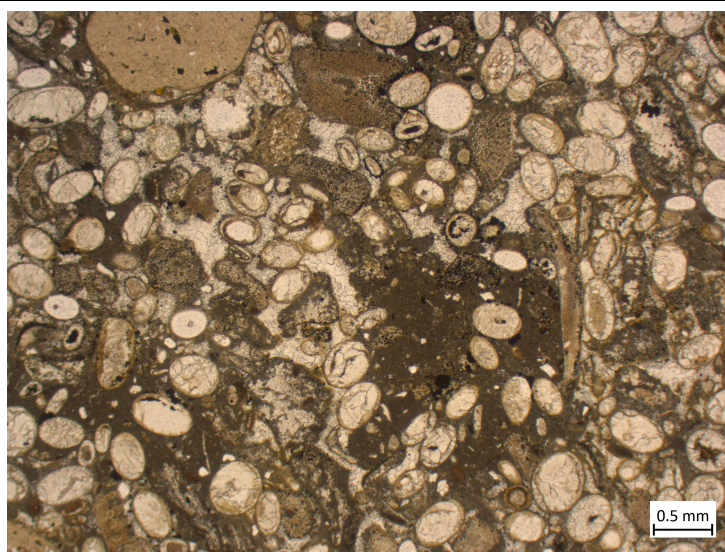
TRU1-1-836.84

Opalinus Clay

Selected photos of microfacies from Staffelegg Fm. and Opalinus Clay

	Fig. B-7: Hardground, lower horizon: pyrite/calcite crust on iron-ooid (now calcitic) bearing micrite Thin section photo TRU1-1-833.00 Opalinus Clay
	Fig. B-8: Hardground, upper horizon: iron-oolite (iron-ooids now calcitic); underneath: calcite (stromatolithe) crust and biomicrite (silty) at the base Thin section photo TRU1-1-833.00 Opalinus Clay
	Fig. B-9: Hardground: iron-oolitic intraclast (iron-ooids now calcitic) in a biomicrite (silty) Thin section photo TRU1-1-826.03 Opalinus Clay

Selected photos of microfacies from Opalinus Clay

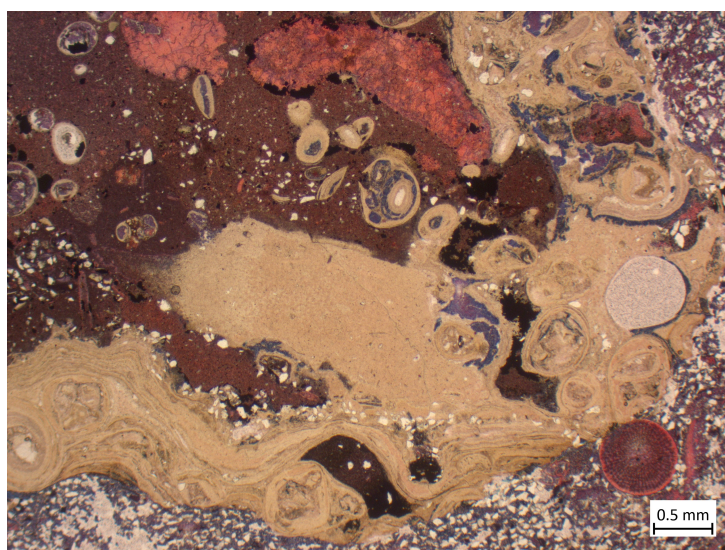
**Fig. B-10:**

Iron-oolite (calcareous, biotrititic):
iron-oids (now calcitic)
with small limonite rim,
crinoids and bivalves, partly
sedimented with micritic
matrix, partly cemented by
calcite

Thin section photo

TRU1-1-816.28

«Murchisonae-Oolith Fm.»

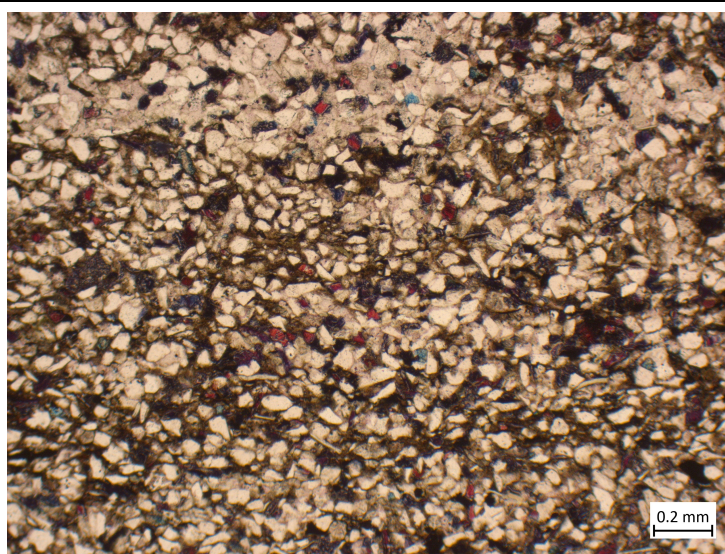
**Fig. B-11:**

Iron-stromatolitic intraclast
in a sandy limestone:
stromatolite damaged due to
thin section preparation,
largely ground away

Thin section photo,
TS stained for calcite=red

TRU1-1-815.44

Wedelsandstein Fm.

**Fig. B-12:**

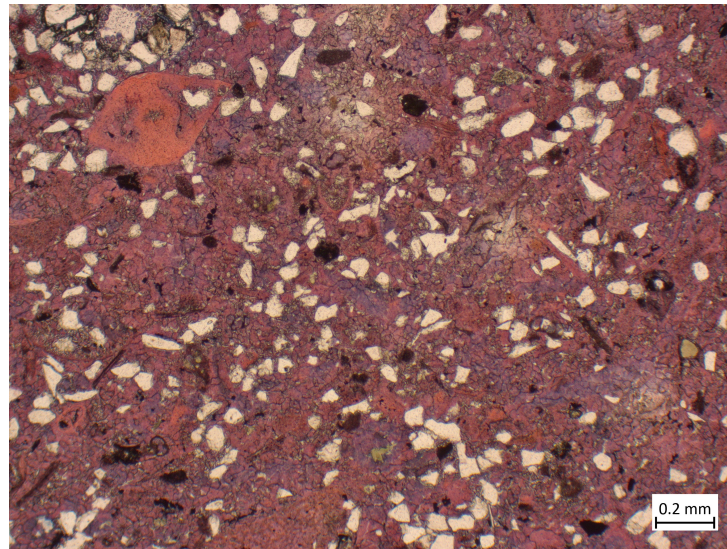
Calcareous sandstone
(biotrititic):
quartz grains and biotritus
cemented by calcite sparite,
sampled from a
calcareous/quartz-rich bed

Thin section photo,
TS stained for calcite=red

TRU1-1-810.82

Wedelsandstein Fm.

Selected photos of microfacies from «Murchisonae-Oolith Fm.» and Wedelsandstein Fm.

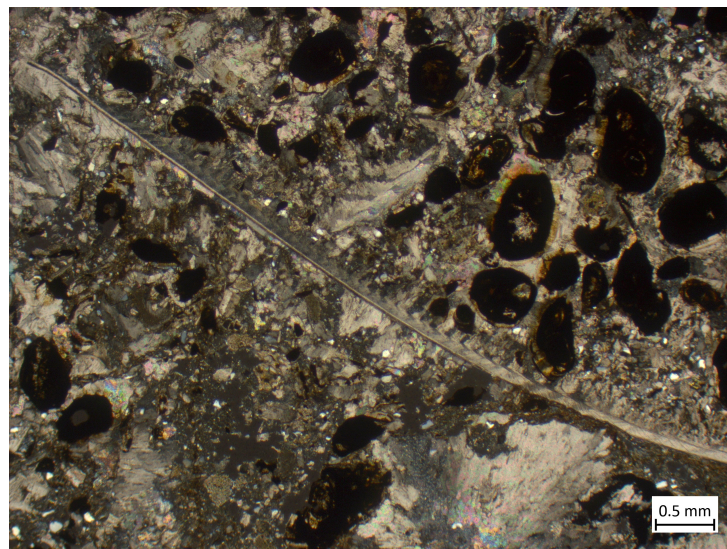
**Fig. B-13:**

Sandy limestone (biosparite): fine-grained biotritus (and one big foraminifera *Lenticulina* sp.) and quartz grains cemented by calcite sparite, sampled from a calcareous/quartz-rich bed

thin section photo,
TS stained for calcite=red

TRU1-1-798.92

Wedelsandstein Fm.

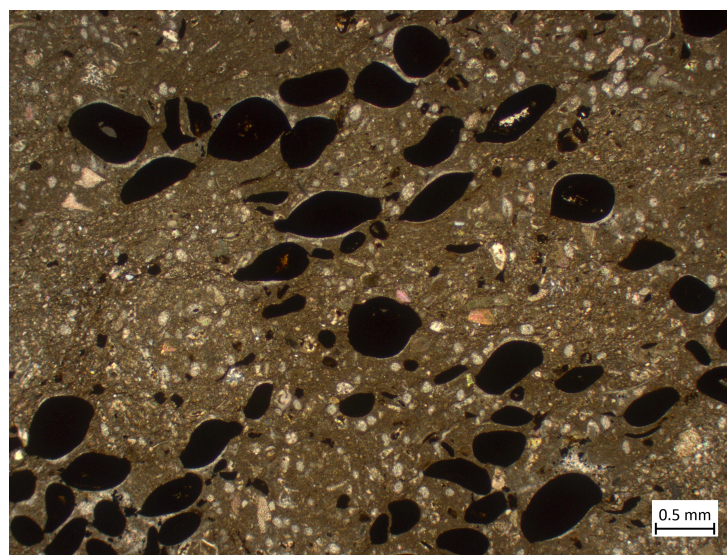
**Fig. B-14:**

Limestone (iron-oolitic): iron-oids and bivalves embedded in micritic matrix, "normal" calcite cement and stellate "hiatus bed" cement

Thin section photo, crossed
nicols

TRU1-1-784.67

«Humphriesioolith Fm.»

**Fig. B-15:**

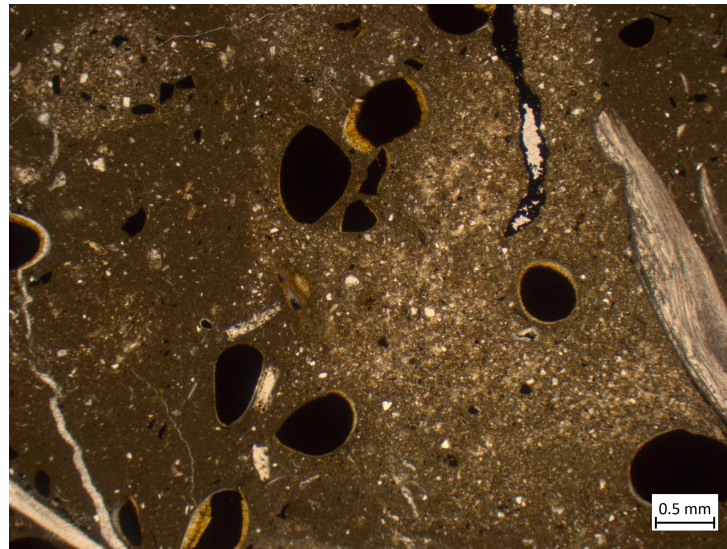
Limestone (iron-oolitic): iron-oids and small biotritus (e.g. sponge spicules) sedimented with micrite matrix

Thin section photo

TRU1-1-776.41

«Humphriesioolith Fm.»

Selected photos of microfacies from Wedelsandstein Fm. and «Humphriesioolith Fm.»

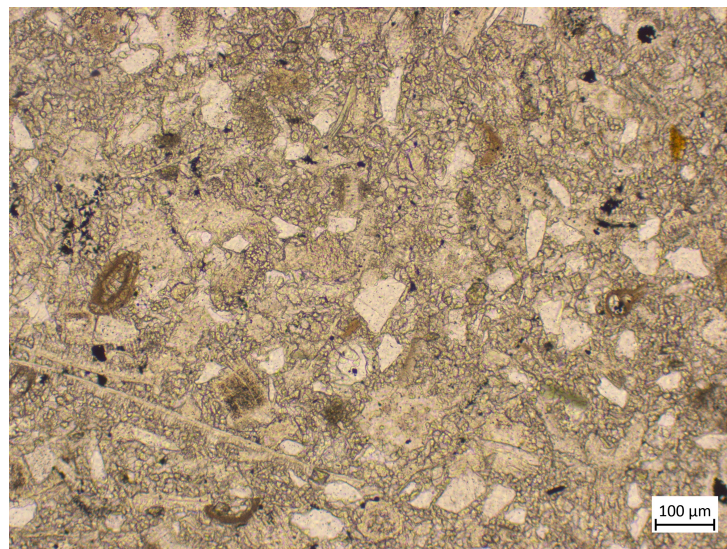
**Fig. B-16:**

Limestone (iron-oolitic):
iron-ooloids with calcite
cement rim, bivalves and
burrows in limonitic micrite
matrix

Thin section photo

TRU1-1-774.93

«Humphriesoolith Fm.»

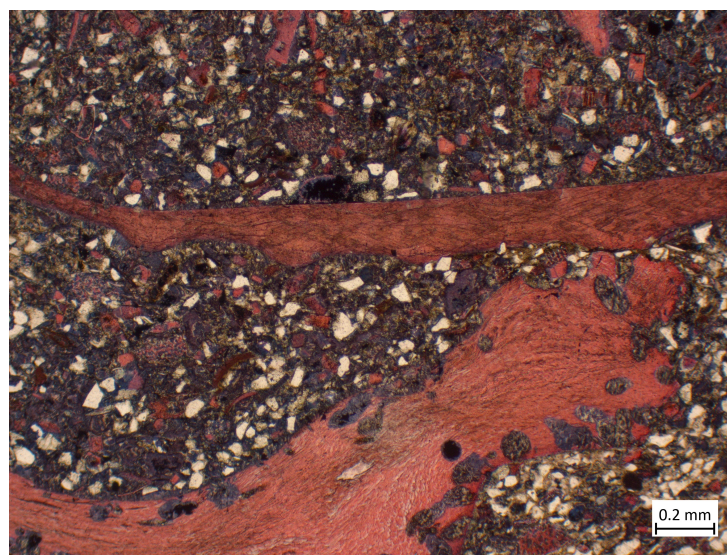
**Fig. B-17:**

Biomicrosparit (silty):
silt-sized quartz grains and
biotritus with stellate
("hiatus bed") cement,
sampled from a
calcareous/quartz-rich bed

Thin section photo

TRU1-1-742.22

«Parkinsoni-Württem-
bergica-Schichten»

**Fig. B-18:**

Biosparite (sandy):
Sand-sized quartz grains,
bivalves (partly bored) and
small biotritus, cemented
by iron-bearing calcite
(bluish-violet coloured),
sampled from a
calcareous/quartz-rich bed

Thin section photo, TS
stained for calcite = red

TRU1-1-735.98

Variansmrgel Fm.

Select. photos of mic.fac. from «Humph.oo. Fm.», «Park.-Württemb.-Sch.», Variansmrgl. Fm.

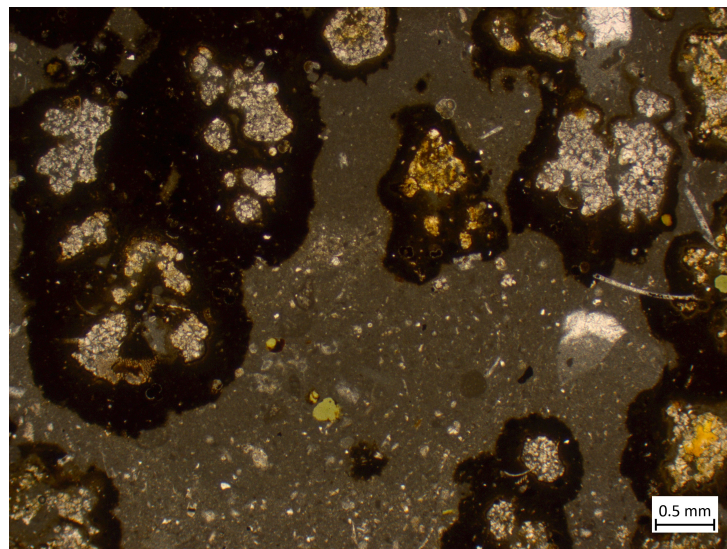
**Fig. B-19:**

Marl with micritic sponge nodules (dark brown, homogeneous part in the centre) and glauconite grains

Thin section photo

TRU1-1-724.25 lower half

Wildegge Fm.
(Birmenstorf Mb.)

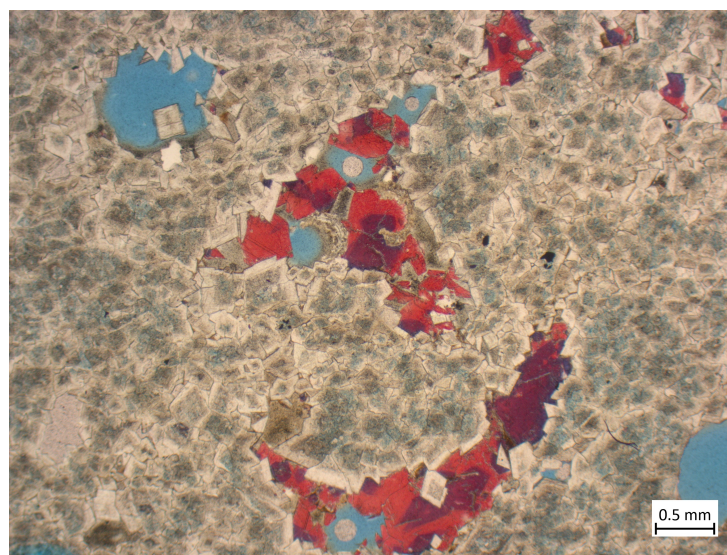
**Fig. B-20:**

"Iron-crust":
strange limonitic crust
consisting of iron-
mineralized "drops" with
calcitic cells inside

Thin section photo

TRU1-1-724.25 upper half

Wildegge Fm.
(Birmenstorf Mb.)

**Fig. B-21:**

Dolostone:
dolomite rhombohedrons
(non-coloured), close-fitted,
and pores (filled with blue
resin), partly cemented by
calcite (red coloured)

Thin section photo,
TS stained for calcite = red

TRU1-1-594.07
«Felsenkalke» +
«Massenkalk»

Selected photos of microfacies from Birmenstorf Mb. and «Felsenkalke» + «Massenkalk»

Appendix C: Plates of ammonites

Plate I:	TRU1-1 (947.91 – 928.03 m)	C-3
Plate II:	TRU1-1 (917.53 – 776.74 m)	C-5
Plate III:	TRU1-1 (766.92 – 732.94 m)	C-7
Plate IV:	TRU1-1 (723.07 – 722.21 m)	C-9

Plate I TRU1-1 (947.91 – 928.03 m)

- Fig. 1: *Amaltheus* ex. gr. *margaritatus* (de Montfort, 1808), depth: 947.41 m, Staffelegg Fm. (Breitenmatt Mb. and Rickenbach Mb.), Margaritatus Zone.
- Fig. 2: *Dactylioceras* (*Orthodactylites*) sp., depth: 943.83 m, Staffelegg Fm. (Rietheim Mb.), Early Toarcian.
- Figs. 3a, 3b: *Haugia?* sp., depth: 933.17 m, Staffelegg Fm. (Gross Wolf Mb.), Variabilis Zone. Fig. 3a: lateral view, 3b: cross section.
- Fig. 4: *Pseudogrammoceras* ex gr. *fallaciosum* (Bayle, 1878), depth: 932.14 m, Staffelegg Fm. (Gross Wolf Mb.), Thouarsense Zone, Fallaciosum Subzone.
- Figs. 5a – 5c: *Pleydellia* sp., depth: 929.18 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, Aalensis Subzone. Fig. 5 shows different specimens: 5a: Fragment in lateral view, 5b: inner whorl, 5c: Fragment in lateral view.
- Fig. 6: *Pleydellia* sp., depth: 928.10 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, possibly Torulosum Subzone.
- Fig. 7: *Pleydellia* ex gr. *buckmani* (Maubeuge, 1947), depth: 928.03 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, Torulosum Subzone.

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

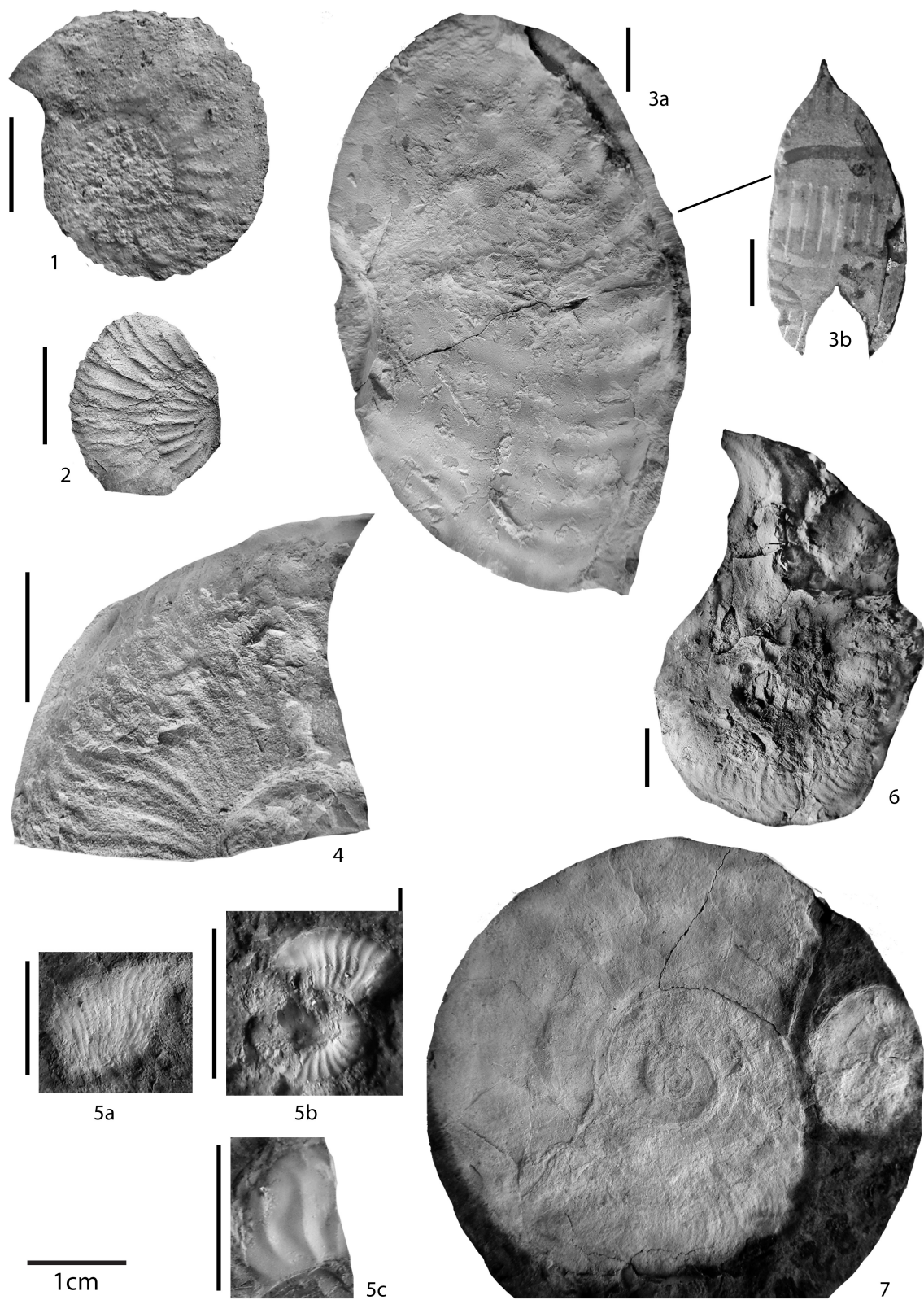


Plate I: TRU1-1 (947.91 – 928.03 m)

Plate II TRU1-1 (917.53 – 776.74 m)

- Fig. 1: *Leioceras opalinum* (Reinecke, 1818), depth: 917.53 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 2: *Leioceras opalinum* (Reinecke 1818), depth: 915.74 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 3: *Leioceras opalinum* (Reinecke, 1818), depth: 913.89 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 4: *Chondroceras* ex gr. *gervillii* (Sowerby, 1818), depth: 776.99 m, «Humphriesioolith Fm.», Humphriesianum Zone, Humphriesianum Subzone, Gervillii-Cycloides faunal horizon.
- Fig. 5: *Chondroceras* ex gr. *gervillii* (Sowerby, 1818), depth: 776.99 m, «Humphriesioolith Fm.», Humphriesianum Zone, Humphriesianum Zone, Gervillii-Cycloides faunal horizon.
- Figs. 6a, 6b: *Stephanoceras* sp., depth: 776.74 m, «Humphriesioolith Fm.», Humphriesianum Zone, Humphriesianum Subzone. Fig. 6a: lateral view, 6b: cross section of the phragmocon.

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

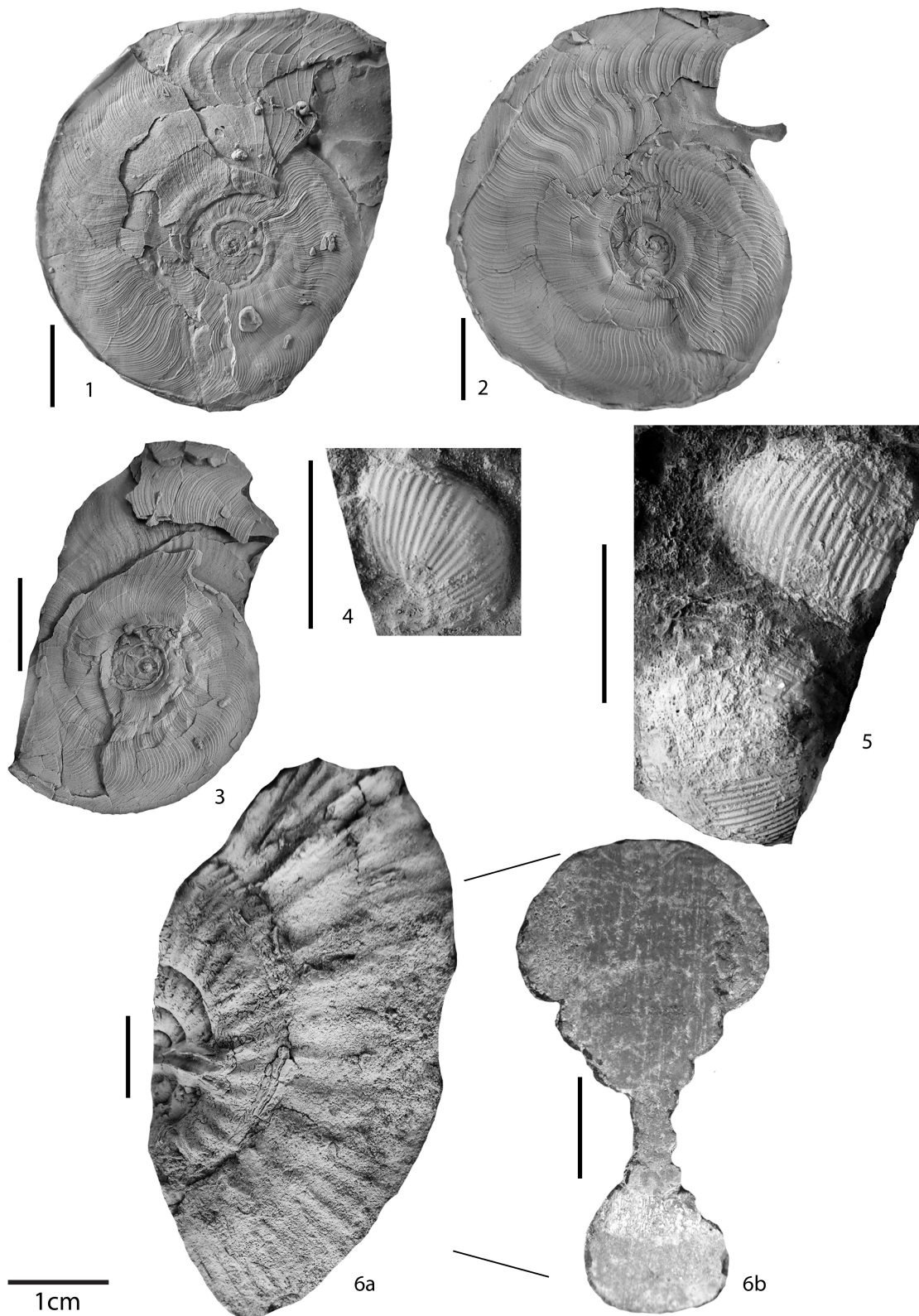


Plate II: TRU1-1 (917.53 – 776.74 m)

Plate III TRU1-1 (766.92 – 732.94 m)

Figs. 1a, 1b: *Parkinsonia* ex gr. *subarietis-rarecostata*, microconch, sharply ripped, depth: 766.92 m, «Parkinsoni-Württembergica-Schichten» (most probably «Parkinsoni-Oolith»), Parkinsoni Zone, Acris Subzone.

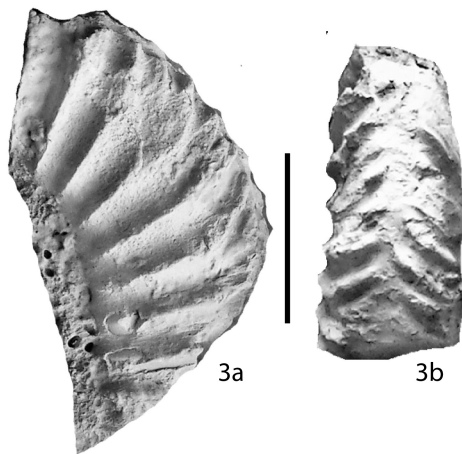
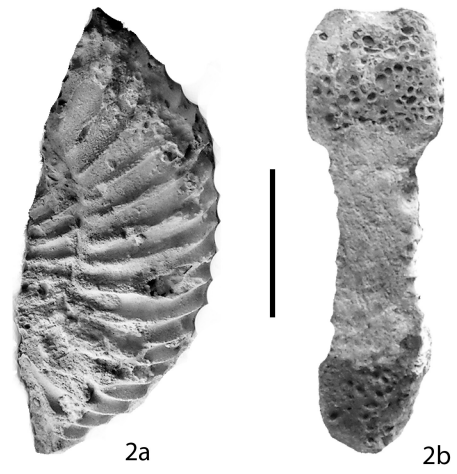
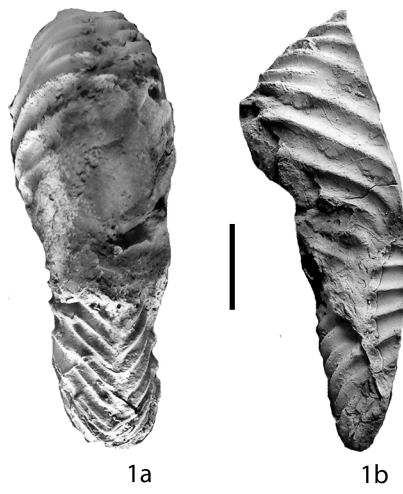
Figs. 2a, 2b: *Parkinsonia* ex gr. *subarietis-rarecostata*, microconch, sharply ripped, depth: 766.76 m, «Parkinsoni-Württembergica-Schichten» (most probably «Parkinsoni-Oolith»), Parkinsoni Zone, Acris Subzone. Fig. 2a: lateral view, 2b: cross section.

Figs. 3a, 3b: *Parkinsonia* ex gr. *subarietis-rarecostata*, microconch, sharply ripped, depth: 766.76 m, «Parkinsoni-Württembergica-Schichten» (most probably «Parkinsoni-Oolith»), Parkinsoni Zone, Acris Subzone. Fig. 3a: lateral view, 3b: ventral view.

Fig. 4: *Parkinsonia?* sp., macroconch, depth: 766.53 m, «Parkinsoni-Württembergica-Schichten», Parkinsoni Zone?

Fig. 5: *Morphoceras* sp., depth: 732.94 m, Variansmergel Fm., Early Bathonian.

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



1cm

Plate IV TRU1-1 (723.07 – 722.21 m)

Fig. 1: *Perisphinctes* sp., depth: 723.07 m, Wildegge Fm. (Birmenstorf Mb.), Transversarium Zone.

Fig. 2: *Dichotomosphinctes?* sp., depth: 722.21 m, Wildegge Fm. (Birmenstorf Mb.), Transversarium Zone, Rotoides Subzone or Bifurcatus Zone, Stenocycloides Subzone.

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



1cm

Plate IV: TRU1-1 (723.07 – 722.21 m)

Appendix D: Palynostratigraphy

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

Appendix D2: Depth/Age plot: Trüllikon-1-1 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 in the Opalinus Clay and its upper 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 upper 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 $\delta^{13}\text{C}_{\text{carb}}$): HB: drilled from a "hiatus bed", HC: drilled from a "hiatus concretion", CC: drilled from a calcareous concretions, SN: drilled from a septarian nodule, MF: drilled from macrofossil, TS: drilled directly from thin section sample (see micro-facies description in Section 3.1).

Depth [m]	Description of sample		TS	$\delta^{13}\text{C}_{\text{carb}}$ [‰ VPDB]	$\delta^{18}\text{O}_{\text{carb}}$ [‰ VPDB]	Carbonate [wt.-%]
824.09	Belemnite	MF		2.23	-0.25	97.2
824.11	Hardground			-4.13	-3.84	34.9
826.03	Intraclast (iron-oolitic)	HC	×	-10.73	-4.59	60.5
831.75	Calcareous bed			-3.35	-3.22	65.5
831.91	Intraclast (micritic)	HC	×	-26.73	-4.27	53.9
832.49	Calcareous bed (silty)		×	-3.34	-1.68	39.3
832.91	Calcareous bed			-6.30	-3.83	69.0
833.00	Micrite (iron-oolitic)			-5.90	-3.13	71.3
836.84	Intraclast (micritic, phosphoritic)		×	-3.59	-7.63	50.2
843.33	Intraclast (micritic, pyritic)		×	1.25	-1.37	32.2
896.67	Calcareous, marly bed	HB	×	-8.98	-7.46	59.9
917.80	Calcareous concretion	CC		-25.58	-1.39	78.0