

Arbeitsbericht NAB 22-01

**TBO Stadel-3-1:
Data Report**

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

June 2022

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

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Dossier IV Microfacies, Bio- and Chemo- stratigraphic Analysis

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Keywords:

STA3-1, Nördlich Lägern, TBO, deep drilling campaign,
microfacies, lithostratigraphy, biostratigraphy, ammonite
stratigraphy, palynostratigraphy, chemostratigraphy,
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 report was finalised in March 2023.

This Dossier was prepared by a project team consisting of:

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

H.R. Bläsi (microfacies)

S. Feist-Burkhardt (palynostratigraphy)

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

G. Deplazes (project management and conceptualisation)

Editorial work: P. Blaser and M. Unger

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

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1 Introduction

1.1 Context

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

In this report, we present the results from the Stadel-3-1 borehole.

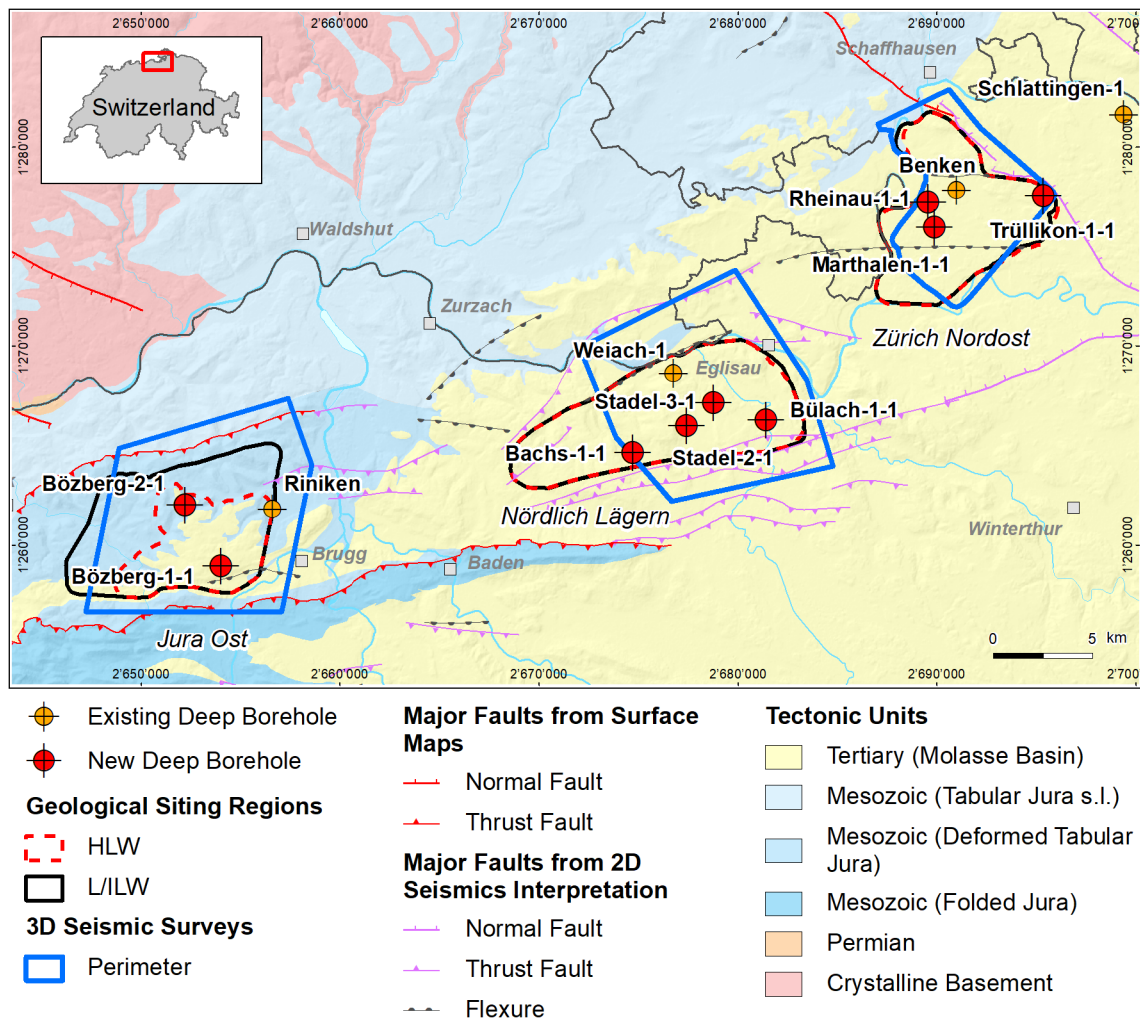


Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Stadel-3-1 (STA3-1) exploratory borehole is the sixth borehole drilled within the framework of the TBO project. The drill site is located in the central part of the Nördlich Lägern siting region (Fig. 1-2). The vertical borehole reached a final depth of 1'280.88 m (MD)¹. The borehole specifications are provided in Tab. 1-1.

Tab. 1-1: General information about the STA3-1 borehole

Siting region	Nördlich Lägern
Municipality	Stadel (Canton Zürich / ZH), Switzerland
Drill site	Stadel-3 (STA3)
Borehole	Stadel-3-1 (STA3-1)
Coordinates	LV95: 2'678'792.885 / 1'267'161.988
Elevation	Ground level = top of rig cellar: 408.74 m above sea level (asl)
Borehole depth	1'280.88 m measured depth (MD) below ground level (bgl)
Drilling period	17th December 2020 – 25th June 2021 (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 : 0.0 – 439.0 m: Polymers 439.0 – 640.0 ³ m: Sodium chloride & polymers 640.0 – 1'035.0 m: Potassium silicate & polymers 1'035.0 – 1'101.0 m: Polymers 1'101.0 – 1'280.9 m: Sodium chloride & polymers

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The main lithostratigraphic boundaries in the STA3-1 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.

³ Borehole uncased below casing shoe at 437.4 m after drilling fluid exchange.

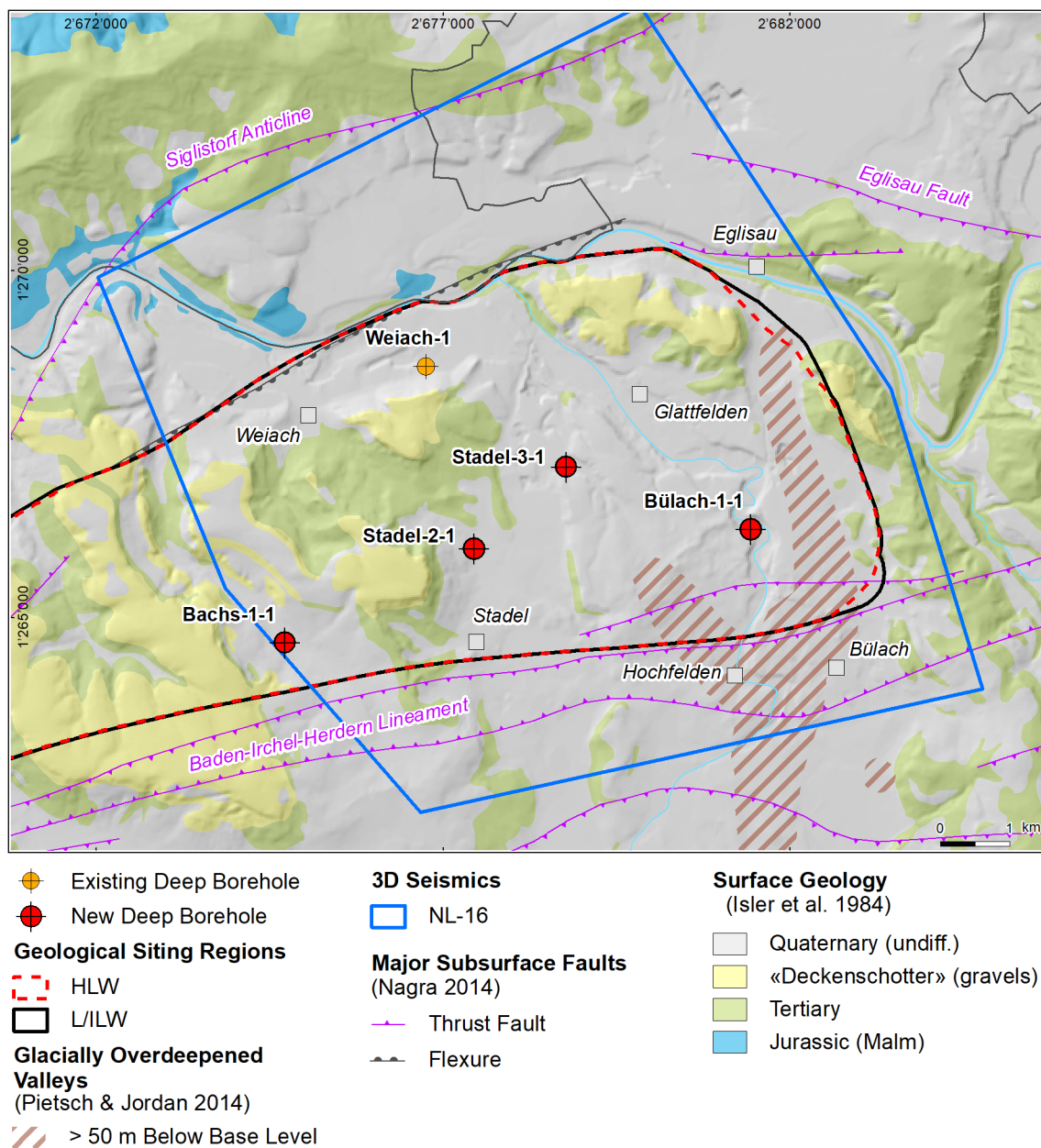


Fig. 1-2: Overview map of the investigation area in the Nördlich Lägern siting region with the location of the STA3-1 borehole in relation to the boreholes Weiach-1, BUL1-1, STA2-1 and BAC1-1

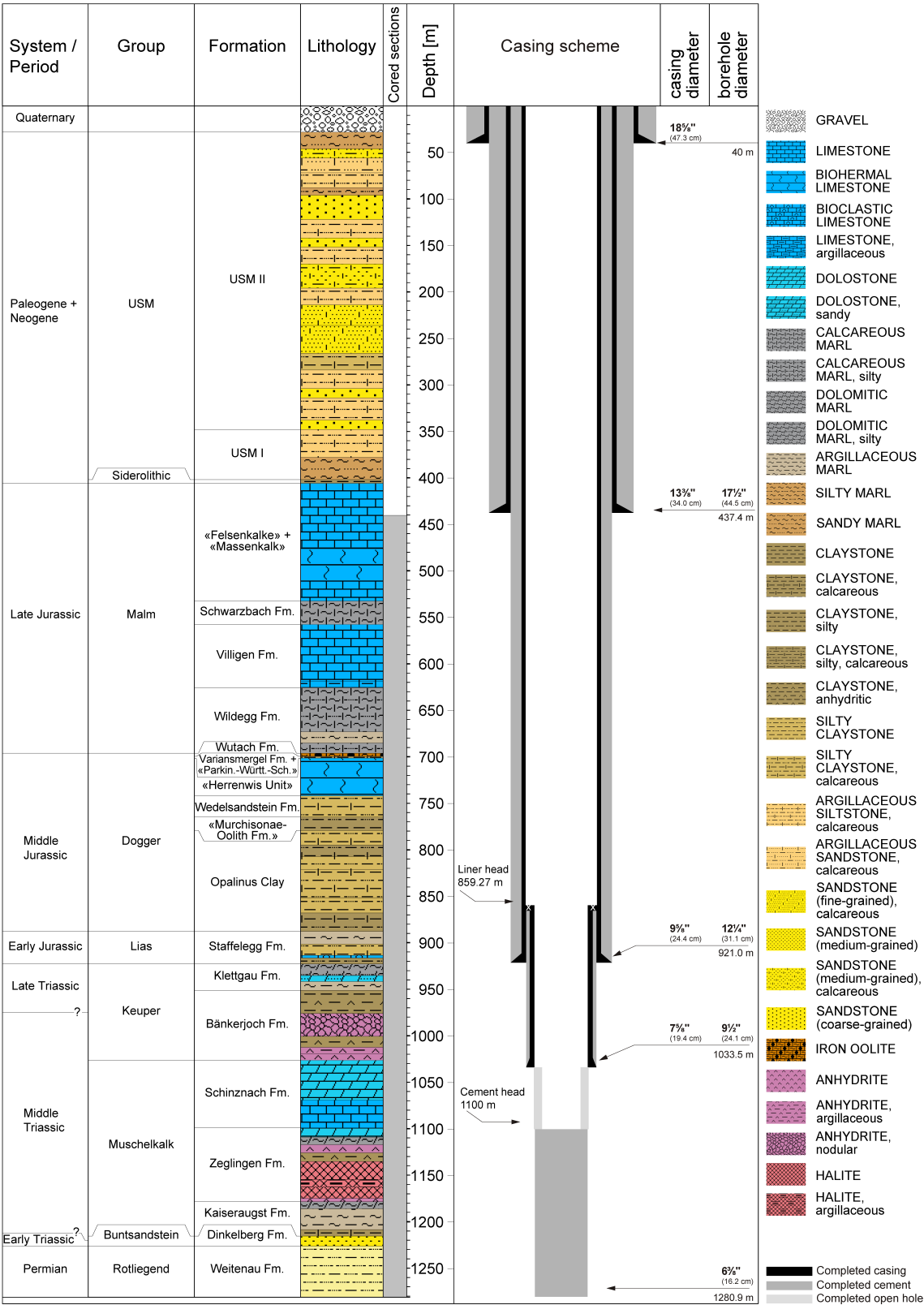


Fig. 1-3: Lithostratigraphic profile and casing scheme for the STA3-1 borehole⁴

⁴ For detailed information see Dossier I and III.

1.3 Documentation structure for the STA3-1 borehole

NAB 22-01 documents the majority of the investigations carried out in the STA3-1 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 STA3-1 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 22-01

Black indicates the dossier at hand.

Dossier	Title	Authors
I	TBO Stadel-3-1: Drilling	M. Ammen & P.-J. Palten
II	TBO Stadel-3-1: Core Photography	D. Kaehr & M. Gysi
III	TBO Stadel-3-1: Lithostratigraphy	P. Schürch, P. Jordan, M. Schwarz, H. Naef, R. Felber, T. Ibele & M. Gysi
IV	TBO Stadel-3-1: Microfacies, Bio- and Chemostratigraphic Analyses	S. Wohlwend, H.R. Bläsi, S. Feist-Burkhardt, B. Hostettler, U. Menkveld-Gfeller, V. Dietze & G. Deplazes
V	TBO Stadel-3-1: Structural Geology	A. Ebert, S. Cioldi, E. Hägerstedt & M. Gysi
VI	TBO Stadel-3-1: Wireline Logging, Microhydraulic Fracturing and Pressure-meter Testing	J. Gonus, E. Bailey, J. Desroches & R. Garrard
VII	TBO Stadel-3-1: Hydraulic Packer Testing	R. Schwarz, M. Willmann, H. Fisch, L. Schlickenrieder, M. Voß & A. Pechstein
VIII	TBO Stadel-3-1: Rock Properties, Porewater Characterisation and Natural Tracer Profiles	L. Aschwanden, L. Camesi, E. Gaucher, T. Gimmi, A. Jenni, M. Kiczka, U. Mäder, M. Mazurek, D. Rufer, H.N. Waber, P. Wersin, C. Zwahlen & D. Traber
IX	TBO Stadel-3-1: Rock-mechanical and Geomechanical Laboratory Testing	E. Crisci, L. Laloui & S. Giger
X	TBO Stadel-3-1: Petrophysical Log Analysis	S. Marnat & J.K. Becker
	TBO Stadel-3-1: Summary Plot	Nagra

1.4 Scope and objectives of this dossier

The dossier at hand complements the lithostratigraphic report (Dossier III) on the STA3-1 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 (26.08.2021), two months after the end of drilling operations and were integrated into the lithostratigraphic discussion and lithostratigraphic boundary definition (Dossier III).

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

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

The detailed stratigraphy of the STA3-1 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 STADEL-3-1							
System / Period	Group	Formation	Metres MD	Member / Sub-unit			
Quaternary			28				
Paleogene / Neogene	Unt. Süsswasser-molasse	USM II	348				
		USM I	402				
	Siderolithic		406				
Jurassic	Late	Malm	«Felsenkalke» + «Massenkalk»				
			Schwarzbach Fm.	532.55			
			Villigen Fm.	557.93			
			Wildeggen Fm.	618.67	Hornbuck Mb.		
	Middle	Dogger		625.58	Effingen Mb.		
				695.71	Birmenstorf Mb. and «Glaukonitsandmergel Bed»		
			Wutach Fm.	696.03			
				699.47			
			Variansmergel Fm. + «Parkinsoni-Württembergica-Sch.»				
			«Herrenwis Unit»	701.65			
			Wedelsandstein Fm.	742.00			
			«Murchisonae-Oolith Fm.»	764.97			
	Early	Lias		779.26	«Sub-unit with silty calcareous beds»		
				807.34	«Upper silty sub-unit»		
				821.09	«Mixed clay-silt-carbonate sub-unit»		
				868.06	«Clay-rich sub-unit»		
				887.94	Gross Wolf Mb.		
				892.79	Rietheim Mb.		
Triassic	Late	Keuper		899.30	Grünschoholz Mb., Breitenmatt Mb. and Rickenbach Mb.		
				901.53	Frick Mb.		
				913.47	Begginnen Mb.		
				916.23	Schambelen Mb.		
	Middle				922.71	Gruhalde Mb.	
					935.22	Seebi Mb.	
					941.66	Gruhalde Mb.	
					943.46	Gansingen Mb.	
						945.28	Ergolz Mb.
						951.13	«Claystone with anhydrite nodules»
						976.08	«Cyclic sequence»
						1'000.71	«Thin-layered anhydrite and claystone sequence»
						1'019.81	«Banded massive anhydrite»
						1'023.45	«Dolomite and anhydrite»
						1'026.62	Asp Mb.
						1'030.65	Stamberg Mb.
						1'069.18	Liedertswil Mb.
						1'071.02	Leutschenberg Mb. and Kienberg Mb.
				1'099.03	«Dolomitzone»		
				1'109.13	«Obere Sulfatzone»		
				1'135.31	«Salzlager»		
				1'174.87	«Untere Sulfatzone»		
				1'178.43	«Orbicularismergel»		
				1'185.81	«Wellenmergel»		
				1'208.52	«Wellendolomit»		
				1'215.50			
	Bsst.	Dinkelberg Fm.	1'226.38				
Permian	Rotlieg.	Weitenau Fm.	1'280.88	Final depth			

Fig. 1-4: Stadel-3-1 stratigraphy with core depth in metres [m MD]

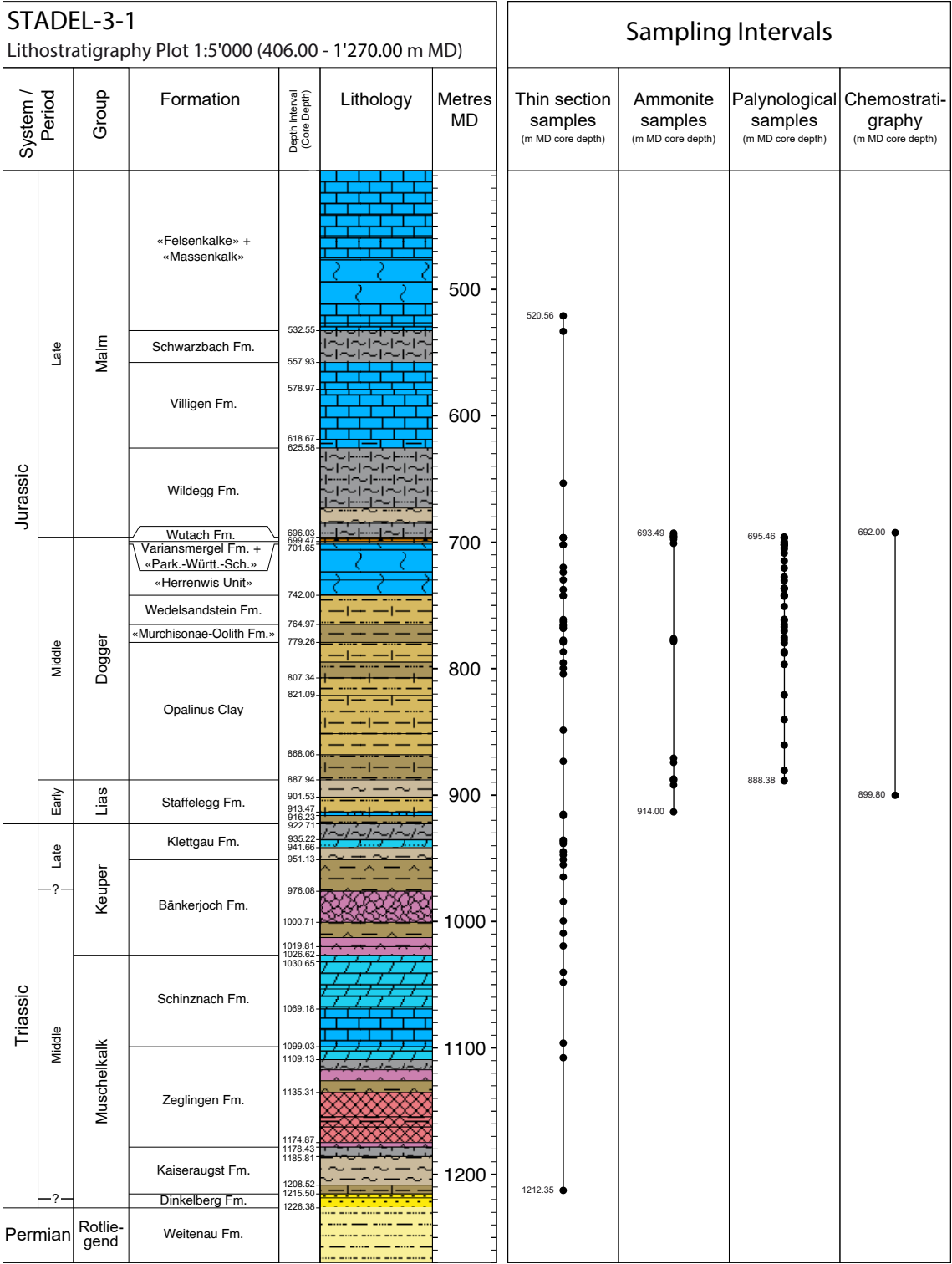


Fig. 1-5: Lithostratigraphy plot (1:5'000) from the Mesozoic succession with the individual sampling intervals for thin sections, macrofossils, palynological analysis and chemostratigraphy.

1:5'000 stratigraphic plot modified from Dossier III, shown is the stratigraphic range from 406 m to 1270 m, final depth at 1280.88 m.

2 Methods

2.1 Microfacies

Thin section preparation

All 48 thin sections (TS) were cut edgewise from the core so that the long side is parallel to the coring direction and therefore covers as much of the stratigraphy as possible. The mean depth of the thin section corresponds to the Sample ID. Therefore, thin sections containing lithological boundaries may have Sample IDs that fall into only one of the two described intervals. However, the lower or upper range on the thin section still covers the interval. A list of all thin sections with their sampling range and Sample ID can be found in Appendix A1 of this report.

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

Thin section analyses

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

Pellets, peloids, aggregates: the column of pellets also contains aggregates (lumps); that means "carbonate grains of various kinds are clumped together to form compound grains" (Bathurst 1975).

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

Fe-ooids or iron-ooids: Limonitic/goethitic or chamositic ooids, with a visible concentric structure; some iron-ooids are replaced by calcite (calcitic iron-ooids), a few of them show relicts of iron mineral layers (see STA3-1-786.32, Fig. B-11, Appendix B).

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

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

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

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

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

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

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

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

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

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

2.2 Ammonite preparation

The STA3-1 cores were carefully examined for macrofossils at the Würenlingen (Canton Aargau) core storage facility. The cores were examined for ammonites and other macrofossils on the bedding and fractured surfaces as well as on the outer surface of the core; the core itself was not broken open. A list of all 17 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 Glovelier where they were prepared and documented. Afterwards they were archived in the earth sciences collection of the Natural History Museum in Bern.

For the preparation, we used mechanical methods such as air tools and fine sandblasting equipment as well as a chemical etching method using potassium hydroxide (KOH). Sodium hydrogen carbonate was mainly used as abrasive. In one case, also some biloxite (corundum) was utilised (specimen from 779.24 m). Residual material from sawing and/or preparing four ammonite samples (marked in grey in Appendix A4) was used as material for palynological samples. Before being photographed, we applied ammonium chloride steam to the fossils to compensate for variation in contrast caused by different colouring. A selection of ammonites is documented on three plates (Plate I – III) 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 using concentrated HCl and concentrated HF, followed by a short oxidation with HNO₃ and, if necessary, treatment with ultrasound (e.g. Wood et al. 1996). The residues are sieved at a mesh size of 15 µm. Residues are mounted on microscope slides and analysed using transmitted light microscopy. A list of all samples with their sampling range and Sample ID can be found in Appendix A4 of this report.

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

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

2.4 Chemostratigraphy

The sampling of the STA3-1 borehole focused primarily on the Dogger and Lias Groups and therefore primarily on clay mineral-rich layers of the Opalinus Clay. The sampling resolution was one metre, except for some intervals with denser sampling density (mainly hardgrounds, condensed intervals and the Rietheim Member of the Staffelegg Formation). All 306 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 ($n = 40$) with results mainly from calcareous beds, calcareous concretions, and macrofossils (e.g. belemnites) can be found in Appendix E1 of this report.

Inorganic (carbonate) analyses

305 samples were analysed for **stable carbon** ($\delta^{13}\text{C}_{\text{carb}}$) and **oxygen isotope** ($\delta^{18}\text{O}_{\text{carb}}$) of bulk carbonate, 243 continuous samples (roughly in metre resolution) and additional 39 samples from specific calcareous beds and concretions in the Opalinus Clay (Appendix E1). The remaining 23 samples were taken for diagenetic comparisons and are not discussed further in this report. Varying amounts of powder to reach approximately 120 μg of carbonate in the vial were weighed using a Mettler Toledo MT5 Fact microbalance in 12 ml vacutainers. The headspace was flushed with pure He, and then the samples were reacted with 100% phosphoric acid at 72 °C in a ThermoFisher GasBench II carbonate device connected to a ThermoFisher Delta V PLUS mass spectrometer. The instrument is calibrated with international carbonate standards NBS19 and NBS18 distributed by the International Atomic Energy Agency (IAEA), Vienna and internal standards (MS2 "Carrara marble"; $\delta^{13}\text{C}_{\text{carb}} = 2.16\text{‰}$, $\delta^{18}\text{O}_{\text{carb}} = -1.85\text{‰}$). The reproducibility of the measurements based on replicated standards was $\pm 0.05\text{‰}$ for $\delta^{13}\text{C}_{\text{carb}}$ and $\pm 0.06\text{‰}$ for $\delta^{18}\text{O}_{\text{carb}}$. All isotope measurements were performed at the Stable Isotope Laboratory of the ETH Zurich (Geological Institute). The isotope values are reported in the conventional delta notation with respect to the Vienna Pee Dee Belemnite (VPDB).

The **Total Carbonate content** (TCarb) was calculated based on a calibration using extracted CO_2 from the known weight of the internal standard material (MS2), which is composed to 100% of carbonate (calcite). The mean area of the m/z 44 peak (corresponding to the most abundant isotopologue $^{12}\text{C}^{16}\text{O}_2$) in the mass spectrometer allows the carbonate content to be estimated from the individual bulk rock samples. The individual uncertainty for TCarb, represents the average from all standard deviations from the MS2 and is $\pm 5.73\%$. 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 (~ 60 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 171 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 $\pm 0.25\%$, respectively $\pm 0.07\%$ 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

Kaiseraugst Formation (STA3-1-1212.35)

The sample STA3-1-1212.35 is a bioclastic limestone (dolomitic) about 3 m above the lower boundary of the Muschelkalk Group. The sediment contains macroscopic white minerals with somewhat strange outlines, somehow growth forms. These are clusters of dolomite rhombohedrons, which are joined closely without interspace (Fig. B-1; Appendix B for all figures in this section). Normally the dolomite crystals are irregularly scattered over the whole sediment. The thin section consists of bivalves (13 vol.-%; Tab. 3-1 for all vol.-% data in this section), echinoderms (5 vol.-%), quartz (4 vol.-%), microsparite (35 vol.-%) and dolomite (41 vol.-%).

Zeglingen Formation (STA3-1-1107.37)

Thin section STA3-1-1107.37 represents an oolitic sediment, which lies intercalated between the dolostones of the «Dolomitzone» of the Zeglingen Formation. But it is neither a dolomitic oolite nor a calcareous oolite. It is now a siliceous or silicified oolite: the original calcitic (aragonitic) ooids are replaced by fine crystalline quartz, and quartz cement also fills the original pore space (Fig. B-2). In Tab. 3-1 the mineral facies are listed according to the mineral replacement: 61 vol.-% quartz, 17 vol.-% dolomite, 14 vol.-% anhydrite, 5 vol.-% dolomicritic matrix and 3 vol.-% pyrite. In the entire thin section, the siliceous ooids represent about 64 vol.-% (not shown separately in Tab. 3-1, only mineral replacements).

Schinznach Formation (STA3-1-1095.82, 1047.76, 1039.78)

The bed, where the thin section STA3-1-1095.82 was taken, seems to consist of oncoids or generally round components. But the analysis did not confirm this. It is more or less a fully dolomitised limestone, where most of the original components are no longer identifiable. The sample consists of dolomite rhombohedrons (64 vol.-%), pellets (8 vol.-%), echinoderms (4 vol.-%), micrite matrix (12 vol.-%), anhydrite crystals (5 vol.-%) and porosity (7 vol.-%).

The two thin sections STA3-1-1047.76 and 1039.78 are dolostones of the Stamberg Member. Both contain more or less ooids (44, resp. 24 vol.-%). The dolomitisation of the original calcitic components caused some porosity (6, resp. 10 vol.-%; Fig. B-3). Bivalves (5, resp. 6 vol.-%), pellets (13 vol.-%, 1039.78), anhydrite (12 vol.-%, 1039.78), dolomitic cement (23, resp. 7 vol.-%) and dolomicritic matrix (22, resp. 28 vol.-%) complete the composition.

Bänkerjoch Formation (STA3-1-1018.99, 1008.96, 999.12, 983.72, 964.44, 954.79)

Starting from below, the two lowermost samples of the Bänkerjoch Formation show an extraordinary (STA3-1-1018.99) and then a special facies (STA3-1-1008.96):

STA3-1-1018.99 is a laminated limestone, which is very atypical within the evaporitic Bänkerjoch Formation, which consists normally of anhydrite – claystone – dolomite sediments. The limestone is composed of extraordinary calcite-rosettes (spheres), which formed as pseudomorphs substituting multiple twinned gypsum crystals (Fig. B-4). The calcite pseudomorph with 85 vol.-% is counted in the column of "calcite cement", dolomite (4 vol.-%), quartz (3 vol.-%) and clay matrix (8 vol.-%) form this sediment.

STA3-1-1008.96 is an intraformational conglomerate, which consists of dolomicritic flat intraclasts (46 vol.-%), sedimented with dolomicritic matrix (48 vol.-%) and few quartz sand components (6 vol.-%).

The four other samples (STA3-1-999.12, 983.72, 964.44 and 954.79) are all dolomitic marls, consisting of clay matrix with countless dolomite rhombohedrons together the lithology is therefore called dolomitic marl. They replace original gypsum crystals, therefore they have elongated rhombohedron crystal shapes (Fig. B-5) and often they are twinned ("Schwalbenschwanz-Zwillinge"). STA3-1-964.44 shows additional dolomite nodules, composed of "normal" rhombohedral dolomite crystals (Fig. B-6). Three samples also contain anhydrite, resulting in the following composition: 32-68 vol.-% dolomite, 12-45 vol.-% anhydrite and 20-28 vol.-% clay matrix. STA3-1-954.79 consists of 43 vol.-% dolomite and 57 vol.-% clay matrix.

Klettgau Formation (STA3-1-950.65, 946.88, 944.45, 938.02, 936.42, 935.27)

The Klettgau Formation is a sedimentary succession with a very variable lithology, so that we analysed two sandstones of the Ergolz Member (STA3-1-950.65 and 946.88), one dolomite of the Gansingen Member (STA3-1-944.45) and three sandy, dolomitic sediments of the Seebi Member (STA3-1-938.02, 936.42 and 935.27).

Thin section STA3-1-950.65 is a fine-layered, fine-grained, argillaceous sandstone, consisting of 62 vol.-% quartz and siliceous rock fragments (for example clay schists), further 7 vol.-% micas, 8 vol.-% anhydrite cement and 23 vol.-% clay matrix, which lies mainly in argillaceous, sandy interlayers.

The sample STA3-1-946.88 is a red sandy claystone with numerous fine-grained sandstone lenses and therefore the lithology is called an argillaceous sandstone. Quartz components and silicate rock fragments have a part of 55 vol.-%, clay matrix in sandstone lenses and claystone layers make 42 vol.-%, as well as few pyrites (3 vol.-%).

STA3-1-944.45 of the Gansingen Member has neither components nor a lamination as expected: it is just a homogeneous dolomicritic (95 vol.-%) sediment with a bit anhydrite (5 vol.-%) in veins.

The lowermost sample of the Seebi Member, STA3-1-938.02, is a sandy dolostone with 22 vol.-% quartz and quartzite components, which are poorly sorted, of very different size between 0.05 and 2.5 mm, as well as few dolomitic intraclasts (2 vol.-%). The sand grains are embedded in a dolomicritic matrix (71 vol.-%) and calcite cement (5 vol.-%).

The two thin sections STA3-1-936.42 and 935.27 are dolomicritic sediments (96, resp. 87 vol.-%) with few quartz components (4, resp. 6 vol.-%). They show a more or less distinct nodular fabric of pedogene origin with few fenestrate little veins, which are more distinct with anhydrite (4 vol.-%) and calcite-fills (3 vol.-%) in STA3-1-935.27.

Staffelegg Formation (STA3-1-915.83, 914.77)

Both samples (STA3-1-915.83 and 914.77) of the Beggingen Member are iron-oolitic, bioclastic limestones, whereby the iron-oolids or the bioclasts are the dominant components.

STA3-1-915.83 looks like an iron ore: the iron-oolite (calcareous) consists of dark red-brown iron-oolids (42 vol.-%), up to 0.7 mm in diameter, and limonitic bioclasts (16 vol.-%), embedded in a very limonitic micrite matrix (38 vol.-%) or nearly limonite matrix, as well as calcite cement

(4 vol.-%). Probably the part of iron-oids is higher than the denoted value, but they are hard to recognise within the limonitic matrix.

Thin section STA3-1-914.77 contains clearly less iron-minerals: it is a bioclastic limestone (iron-oolitic) with 17 vol.-% iron-oids, 23 vol.-% bivalves, 5 vol.-% echinoderms, 4 vol.-% limonitic bioclasts, 37 vol.-% micrite matrix and 11 vol.-% limonitic matrix.

Opalinus Clay (STA3-1-872.92, 848.30, 803.85, 799.36, 794.95, 786.32)

In the Opalinus Clay, the focus of the thin section analyses was mainly on the different calcareous horizons, which interrupt as "hiatus beds" or firm- to hardgrounds the normal Opalinus Clay succession of silty claystones and claystones. Microfacies of the Opalinus Clay subunits have been described in other reports, as for example BOZ1-1 (Section 3.1 in Wohlwend et al. 2022).

STA3-1-872.92 comes from a calcite rich layer about 15 m above the lower Opalinus Clay boundary. The thin section documents a 1.5 cm thick "cone-in-cone" calcite horizon (50 vol.-%), thin-shelled bivalves (6 vol.-%), clay matrix (40 vol.-%) and pyrite (4 vol.-%) form this calcareous marl.

STA3-1-848.30 and 803.85 are two nodular, calcareous, sideritic beds: The lower is a pyrite-rich horizon with, up to 2 cm nodules of clear calcites, which are similar to "stellate calcite". The nodules are a product of diagenesis, the bed is a "hiatus bed". STA3-1-848.30 consists of calcareous nodules (11 vol.-%), pyrite (11 vol.-%), often as rim of the nodules (Fig. B-7), quartz fine-sand (15 vol.-%), bioclasts (echinoderms and bivalves, 11 vol.-%) and clay matrix (35 vol.-%) with stellate calcite (12 vol.-%).

STA3-1-803.85 shows a similar composition and origin, but with much more bioclasts and less pyrite. The sampled bed covers the lower part of the «Sub-unit with silty calcareous beds» where the beds still partly contain calcareous sandstone lenses. It consists of echinoderm skeletal elements (26 vol.-%), bivalves (8 vol.-%), nodules and intraclasts (18 vol.-%, Fig. B-8), quartz silt (12 vol.-%), pyrite (3 vol.-%) and a sideritic clay matrix (30 vol.-%).

The three samples STA3-1-799.36, 794.95 and 786.32 have been taken from the calcareous firm to hardgrounds of the uppermost 20 m of the Opalinus Clay. They have all at least some iron-oids and/or calcitic iron-oids. The here mentioned calcitic iron-oids (also applies for the following thin section descriptions) have been noted in the "Fe-oids" column in Tab. 3-1 with an asterisk behind the number. The individual calcareous beds of STA3-1-799.36 and 794.95 are embedded in a silty, sandy claystone (partly calcareous). STA3-1-786.32, however, covers a succession of few silty to sandy, bioclastic limestone beds.

Thin-section STA3-1-799.36 shows a multi-layered bed with a limestone (iron-oolitic) horizon, then a bioclastic marl and a marl with iron-stromatolitic flasers. Overall, the analyses document the following composition: calcitic iron-oids (11 vol.-%), intraclasts (7 vol.-%), iron-stromatolitic components (4 vol.-%), biogenes (12 vol.-%), quartz silt (5 vol.-%), pyrite (4 vol.-%) and micrite- and clay matrix (57 vol.-%, Fig. B-9).

STA3-1-794.95 is a bioclastic limestone, in some parts of the thin section also partly argillaceous with spheroidal calcitic components. Because some of these have original chamositic iron-oid cores (Fig. B-10), they have been interpreted all as iron-oids or calcitic iron-oids. Therefore, STA3-1-794.95 consists of iron-oids (11 vol.-%), nodules and intraclasts (6 vol.-%), echinoderms (24 vol.-%), bivalves (7 vol.-%), other biogenes (3 vol.-%), quartz silt (6 vol.-%)

and a matrix of micrite and clay (18 vol.-%) with siderite (11 vol.-%), "stellate calcite" (10 vol.-%) and pyrite (4 vol.-%).

STA3-1-786.32 has the highest content of iron-oids from all thin sections analysed from the calcareous beds of the Opalinus Clay: 23 vol.-% iron-oids, whereof most of them are of calcite replacing iron-minerals, but still with an iron-mineral core or mixed with limonite or with pyrite (Fig. B-11). The other components are nodules and intraclasts (7 vol.-%), echinoderms (16 vol.-%), bivalves (11 vol.-%), other biogenes (9 vol.-%, e.g. serpulids and corals), quartz sand (8 vol.-%) and pyrite (5 vol.-%). They are sedimented with micrite matrix (21 vol.-%).

«Murchisonae-Oolith Formation» (STA3-1-778.66, 777.83, 777.00, 767.76, 767.44, 765.94)

All analysed thin sections from the «Murchisonae-Oolith Formation» contain limonitic components. During the drill core description, it was not always clear if they are iron-oids or limonitic bioclasts?

All thin section have iron-oids, with the exception of STA3-1-767.44, but the most dominant components in all thin sections are echinoderm skeletal elements (14 – 38 vol.-%) and/or limonitic bioclasts (12 – 23 vol.-%). The iron-oids measure 0.1 – 0.5 mm, and are, contrary to the Opalinus Clay, still of iron-mineral composition.

STA3-1-778.66 consists of three different intervals: a sandy, bioclastic marl layer at the bottom (ca. 35 vol.-% quartz sand), then a thin limonitic crust, and at the top a bioclastic limestone (iron-oolitic). The latter has 13 vol.-% iron-oids, 3 vol.-% intraclasts, 5 vol.-% limonitic pellets (in Tab. 3-1 counted as "limonite, Fe-mineralised nodules"), 31 vol.-% echinoderms, 5 vol.-% bivalves, 3 vol.-% other biogenes, then 6 vol.-% quartz sand, 5 vol.-% micrite, 15 vol.-% sparite cement, 10 vol.-% "stellate calcite" and 4 vol.-% iron dolomite rhombohedrons.

The sample STA3-1-777.83, a bioclastic limestone (iron-oolitic), of red-brown colour, is distinctly more limonitic: iron-oids (24 vol.-%), limonitic bioclasts (23 vol.-%), limonitic pellets (4 vol.-%, counted as "limonite, Fe-mineralised nodules" in Tab. 3-1) and limonitic matrix (15 vol.-%) make the main part of the sediment. Quartz sand (12 vol.-%), bivalves (4 vol.-%), other biogenes (2 vol.-%), calcite cement (8 vol.-%) and iron dolomite rhombohedrons (8 vol.-%) complete the composition.

STA3-1-777.00 looks similar to STA3-1-777.83, but is very heterogenous: lenses and layers, which are rich in limonite, alternate with such without limonitic components. The thin section documents a notable limonitic sponge component (Fig. B-12), a component which has never been seen before. Altogether echinoderms (14 vol.-%), limonitic bioclasts (13 vol.-%), bivalves and others (6 vol.-%), iron-oids (14 vol.-%), intraclasts (5 vol.-%), limonitic pellets (4 vol.-%) and quartz sand (8 vol.-%) with micrite matrix (10 vol.-%) and iron dolomitic rhombohedrons (16 vol.-%) build this bioclastic limestone (iron-oolitic).

The two thin section STA3-1-767.76 and 767.44, taken from the uppermost succession of the «Murchisonae-Oolith Formation», are once a bioclastic limestone (sandy) and second a bioclastic limestone, both with echinoderm skeletal elements as the dominant components. They consist of echinoderms (22, resp. 38 vol.-%), limonitic bioclasts (16, resp. 12 vol.-%), bivalves (10, resp. 14 vol.-%), others biogenes (4, resp. 2 vol.-%) and quartz sand (16, resp. 8 vol.-%). STA3-1-767.76 contains few iron-oids (5 vol.-%) and iron-oolitic intraclasts (4 vol.-%, Fig. B-13), as well as few pellets (4 vol.-%). This sample is a micritic (10 vol.-%) limestone with some limonitic patches. STA3-1-767.44 on the other hand is a sparitic cemented (26 vol.-%) limestone.

STA3-1-765.94 is a bioclastic, calcareous marl with iron-oooids (10 vol.-%), limonitic bioclasts (12 vol.-%) and limonitic matrix (8 vol.-%). Further components are non-limonitic echinoderms (16 vol.-%), bivalves (4 vol.-%), other biogenes (2 vol.-%), quartz silt (12 vol.-%). Clay matrix (14 vol.-%), calcite cement (13 vol.-%), "stellate calcite" (5 vol.-%) and pyrite (4 vol.-%) encompass the components.

Wedelsandstein Formation (STA3-1-764.86, 762.44, 760.80, 742.02)

The four samples STA3-1-764.86, 762.44, 760.80 and 742.02 are representatives of the calcareous beds, which are intercalated in the silty, sandy marl and silty, sandy claystone succession of the Wedelsandstein Formation. They all contain quartz sand (15 – 35 vol.-%), echinoderm skeletal elements (22 – 25, resp. 8 vol.-%) and bivalves (5 – 7, resp. 17 vol.-%).

STA3-1-764.86, a bioclastic limestone (sandy, iron-oolitic) taken near the base of the Wedelsandstein Formation, contains moreover greenish, chamositic iron-stromatolitic flasers (3 vol.-%) and iron-oooids (11 vol.-%), which are deformed due to compaction (Fig. B-14).

STA3-1-764.86 and 762.44 as well as 760.80 have a micritic, partly argillaceous matrix (18 – 25 vol.-%), mixed with little siderite crystals (10 – 12 vol.-%) and pyrite (2 – 4 vol.-%). All three thin sections contain calcitic biogenes (echinoderms and bivalves) (28 – 30 vol.-%). Thin section STA3-1-760.80 shows additional intraclasts and nodules (13 vol.-%), what supports the aspect of a "hiatus bed".

STA3-1-742.02 has a microsparitic, partly micritic matrix (32 vol.-%), which could also be mixed with siderite, but also sparite cement (7 vol.-%) in the shelter of big bivalves. Few of the last ones contains quartz cement (2 vol.-%).

«Herrenwis Unit» (STA3-1-741.84, 737.04, 729.39, 723.46, 719.48, 701.67)

The lowermost sample from the «Herrenwis Unit» (STA3-1-741.84), was taken to have an impression about the matrix surrounding the coral branches. It is a microsparitic, coral bearing limestone. Originally a micrite matrix (31 vol.-%), with some quartz silt (7 vol.-%) and pyrite (5 vol.-%). The corals (52 vol.-%) consist of calcite, replacing the original aragonite, and of calcite cement. The thin section also contains a gastropod (5 vol.-%).

The two thin sections, STA3-1-737.04 and 729.39 are both bioclastic limestones, composed of numberless fossil debris. In the lower sample coral bioclasts dominate and bivalves in the upper one. STA3-1-737.04 looks coarser crystalline than STA3-1-729.39, due to the coral fragments and coarser calcite crystals. The composition is: corals (33 vol.-%), bivalves (16 vol.-%), echinoderms (13 vol.-%), microsparitic matrix (17 vol.-%), calcite cement (17 vol.-%) and quartz cement (4 vol.-%) within bivalve shells. STA3-1-729.39 consists of bivalves (32 vol.-%), echinoderms (10 vol.-%), corals (3 vol.-%), other biogenes (3 vol.-%), intraclasts (3 vol.-%), microsparitic matrix (25 vol.-%) and calcite cement (24 vol.-%).

STA3-1-723.46 is a bioclastic limestone too, but a rather porous one. The thin section documents in some parts how cementation started at the rims of primary pore space and partly leached biogenes (Fig. B-15) and in another part in leached corals, that are only partially cemented (Fig. B-16). The sample consists of corals (20 vol.-%), echinoderms (15 vol.-%), bivalves (10 vol.-%), other biogenes (5 vol.-%), calcite cement (30 vol.-%), micrite matrix (5 vol.-%), as well as inter- and intragranular porosity (15 vol.-%).

The sample STA3-1-719.48 is a bioclastic limestone too and contains some micritic intraclasts (11 vol.-%) and a lot of different fossil clasts: echinoderms (18 vol.-%), corals (12 vol.-%), bivalves (5 vol.-%), serpulids (2 vol.-%) and others (12 vol.-%) with microsparite and micrite matrix (22 vol.-%), as well as calcite cement (18 vol.-%) (Fig. B-17).

The top of the «Herrenwis Unit» and the hanging basal layer were analysed by thin section STA3-1-701.67. The coral reef, or at least a part, is covered by a limonitic hardground (Fig. B-18), partly a stromatolitic crust. This itself is overlain by a limonitic, bioclastic layer (Fig. B-19). Overall, the thin section consists of corals (13 vol.-%), an iron-stromatolitic crust (8 vol.-%), echinoderms (14 vol.-%), bivalves (4 vol.-%), other biogenes (5 vol.-%), limonitic matrix (23 vol.-%), calcite cement (13 vol.-%), "stellate calcite" (8 vol.-%) and iron-dolomite rhombohedrons (12 vol.-%).

«Parkinsoni-Württembergica-Schichten» (STA3-1-701.59)

The only analysed sample from the «Parkinsoni-Württembergica-Schichten» (STA3-1-701.59) was taken from an 8 cm thick iron-oolite in the lower part of the succession. Iron-ooids (32 vol.-%), up to 2 mm big, with limonitic cores and wide calcite rims (Fig. B-20) are the main components. Quartz silt (8 vol.-%), echinoderms (7 vol.-%), bivalves (2 vol.-%) and pyrite (3 vol.-%), together with micrite matrix (48 vol.-%) complete the sediment.

Wutach Formation (STA3-1-696.10, 696.05)

Both thin sections (STA3-1-696.10 and 696.05) come from the uppermost horizons of the Wutach Formation, whose top is at 696.03 m. Both are iron-oolites: STA3-1-696.10 has limonitic, chamositic iron-ooids (46 vol.-%) with calcite rims, or few of them are replaced by calcite (Fig. B-21). But in STA3-1-696.05, only 5 cm above, almost all iron-ooids (42 vol.-%) are replaced completely by calcite. Only an outer rim of chamosite is still visible.

The thin section STA3-1-696.05 was also prepared to answer another question. The question refers to the correct definition of the lower limit of the Birmenstorf Member, which was normally defined with the onset of the glauconite. The answer is yes, although few glauconite grains (3 vol.-%) are present, but they are in a vug, filled by marl, coming from the hanging.

The iron-ooids are accompanied by some bivalves (8, resp. 7 vol.-%), echinoderms (4, resp. 5 vol.-%), other biogenes (3 vol.-%), quartz sand (5 vol.-%), pyrite (2, resp. 4 vol.-%) and limonitic micrite matrix (32, resp. 34 vol.-%).

Wildegge Formation (STA3-1-696.00, 652.83)

This lowermost horizon of the Wildegge Formation delivered sample STA3-1-696.00, which contains a belemnite horizon, a silty horizon, a horizon with glauconite and a big, bored, limonitic intraclast. The analyses document the following composition of a silty marl (bioclastic): belemnites (24 vol.-%), bivalves (3 vol.-%), intraclasts (15 vol.-%), quartz silt (13 vol.-%), glauconite (6 vol.-%), limonitic nodules (3 vol.-%), pyrite (2 vol.-%), mica (2 vol.-%) and clay matrix (32 vol.-%).

STA3-1-652.83, a bed of a biomicritic limestone succession, consists of small crinoids (13 vol.-%), bivalves (3 vol.-%), other biogenes (3 vol.-%), quartz silt (3 vol.-%), small pyritic nodules and pyritised little fossils (9 vol.-%), glauconite (2 vol.-%) and micrite matrix (67 vol.-%).

Schwarzbach Formation (STA3-1-532.80)

Sample STA3-1-532.80 was taken out of a nodular limestone, which contains several little blackish nodules. The thin section shows a biogene-rich limestone, consisting of sponge nodules (17 vol.-%), oncoids (18 vol.-%), pellets (13 vol.-%), thin-shelled bivalves (14 vol.-%), echinoderms (6 vol.-%), glauconite (5 vol.-%), sedimented with micrite matrix (23 vol.-%).

«Felsenkalke» and «Massenkalk» (STA3-1-520.56)

The bed or succession, where the thin section STA3-1-520.56 was taken from, looks in a macroscopic view more as a greenish calcareous marl than a limestone. The succession may be addressed as the informal «Glaukonitbank». However, the thin section shows a dedolomite (80 vol.-%) with pyrite (5 vol.-%), glauconite (3 vol.-%), few biogenes (3 vol.-%), a vein with calcite cement (3 vol.-%) and some porosity (6 vol.-%).

Tab. 3-1: Microfacies analysis from STA3-1 (1'212.35 – 520.56 m); numbers in vol.-%

Microfacies analysis STA3-1 (1'212.35 - 520.56 m)	clay matrix, micrite, microsparite	dolomitic matrix	limonitic matrix	components (and biohermal organisms)										cements, diagenesis														
				calclitic biogenes						allochems				cements, diagenesis														
				echinoderms	bivalves	limonitic echinod. + bivalves	serpulids	corals	sponges, spicules	other biogenes	Fe-stromatolitic clasts	aggregates, pellets, peloids	oncoids	Fe-ooids	intraclasts, nodules	detrital quartz + silic. rock fragm.	quartz grainsize (mm)	calcite cement	"stellate cement" (s) cone-in-cone calcite (c)	(Fe)-dolomite	dedolomite	anhydrite, gypsum	pyrite	limonite, Fe-min. nodules	siderite	glauconite	mica	porosity
520.56m: dedolomite «Felsenkalkes» + «Massenkalk»										3							3											6
532.80m: biomicrite Schwarzbühl Fm.	23			6	14					17	4	13	18													5		
652.83m: biomicrite Wildegg Fm. (Efringen Mb.)	67			13	3																					2		
696.00m: silty marl (bioclastic) Wildegg Fm. (Birmensdorf Mb. + Gählenkirchensandsteine Bed.)	32				3						24															6	2	
696.05m: iron-oolite (calcareous) Wildegg Fm.			34	5	7						3															4		
696.10m: iron-oolite (calcareous) Wildegg Fm.			32	4	8						3															2		
701.59m: iron-oolite (calcareous) «Parkinson-Württemberg-Schichten»	48			7	2																							
701.67m: hardground «Herrenwies Units»			23	14	4			13			5	8																
719.48m: bioclastic limestone «Herrenwies Units»	22			18	5	2	12				12																	
723.46m: bioclastic limestone «Herrenwies Units»	5			15	10			20			5																	15
729.39m: bioclastic limestone «Herrenwies Units»	25			10	32			3			3																	
737.04m: bioclastic limestone «Herrenwies Units»	17			13	16			33																				
741.84m: coral-limestone «Herrenwies Units»	31							52			5																	
742.02m: bioclastic limestone (sandy) Wedelsandstein Fm.	32			8	17						5	6																
760.80m: bioclastic calc. marl (sandy) Wedelsandstein Fm.	25			23	5	2					4																	
762.44m: bioclastic limestone (sandy) Wedelsandstein Fm.	18			25	5						3																	
764.86m: biocl. limest. (sandy, Fe-ool.) Wedelsandstein Fm.	18			22	7						3	3																
765.94m: biocl., calc. marl (iron-oolitic) «Murchisonae-Oolith Fm.»	14		8	16	4	12					2																	
767.44m: bioclastic limestone «Murchisonae-Oolith Fm.»				38	14	12					2																	
767.76m: bioclastic limestone (sandy) «Murchisonae-Oolith Fm.»	10		5	22	10	16					4																	
777.00m: biocl. limestone (iron-oolitic) «Murchisonae-Oolith Fm.»	10		10	14	4	13					2																	
777.83m: biocl. limestone (iron-oolitic) «Murchisonae-Oolith Fm.»			15		4	23					2																	
778.66m: biocl. limestone (iron-oolitic) «Murchisonae-Oolith Fm.»	5			31	5						3																	
786.32m: biocl. limestone (iron-oolitic) Opalinus Clay	21			16	11		3	3			3																	
794.95m: biocl. limestone (argilla.) Opalinus Clay	18			24	7						3																	
799.36m: limestone (iron-oolitic) Opalinus Clay	57			8	3						1	4																
803.85m: biocl. limestone with nodules Opalinus Clay	30			26	8						3																	
848.30m: biocl. marl (sandy) + nodules Opalinus Clay	35			8	3						5																	
872.92m: calcareous marl Opalinus Clay	40				6																							
914.77m: biocl. limestone (iron-oolitic) Starfegg Fm. (Begrüben Mb.)	37		11	5	23	4					3																	
915.83m: iron-oolite (calcareous) Starfegg Fm. (Begrüben Mb.)			38			16																						
935.27m: dolomicrite Klettgau Fm. (Seebi Mb.)		87																										
936.42m: dolomicrite Klettgau Fm. (Seebi Mb.)		96																										
938.02m: sandy dolostone Klettgau Fm. (Seebi Mb.)		71																										
944.45m: dolomicrite Klettgau Fm. (Gansingen Mb.)		95																										
946.88m: argillaceous sandstone Klettgau Fm. (Ergolz Mb.)	42																											
950.65m: argillaceous sandstone Klettgau Fm. (Ergolz Mb.)	23																											
954.79m: dolomitic marl Bänkerpösch Fm.	57																											
964.44m: dolo. marl + dolo. & anh. nod. Bänkerpösch Fm.	20																											
983.72m: dolomitic marl (anhydritic) Bänkerpösch Fm.	28																											
999.12m: dolomitic marl and anhydrite Bänkerpösch Fm.	23																											
1'008.96m: flat pebble conglomerate Bänkerpösch Fm.		48																										
1'018.99m: limestone, laminated Bänkerpösch Fm.	8																											
1'039.78m: dolostone (originally oomicrite) Schinzräch Fm. (Sarnberg Mb.)		28			6																							
1'047.76m: dolostone (originally oomicrite) Schinzräch Fm. (Sarnberg Mb.)		22																										
1'095.82m: dolostone, calcareous Schinzräch Fm. (Leutschenberg Mb. + Kienberg Mb.)	12			4																								
1'107.37m: silicified oolite Zeglingen Fm. («Dolomitezone»)		5																										
1'212.35m: bioclastic limestone (dolom.) Kaiseraugst Fm. («Weledolomite»)	35			5	13																							

3.2 Ammonite stratigraphy

From STA3-1 seventeen ammonite specimens were recovered, only two of them (depth 779.24 m and 777.72 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 borehole. They are relatively common in the Toarcian and Early Aalenian, where ammonite fragments and cross sections are locally common in the range between 889.12 m and 871.14 m (see Appendices A2 and A3). In the Late Aalenian, ammonites are rare. In the Bajocian, no ammonites were found. From the Bathonian and Callovian, three ammonites were found but all were so badly cut that an exact determination is not possible. Somewhat more frequent are the ammonites again in the Middle Oxfordian. Due to the generally small sample size and the poor, often incomplete preservation of the ammonites, a more-or-less large uncertainty in the age determinations must be expected, and this can have an effect on the biostratigraphic classification.

The names of several ammonite taxa are followed by a question mark, for example in *Leioceras?* 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.

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

In general, the more ammonites are present in a specific profile section, the more precisely the biostratigraphic classification of that section can be determined (Tab. 3-2). 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 the biostratigraphic determination. 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

- 914.00 m: Arietitidae indet. The truncated ammonite is a partially mineralised steinkern (geopetal fabric). Age: Early Sinemurian. Lithology: hard, grey bioclastic limestone. This ammonite is not illustrated.
- 892.74 m: *Hildoceras* sp. Truncated phosphoritic steinkern with flattened pyritised inner coils. Age: Variabilis Zone. Lithology: hard, dark-grey limestone with pyrite. The ammonite fragment is illustrated on Plate I, Fig. 1 (Appendix C, for all figures in this chapter).
- 889.12 m: *Cotteswoldia* sp. Three specimens: Two flattened steinkerne and a 3D-preserved fragment of a body chamber. Age: Aalensis Zone, probably Aalensis Subzone. Lithology: Grey calcareous marl with some bioclasts. The ammonites are illustrated on Plate I, Fig. 2.

888.36 m: *Cotteswoldia* ex gr. *lotharingica* (Branco, 1879) or *C. pseudolotharingica* (Maubeuge, 1950). Flattened steinkern. Age: Aalensis Zone, Torulosum Subzone. Lithology: grey bioclastic marl. The bioclasts consist mainly of echinoderm skeletal elements. Other fossils are ammonite fragments. The ammonite is illustrated on Plate I, Fig. 3.

888.02 m: *Pleydellia* ex gr. *buckmani* (Maubeuge, 1947). Age: Aalensis Zone, Torulosum Subzone. Lithology: grey bioclastic marl. The bioclasts consist mainly of echinoderm skeletal elements. The ammonite is illustrated on Plate I, Fig. 4.

Opalinus Clay

874.91 m: *Leioceras* ex gr. *opalinum* (Reinecke, 1818). Phragmocone in 3D-preservation with flattened body chamber. Age: Opalinum Zone, Opalinum Subzone. Lithology: dark-grey, somewhat silty claystone. Further fossils are ammonite fragments. The ammonite is illustrated on Plate II, Fig. 1.

871.56 m: *Leioceras* ex gr. *opalinum* (Reinecke, 1818). Flattened specimen with calcite shell preservation. Age: Opalinum Zone, Opalinum Subzone. Lithology: dark-grey, mica-bearing claystone. The ammonite is illustrated on Plate II, Fig. 2.

«Murchisonae-Oolith Fm.»

779.24 m: *Leioceras*? sp. Age: Early Aalenian. Lithology: hard, dark-grey bioclastic (echinoderm) limestone with intraclasts. The ammonite is not illustrated.

778.54 m: *Staufenia*? sp. Age: Murchisonae Zone? Lithology: brown, bioclastic (echinoderm and others) limestone with limonitised components. The ammonite is illustrated on Plate II, Fig. 3.

777.72 m: Graphoceratidae indet. Age: Aalenian. Lithology: hard, red-brown, iron-ooide-bearing limestone. The iron-ooide measure up to ca. 0.2 mm in diameter. Other fossils: shell fragments. The ammonite is not illustrated.

776.94 m: *Staufenia* ex gr. *staufensis* (Oppel, 1856). Age: Bradfordensis Zone, Bradfordensis Subzone. Lithology: dark, brown-black limestone (argillaceous) with very small (mostly < 1 mm) limonitised components. Other fossils are a belemnite and a bivalve of the species *Eopecten*. In addition, some shell fragments. The ammonite is illustrated on Plate II, Figs. 4a and 4b.

«Parkinsoni-Württembergica-Schichten»

701.64 m: Pseudoperisphinctidae indet. Truncated ammonite with flattened steinkern. Age: Bathonian? Lithology: grey, limestone (argillaceous) with large limonitic-goethitic iron-ooide (diameters up to ca. 2 mm). Other fossils: shell fragments. The ammonite is not illustrated.

Wutach Formation

- 698.34 m: *Oecotraustes* sp. Truncated specimen with shell preservation. Age: Bathonian. Lithology: red, iron-oolitic limestone (argillaceous). The iron-oolids are limonitic/goethitic (diameters up to ca. 1.6 mm). Other fossils are a single coral and a shell fragment. The ammonite is illustrated on Plate III, Figs. 1a and 1b.
- 696.36 m: Pseudoperisphinctidae indet. Truncated ammonite. Age: Bathonian or Callovian. Lithology: red, iron-oolitic limestone (argillaceous). The iron-oolids are limonitic/goethitic (diameters up to ca 1 mm). Other fossils comprise a belemnite, bivalves, a gastropod, and a terebratulid brachiopod. The ammonite is not illustrated.
- 696.29 m: *Macrocephalites* sp. Truncated specimen with shell preservation. Age: Late Bathonian to Early Middle Callovian, probably Early Callovian. Lithology: somewhat argillaceous, rust-red to grey iron-oolitic limestone. The iron-oolids measure up to max. 1 mm in diameter. Other fossils: shell fragments. The ammonite is illustrated on Plate III, Figs. 2a and 2b.

Wildegge Formation

- 694.82 m: *Perisphinctes* sp. Microconch in flattened steinkern preservation. Age: Transversarium Zone to Early Bifurcatus Zone. Lithology: grey, bioturbated limestone (argillaceous) with some bioclasts (echinoderms). The ammonite is illustrated on Plate III, Fig. 3.
- 693.49 m: *Taramelliceras* ex gr. *dentostriatum* (Quenstedt, 1887). Flattened steinkern. Age: Transversarium Zone, Luciaeformis Subzone. Lithology: grey, mica-bearing, bioturbated calcareous marl. The ammonite is illustrated on Plate III, Fig. 4.

Tab. 3-2: Ammonite and other macrofossil determination from STA3-1

Depth [m MD]	Identification	Ammonite Zone (Subzone) or Age
693.49	<i>Taramelliceras</i> ex gr. <i>dentostriatum</i> (Quenstedt, 1887)	Transversarium Z (Luciaeformis SZ)
694.82	<i>Perisphinctes</i> sp.	Transversarium Z to Early Bifurcatus Z
696.29	<i>Macrocephalites</i> sp.	Early Callovian?
696.36	Pseudoperisphinctidae indet.	Bathonian or Callovian
698.34	<i>Oecotraustes</i> sp.	Bathonian
701.64	Pseudoperisphinctidae indet.	Bathonian?
776.94	<i>Staufenia</i> ex gr. <i>staufensis</i> (Oppel, 1856)	Bradfordensis Z (Bradfordensis SZ)
777.72	Graphoceratidae indet.	Aalenian
778.54	<i>Staufenia</i> ? sp.	Murchisonae Zone?
779.24	<i>Leioceras</i> ? sp.	Early Aalenian
871.56	<i>Leioceras</i> ex gr. <i>opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum Subzone)
874.91	<i>Leioceras</i> ex gr. <i>opalinum</i> (Reinecke, 1818)	Opalinum Zone (Opalinum Subzone)
888.02	<i>Pleydellia</i> ex gr. <i>buckmani</i> (Maubeuge, 1947)	Aalensis Zone (Torulosum Subzone)
888.36	<i>Cotteswoldia</i> ex gr. <i>lotharingica</i> (Branco, 1879) or <i>C. pseudolotharingica</i> (Maubeuge, 1950)	Aalensis Zone (Torulosum Subzone)
889.12	<i>Cotteswoldia</i> sp.	Aalensis Zone (probably Aalensis Subzone)
892.74	<i>Hildoceras</i> sp.	Variabilis Zone
914.00	Arietitidae indet.	Early Sinemurian

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

STA2-1

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 STA3-1

STA2-1

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

3.3 Palynostratigraphy

The 40 studied samples yielded mostly a good palynological residue with rich and diverse palynofloras. Preservation is good. The palynomorph assemblages are composed of mainly dinoflagellate cysts and pollen and spores. Minor components are prasinophytes, acritarchs, foraminiferal test linings and green algae (e.g. *Botryococcus*). A total of 174 dinoflagellate cyst taxa, 20 other aquatic palynomorphs and 46 pollen and spore taxa are recorded.

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

The studied samples from STA3-1 cores are dated to span the interval from the latest Toarcian to the Oxfordian. 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 888.38 m (1 sample): Late Toarcian, Aalensis Zone to Early Aalenian, Opalinum Zone, Opalinum Subzone

The palynoflora in this sample is characterised by the very high abundance of one dinoflagellate cyst species, *Evansia*? cf. *granochagrinata*. The species dominates the palynoflora, reaching 83% of all palynomorphs counted. Other dinoflagellate cysts present, though in low numbers, are a few representatives of the families Phallocystaceae (*Andreedinium* sp. 2) and Valvaeodiniaceae (*Valvaeodinium brevipellitum*, *V. cavum*, *V. sphaerechinatum*) as well as *Hystrichodinium*? sp. in Feist-Burkhardt & Pross (2010), *Kallosphaeridium praussii*, *Mancodinium semitabulatum*, *Nannoceratopsis* spp., *N. gracilis* s.s. and s.l., *Scrinocassis limbicavatus*, *S. priscus* and *S. weberi*.

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

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

Sample interval 880.18 – 796.27 m (5 samples): Early Aalenian, Opalinum Zone, Opalinum Subzone

Dinoflagellate cyst assemblages of this sample interval are rich and diverse. They are composed of common to abundant *Evansia*? cf. *granochagrinata*, diverse Phallocystaceae (*Andreedinium* aff. *elongatum*, *Andreedinium* sp. 2, *Dodekovia* spp., *D. bullula*, *D. pseudochytrooides*, *Parvocysta bjaerkei*, *Phallocysta*? *frommernensis*, *Reutlingia cardobarbata*, *R. nasuta*,

Susadinium scrofoides) and Valvaeodiniaceae (*Comparodinium aquilonium*, *Valvaeodinium* spp., *V. brevepellitum*, *V. cavum*, *V. sphaerechinatum*, *V. spongiosum*, *V. vermipellitum*), species of *Nannoceratopsis* (*Nannoceratopsis* spp., *N. dictyambonis*, *Nannoceratopsis gracilis* s.s. and s.l., *N. triangulata*) and *Scriniocassis* (*S. limbicavatus*, *S. priscus*, *S. weberi*) as well as *Bradleyella* spp., *Hystrichodinium*? sp. in Feist-Burkhardt & Pross (2010), *Kallosphaeridium praussii*, *Mancodinium semitabulatum* and *Wallodinium laganum*. The species *Evansia*? cf. *grano-chagrinata* is still superabundant in the sample at the base of the interval but its abundance decreases up section. *Phallocysta*? *frommernensis* is fairly common throughout and shows an acme up to the top of the interval. Last occurrences at the top of the interval are those of *Nannoceratopsis triangulata* and *Phallocysta*? *frommernensis*.

The interval is defined as from the first to the last occurrence of *Phallocysta*? *frommernensis*.

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

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

Sample 787.31 m (1 sample): Early Aalenian, Opalinum Zone, Opalinum to possibly Bifidatum Subzone

The assemblage in this sample is reduced in diversity of the phallocystacean dinoflagellate cysts. The sample is characterised by the first common occurrences of several subspecies of *Nannoceratopsis plegas* (*N. plegas brevicornis*, *N. plegas plegas*) and *Nannoceratopsis* sp. 1. Last occurrences in this sample are unquestionable *Scriniocassis weberi* and *Wallodinium laganum*.

The interval is defined from the first common and diverse occurrences of subspecies of *Nannoceratopsis plegas* and the last occurrence of *Wallodinium laganum* on the one hand to the first and common occurrence of *Batiacasphaera* sp. A in the interval above.

The common occurrence of subspecies of *Nannoceratopsis plegas* and the increase in diversity of *Nannoceratopsis* species in general has been observed to be typical from the upper part of the Opalinum Zone onwards. The LADs (Last Appearance Datums) of *Scriniocassis weberi* and *Wallodinium laganum* are considered to be at the top of the Opalinum Zone. The FAD of the genus *Batiacasphaera* is in the upper part of the Opalinum Zone.

The interval is interpreted Opalinum Zone, Opalinum to possibly Bifidatum Subzone.

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

Sample 786.21 m (1 sample): Early Aalenian, Opalinum Zone, Bifidatum Subzone

The assemblage in this sample is characterised by the first and common occurrence of the genus *Batiacasphaera*, with *Batiacasphaera* spp., *Batiacasphaera* sp. A in Feist-Burkhardt & Pross (2010) and *Batiacasphaera* sp. B in Feist-Burkhardt & Pross (2010), the increase in diversity of *Nannoceratopsis*, with *N. plegas dictyornata*, *Nannoceratopsis* sp. B. in Feist (1987) and *N. tricerias*, as well as the first occurrences of *Andreedinium elongatum* and *Kallosphaeridium* spp.

The interval is defined by the first common occurrence of *Batiacasphaera* sp. A to the first occurrence of *Evansia? spongogranulata* in the interval above.

The genus *Batiacasphaera* has its FAD in the upper part of the Opalinum Zone with *Batiacasphaera* sp. A often being abundant in the Bifidatum Subzone of Opalinum Zone. The FAD of *Evansia? spongogranulata* is in the Murchisonae Zone.

The sample is dated Bifidatum Subzone of the Opalinum Zone.

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

Sample 779.24 m (1 sample): Middle Aalenian, Murchisonae Zone

The assemblage in this sample is quite similar to the interval below, but it shows the first occurrence of *Evansia? spongogranulata*. *Evansia? cf. granochagrinata* shows its last common occurrence in this sample. Representatives of the genus *Dissiliodinium* are not yet present but have their first occurrence in the interval above.

The interval is defined by the first occurrences of *Evansia? spongogranulata* to the first occurrence of *Dissiliodinium* spp. in the interval above.

The FAD of *Evansia? spongogranulata* is in the Murchisonae Zone, that of *Dissiliodinium* spp. is within the Bradfordensis Zone.

The sample is dated Murchisonae Zone.

Sample interval 776.94 – 769.79 m (3 samples): Middle Aalenian, Bradfordensis Zone

The assemblages are characterised by the first species of *Dissiliodinium*, *Dissiliodinium* spp. and *D. lichenoides*. Species of *Scriniocassis* (*S. limbicavatus*, *S. priscus*, questionable *S. weberi*) have their last occurrence in this interval. *Nannoceratopsis dictyambonis* is superabundant in sample 774.96 m and *Hystriodinium? sp.* is superabundant in sample 776.94 m. *Andreedinium elongatum* is quite common in the interval.

The interval is defined by the first occurrence of *Dissiliodinium lichenoides* to the first occurrence of *Evansia? Eschachensis* in the interval above. The FADs of *Dissiliodinium* spp. And *D. lichenoides* are within the Bradfordensis Zone. The LAD of *Scriniocassis* spp. Is in the Bradfordensis Zone. The FAD of *Evansia? Eschachensis* is in the Concavum Zone.

The interval is dated Bradfordensis Zone.

Sample 766.62 m (1 sample): Late Aalenian Concavum Zone to ?Early Bajocian Discites Zone

The assemblage in this sample differs from the interval below in that *Dissiliodinium* spp. And *D. lichenoides* are common. At the base of the interval the first occurrence of *Evansia? Eschachensis* is recorded. *Andreedinium elongatum*, which is common, and *Nannoceratopsis* sp. B have their last occurrences.

The interval is defined by the first occurrence of *Evansia? Eschachensis* to the last occurrence of *Nannoceratopsis* sp. B and the first occurrence of *Dissiliodinium* aff. *Giganteum* in the interval above.

The FAD of *Evansia? Eschachensis* is in the Concavum Zone, that of *Dissiliodinium* aff. *Giganteum* is in the Discites Zone. The LAD of *Nannoceratopsis* sp. B is in the Discites Zone.

The interval is interpreted Concavum to questionably Discites Zone.

Sample interval 764.68 – 761.56 m (2 samples): Early Bajocian, Ovale Zone

Assemblages in this interval are characterised by the first occurrences of *Dissiliodinium* aff. *Giganteum*, *D. giganteum*, *Durotrigia* spp., questionable *Gongylodinium erymnoteichon* and *Pareodinia* spp. The last occurrence of *Evansia? Eschachensis* is at the base of the interval.

The interval is defined by the co-occurrence of *Dissiliodinium giganteum* and *Evansia? Eschachensis* to the first occurrences of *Cavatodissiliodinium hansgochtii* and *Batiacasphaera laevigata* in the interval above.

The FAD of *Dissiliodinium giganteum* is in the Ovale Zone. The LAD of *Evansia? Eschachensis* is also in the Ovale Zone. The FADs of *Cavatodissiliodinium hansgochtii* and *Batiacasphaera laevigata* are in the Laeviuscula Zone.

The sample is interpreted Ovale Zone.

Sample interval 760.65 – 742.33 m (3 samples): Early Bajocian, Laeviuscula Zone

Assemblages in this interval show the first occurrences of *Batiacasphaera laevigata*, *Cavatodissiliodinium hansgochtii* and *Durotrigia daveyi* at the base. *Dissiliodinium giganteum* is common to abundant. *Bradleyella adela* is recorded in the topmost sample. *Nannoceratopsis dictyambonis* shows its last occurrence within the interval.

The interval is defined by the first occurrences of *Batiacasphaera laevigata* and *Cavatodissiliodinium hansgochtii* at the base of the interval to the first occurrence of *Kallosphaeridium hypornatum* in the interval above.

The FADs of *Batiacasphaera laevigata* and *Cavatodissiliodinium hansgochtii* are in the Laeviuscula Zone. The LAD of *Nannoceratopsis dictyambonis* is also in the Laeviuscula Zone. The FAD of *Kallosphaeridium hypornatum* is in the Sauzei Zone.

The interval is dated Laeviuscula Zone.

Sample interval 741.99 – 736.02 m (5 samples): Early Bajocian, Sauzei Zone

Assemblages in this interval are quite similar to below but show the first occurrence of *Kallosphaeridium hypornatum*. *Hystriodinium?* sp. occurs for the last time in the sample at 741.41 m.

The interval is defined from the first occurrence of *Kallosphaeridium hypornatum* to the first occurrence of questionable *Phallocysta thomasii* in the interval above.

The FAD of *Kallosphaeridium hypornatum* is in the Sauzei Zone. The FAD of *Phallocysta thomasii* is in the Humphriesianum Zone.

The interval is dated Sauzei Zone.

Sample interval 729.98 – 727.06 m (2 samples): Early Bajocian, Sauzei to Humphriesianum Zone

The assemblages in this interval show the first occurrences of questionable *Phallocysta thomasii* and questionable *Durotrigia filapicata*. Last occurrences show questionable *Cavatodissiliodinium hansgochtii*, *Dissiliodinium giganteum* and *Moesiodinium raileanui* at the base, and *Evansia? spongogranulata* at the top of the interval.

The interval is defined by the first occurrence of questionable *Phallocysta thomasii* to the last occurrence of *Evansia? spongogranulata*.

The LADs of *Cavatodissiliodinium hansgochtii*, *Dissiliodinium giganteum*, *Evansia? Spongogranulata* and *Moesiodinium raileanui* are all in the Sauzei Zone. The range of *Phallocysta thomasii* is considered to be restricted to the Romani and Humphriesianum Subzones of the Humphriesianum Zone. The FAD of *Durotrigia filapicata* is in the Humphriesianum Zone.

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

Sample 720.09 m (1 sample): Bajocian to Early Bathonian, possibly Humphriesianum to Zigzag Zone

The assemblage in this sample is very different to below with a mixture of dinoflagellate cysts of different age. The recorded dinoflagellate cysts include i.a. *Acanthaulax crispa*, *Cavatodissiliodinium* spp., *Ctenidodinium continuum*, *Ct. sellwoodii* group, *Dissiliodinium* spp., *Endoscrinium asymmetricum*, *Gonyaulacysta eisenackii*, *G. pectinigera*, *Korystocysta gochtii*, *Mancodinium semitabulatum*, *Meiourogonaulax valensii*, *Nannoceratopsis spiculata*, *Orobodinium* spp., *Sirmiodiniopsis* sp. of Feist-Burkhardt & Wille (1992), *Valensiella/Ellipsoidictyum* spp. and *Valvaeodinium spinosum*.

Constraining the age of the sample is difficult. There are a few specimens of taxa that are restricted to the Early Bajocian, but most taxa recorded are typical for a Late Bajocian or somewhat younger age, with some of them having an LAD in the Early Bathonian Zigzag Zone.

Typical for the Early Bajocian are *Cavatodissiliodinium* spp. and *Mancodinium semitabulatum*, the latter having an LAD in the Humphriesianum Zone. Taxa with an FAD in the Humphriesianum Zone, but also common later in the Late Bajocian are *Acanthaulax crispa*, *Meiourogonaulax valensii*, *Nannoceratopsis spiculata* and *Valensiella/Ellipsoidictyum* spp. Taxa with an FAD in the Niortense Zone are *Ctenidodinium continuum*, *Endoscrinium asymmetricum*,

Gonyaulacysta pectinigera, *Korystocysta gochtii* and *Valvaeodinium spinosum*. The taxa *Orobodinium* spp., *Gonyaulacysta eisenackii* and *Sirmiodiniopsis* sp. have their FADs in the Parkinsoni Zone. The LAD of *Acanthaulax crispa* is in the Parkinsoni Zone, and that of *Meiourogoniaulax valensii* and *Sirmiodiniopsis* sp. are in the Zigzag Zone.

The sample is interpreted to range from possibly Humphriesianum Zone to Zigzag Zone, with most constituents indicating Parkinsoni Zone.

Sample interval 714.37 – 705.02 m (3 samples): Early Bajocian, Humphriesianum Zone

The dinoflagellate cyst assemblages in this interval include *Acanthaulax crispa*, *Batiacasphaera* spp., *B. laevigata*, *Dissiliodinium* spp., *Durotrigia daveyi*, *Gongylodinium erymnoteichon*, *Kallosphaeridium hypornatum*, *Nannoceratopsis gracilis* s.l. and *Valensiella/Ellipsoidictyum* spp. *Cavatodissiliodinium* sp. 3 is recorded in the sample at 714.37 m, "*Hypolytodium*" sp. and *Mancodinium semitabulatum* are recorded in the sample at 708.23 m.

The interval is defined by the occurrence of *Acanthaulax crispa* to the last occurrence of *Mancodinium semitabulatum*.

Acanthaulax crispa has its FAD in the Humphriesianum Zone. *Mancodinium semitabulatum* has its LAD also in the Humphriesianum Zone. The range of "*Hypolytodium*" sp. is considered to be restricted to the Romani and Humphriesianum Subzones of the Humphriesianum Zone.

The sample interval is interpreted Humphriesianum Zone.

Sample interval 703.71 – 701.64 m (4 samples): Late Bajocian Parkinsoni Zone to Early Bathonian Zigzag Zone (plus Early Bajocian)

Composition of the dinoflagellate cyst assemblages in these samples is very different to below. Assemblages are rich and diverse. Taxa recorded regularly in these assemblages include i.a. *Acanthaulax crispa*, *Atopodinium polygonale*, *Ctenidodinium* spp., *Ct. continuum*, *Ct. sellwoodii* group, *Durotrigia daveyi*, *Gongylodinium hocneratum*, *Korystocysta gochtii*, *Meiourogoniaulax valensii*, *Nannoceratopsis spiculata*, *Orobodinium* spp., *O. automobile*, *Rhynchodiniopsis? regalis*, *Sirmiodiniopsis* sp. in Feist-Burkhardt & Wille (1992) and *Valvaeodinium spinosum*.

In all four samples of the interval there are some unexpected occurrences that are in conflict with the age suggested by the majority of taxa. These are *Dissiliodinium giganteum* and *Hystrichodinium?* sp. in the sample at 703.71 m, questionable *Ctenidodinium combazii* at 703.71 m and 701.79 m, *Cavatodissiliodinium* spp., *Lithodinia* spp. and *Tubotuberella dangeardii* at 701.79 m, *Nannoceratopsis plegas plegas* at 701.66 m, and *Nannoceratopsis gracilis* s.l. at 701.64 m.

Based on the majority of taxa recorded, the assemblages in this interval correspond best to the Parkinsoni Zone, as *Orobodinium automobile* and *Sirmiodiniopsis* sp. have their FADs in the Parkinsoni Zone and *Acanthaulax crispa* has its LAD also in the Parkinsoni Zone. Conflicting with this age assignment are the odd occurrences of taxa with an FAD in the Zigzag Zone (*Ctenidodinium combazii*, *Lithodinia* spp., *Tubotuberella dangeardii*) and of taxa with their main distribution or LADs in the Early Bajocian (*Dissiliodinium giganteum*, *Cavatodissiliodinium* spp., *Hystrichodinium?* sp., *Nannoceratopsis gracilis* s.l., *Nannoceratopsis plegas plegas*).

The samples in this interval are interpreted Parkinsoni to Zigzag Zone, with some Early Bajocian.

Sample 701.38 m (1 sample): Early Bathonian Zigzag Zone

The assemblage is characterised by the abundant and diverse occurrence of species of the genus *Ctenidodinium*, including *Ctenidodinium* spp., *Ct. combazii*, *Ct. continuum*, *Ct. cornigerum*, *Ct. ornatum* and *Ct. sellwoodii* group. *Ctenidodinium combazii* and *Dissiliodinium minimum* are common. First occurrences include *Lithodinia jurassica* and the first chorate dinoflagellate cyst *Cleistosphaeridium* spp. Last occurrences include questionable *Acanthaulax crispa*, *Endoscriinium asymmetricum* and *Meiourogoniaulax valensii*.

The interval is defined by the first occurrence of unequivocal *Ctenidodinium combazii* and *Lithodinia jurassica* to the last occurrence of *Meiourogoniaulax valensii* and the first occurrence of *Cleistosphaeridium* spp.

The FAD of *Ctenidodinium combazii* is within the upper part of Parkinsoni Zone, that of *Lithodinia jurassica* is in the Zigzag Zone, and that of *Cleistosphaeridium* spp. in the Tenuiplicatus Subzone of Zigzag Zone. The LAD of *Meiourogoniaulax valensii* is in the Zigzag Zone.

The sample is interpreted Zigzag Zone.

Sample interval 699.74 – 699.22 m (2 samples): Late Bathonian, Hodsoni Zone

The assemblages in this interval are similar to below with abundant and diverse representatives of the genus *Ctenidodinium*. *Ct. cornigerum* is superabundant. In addition, there are the first occurrences of *Atopodinium prostatum*, *Pareodinia prolongata* and *Sirmiodiniopsis orbis* at the base, and the first complex skolochorate dinocysts indet. at the top of the interval. Last occurrences include *Carpathodinium predae* at the base, and *Gongylodinium erymnoteichon*, *G. hocneratum*, *Rhynchodiniopsis? regalis* and *Valvaeodinium spinosum* at the top of the interval.

The interval is defined by the first occurrences of *Atopodinium prostatum*, *Pareodinia prolongata* and *Sirmiodiniopsis orbis* to the last occurrences of *Gongylodinium erymnoteichon* and *Rhynchodiniopsis? regalis*.

The FADs of *Atopodinium prostatum*, *Pareodinia prolongata* and *Sirmiodiniopsis orbis* are in the Hodsoni Zone. The LADs of *Gongylodinium erymnoteichon* and *Rhynchodiniopsis? regalis* are also in the Hodsoni Zone.

The sample is dated Hodsoni Zone.

Sample interval 696.29 – 696.10 m (2 samples): Early Callovian, Herveyi Zone

Composition of the dinoflagellate cyst assemblages in this interval is different to below. Complex skolochorate dinocysts indet. are common. Species of *Ctenidodinium* are less abundant. There are several first occurrences, i.a. *Korystocysta pachyderma*, *Lithodinia caytonensis*, *Mosaicodinium mosaicum*, *Sentusidinium? varispinosum* and *Stephanelytron scarburghense* at the base and *Eodinia pachythea*, *Rhynchodiniopsis cladophora* and *Sirmiodinium grossii* at the top of the interval. Last occurrences include *Ctenidodinium combazii* and *Valvaeodinium vermicylindratum* at the base, and *Aldorfia aldorfensis*, *Atopodinium polygonale*, *Gonyaulacysta pectinigera*, *Lithodinia caytonensis*, *Nannoceratopsis spiculata* and *Sentusidinium? varispinosum* at the top of the interval.

The interval is defined by the first occurrences of *Sentusidinium? varispinosum* and *Stephanelytron scarburghense* to the last occurrences of *Atopodinium polygonale*, *Ctenidodinium combazii* and *Gonyaulacysta pectinigera*.

The FADs of *Sentusidinium? varispinosum* and *Stephanelytron scarburghense* are in the Herveyi Zone. The LADs of *Atopodinium polygonale*, *Ctenidodinium combazii* and *Gonyaulacysta pectinigera* are also in the Herveyi Zone.

The interval is interpreted Herveyi Zone.

Sample 696.00 m (1 sample): Early Oxfordian, Mariae Zone

Composition of the dinoflagellate cyst assemblage in this sample is different to below. Chorate dinoflagellate cysts are superabundant. There are numerous first occurrences. These include *Acanthaulax granulata/venusta* spp., *Compositosphaeridium polonicum*, questionable *Endoscrinium galeritum*, questionable *Liesbergia liesbergensis*, *L. scarburghensis*, *Limbodinium absidatum*, *Omatidium amphiacanthum*, *Prolixosphaeridium* spp., *Rigaudella aemula*, *Scriniodinium crystallinum*, *Stephanelytron redcliffense*, *Wanaea digitata*, *W. fimbriata* and *W. thysanota*. Important last occurrences in this sample are *Ctenidodinium continuum*, questionable *Liesbergia liesbergensis* and *Wanaea digitata*.

The interval is defined by the first occurrences of *Omatidium amphiacanthum* and *Wanaea fimbriata* to the last occurrences of *Ctenidodinium continuum*, questionable *Liesbergia liesbergensis* and *Wanaea digitata*.

The FADs of *Omatidium amphiacanthum* and *Wanaea fimbriata* are in the Mariae Zone. The LADs of *Ctenidodinium continuum*, *Liesbergia liesbergensis* and *Wanaea digitata* are also in the Maria Zone.

The interval is dated Mariae Zone.

Sample 695.46 m (1 sample): Middle Oxfordian, Transversarium Zone to Late Oxfordian, Bifurcatus Zone

The sample shows the first occurrences of *Dingodinium tuberosum*, *Glossodinium dimorphum*, questionable *Lithodinia arcanitabulata* and *Occisucysta balios*. Important taxa still present in the sample are *Compositosphaeridium polonicum*, *Endoscrinium galeritum*, *Gonyaulacysta eisenackii*, *Nannoceratopsis pellucida*, *Scriniodinium crystallinum* and *Sirmiodiniopsis orbis*.

The interval is defined by the co-occurrence of *Compositosphaeridium polonicum*, *Endoscrinium galeritum*, *Gonyaulacysta eisenackii*, *Nannoceratopsis pellucida* and *Sirmiodiniopsis orbis* on the one hand, and *Dingodinium tuberosum* and questionable *Lithodinia arcanitabulata* on the other.

The LADs of *Compositosphaeridium polonicum*, *Endoscrinium galeritum*, *Gonyaulacysta eisenackii*, *Nannoceratopsis pellucida* and *Sirmiodiniopsis orbis* are in the Transversarium Zone. The FADs of *Dingodinium tuberosum* and *Lithodinia arcanitabulata* are considered to be in the Bifurcatus Zone.

The interval is interpreted Transversarium to Bifurcatus Zone, with most constituents indicating Transversarium Zone.

Tab. 3-3: List of analysed palynology samples from STA3-1

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

Depth [m MD]	Age	Zone & Subzone
695.46	Late to Middle Oxfordian	Bifurcatus – Transversarium Zone
696.00	Early Oxfordian	Mariae Zone
696.10	Early Callovian	Herveyi Zone
696.29	Early Callovian	Herveyi Zone
699.22	Late Bathonian	Hodsoni Zone
699.74	Late Bathonian	Hodsoni Zone
701.38	Early Bathonian	Zigzag Zone
701.64	Early Bathonian – Bajocian	Zigzag – Parkinsoni Zone (plus Early Bajocian)
701.66	Early Bathonian – Bajocian	Zigzag – Parkinsoni Zone (plus Early Bajocian)
701.79	Early Bathonian – Bajocian	Zigzag – Parkinsoni Zone (plus Early Bajocian)
703.71	Early Bathonian – Bajocian	Zigzag – Parkinsoni Zone (plus Early Bajocian)
705.02	Early Bajocian	Humphriesianum Zone
708.23	Early Bajocian	Humphriesianum Zone
714.37	Early Bajocian	Humphriesianum Zone
720.09	Early Bathonian – Bajocian	Zigzag – possibly Humphriesianum Zone
727.06	Early Bajocian	Humphriesianum – Sauzei Zone
729.98	Early Bajocian	Humphriesianum – Sauzei Zone
736.02	Early Bajocian	Sauzei Zone
736.06	Early Bajocian	Sauzei Zone
736.49	Early Bajocian	Sauzei Zone
741.41	Early Bajocian	Sauzei Zone
741.99	Early Bajocian	Sauzei Zone
742.33	Early Bajocian	Laeviuscula Zone
750.42	Early Bajocian	Laeviuscula Zone
760.65	Early Bajocian	Laeviuscula Zone
761.56	Early Bajocian	Ovale Zone
764.68	Early Bajocian	Ovale Zone
766.62	Early Bajocian – L. Aalenian	?Discites – Concavum Zone
769.79	Middle Aalenian	Bradfordensis Zone
774.96	Middle Aalenian	Bradfordensis Zone
776.94	Middle Aalenian	Bradfordensis Zone
779.24	Middle Aalenian	Murchisonae Zone
786.21	Early Aalenian	Opalinum Zone (Bifidatum SZ)
787.31	Early Aalenian	Opalinum Zone (possibly Bifidatum – Opalinum SZ)
796.27	Early Aalenian	Opalinum Zone (Opalinum SZ)
820.33	Early Aalenian	Opalinum Zone (Opalinum SZ)
840.00	Early Aalenian	Opalinum Zone (Opalinum SZ)
860.03	Early Aalenian	Opalinum Zone (Opalinum SZ)
880.18	Early Aalenian	Opalinum Zone (Opalinum SZ)
888.38	Early Aalenian – L. Toarcian	Opalinum Zone (Opalinum SZ) – Aalensis Zone

3.4 Chemostratigraphy

The sampling of the STA3-1 cores focused primarily on the upper part of the Lias Group (Figs. 3-2 and 3-3) and Dogger Group (Figs. 3-4 to 3-7) and, therefore inter alia on clay mineral-rich layers of the Opalinus Clay. The summary Figs. 3-8 and 3-9 illustrate the fully analysed interval from the upper part of the Staffelegg Formation up to the lowermost part of the Wildeggen Formation (899.80 – 692.00 m). The data presented here (applies for all subsequent figures in this section) is shown in comparison to other data collected during the drilling campaign: Stratigraphic profile after Dossier III, DryClay (values in wt.-%, vertical axis in m MD log depth; cf. Dossier X), XRD measurements (horizontal bars; calcite: blue, dolomite and ankerite: green, siderite: red; cf. Dossier VIII) and C(org) measurements also with blue horizontal bars (cf. Dossier VIII). In addition, formation boundaries were highlighted with black lines and other formal or informal subintervals with grey lines. The following stratigraphic abbreviations were used in Figs. 3-2 to 3-9: F. = Frick Member; G.B.R = Grünschholz Member, Breitenmatt Member and Rickenbach Member; Rieth. = Rietheim Member; G. W. = Gross Wolf Member; «M.-O. Fm.» and «M.-O.» = «Murchisonae-Oolith Formation»; Wedelsst. = Wedelsandstein Formation; V.+PW. = Variansmergel Formation and «Parkinsoni-Württembergica-Schichten».

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

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

Although, the calculated carbonate content (TCarb) is only a semi-quantitative method, the values presented here correspond quite good to the XRD values measured at the University of Bern (cf. Dossier VIII). The XRD data are illustrated in the following Figs. 3-2, 3-4 and 3-6 to provide a visual comparison between the data presented here and those from Dossier VIII. As discussed in Wohlwend et al. (2019b) based on measurements from the BDB-1 borehole at the Mont Terri Rock Laboratory, the values calculated here follow nicely the calcite and dolomite wt.-% with an additional mixed signal from the other carbonates (mainly siderite). Because during the reaction time of 60 min at 72 °C, a complete reaction for example for siderite does not take place. The TCarb values are slightly too low in siderite-rich successions (red bars in the XRD data), which is for example often the case in the «Mixed clay-silt-carbonate sub-unit» (868.06 – 821.09 m; Fig. 3-4).

In contrast to the carbonate measurements (bulk samples), the organic measurements were not always measured in metre resolution, depending on the variability of the expected isotope data and the TCarb content. If no major isotope changes were expected, as for example during the middle part of the Opalinus Clay, only every second sample (mainly 2 m interval) was analysed. Of the entire «Herrenwis Unit» only 5 more argillaceous interlayers were analysed.

Lias Group

Starting from the bottom up (Fig. 3-2), the oldest sediments measured belong to the Early Jurassic (probably Late Pliensbachian). The lowermost three measurements (899.80 m, 899.60 m and 899.40 m) belong to the uppermost combined Grünschholz Member, Breitenmatt Member and Rickenbach Member. The following ones, between 899.25 m and 887.98 m, represent the upper two members of the Staffelegg Formation. They show larger variations in their individual data, which can be explained by the overall higher sampling resolution in the Lias Group (some intervals in the Rietheim Member with around 20 cm spacing) as well as by the nodular calcareous lithology of the Gross Wolf Member.

The semi-quantitative carbonate content (TCarb, Fig. 3-2) represents the lithological variations in the Rietheim Member and the hanging Gross Wolf Member up to the Opalinus Clay. In the Rietheim Member the TCarb values show an increasing trend from around 17 wt.-% to values slightly above 50 wt.-%. The interval from 899.30 m to 898.55 m, the base of the Rietheim Member and up to the «Unterer Stein», clearly contains less carbonate than the hanging interval to the top of the Rietheim Member. The whole succession of the member is interrupted by higher values measured from the three calcareous interbeds in the middle part of the member («Unterer Stein»: 898.52 – 898.28 m, «Homogene Kalkbänke»: 897.97 – 897.82 m and «Oberer Stein»: 897.11 – 896.90 m). The uppermost more calcareous interval is represented by one sample (questionable «Monotisbank» between 893.74 – 893.20 m). The nomenclature of these beds is *sensu* Kuhn & Etter (1994). The TCarb data from these three beds is documented in Appendix E1 and marked by blue dots in Fig. 3-2. The overlying Gross Wolf Member shows similar values as in the succession below, but only the once measured from the argillaceous to calcareous marl sediment. Although, the calcareous nodules to nodular layers, which are typical for the Gross Wolf Member clearly show higher values 89.7 wt.-% (892.58 m) and 95.0 wt.-% (890.50 m).

The $\delta^{13}\text{C}_{\text{carb}}$ values document at the base of the Rietheim Member a negative trend with the most negative value coinciding with the «Unterer Stein» (-2.5‰ at 898.40 m). The negative trend is subsequently followed by a rapid increase. The most positive $\delta^{13}\text{C}_{\text{carb}}$ value thereafter was documented just above the «Oberer Stein» with +2.0‰ at 896.47 m. Further up to the top of the Gross Wolf Member the values show a continuous decreasing trend to values around +0.6‰ at 888.99 m, followed by a clear jump to more negative values around the lithological boundary (887.94 m) into the lowermost Opalinus Clay. The discussed negative carbon isotope excursion (CIE) up to and including here also the «Unterer Stein» represents one of the major Mesozoic perturbations of the carbon cycle. This CIE, documented here in the Rietheim Member, can be correlated with the global Toarcian-CIE (T-CIE). In many places the T-CIE is also linked with an organic-rich succession (also in STA3-1, discussion follows below), and therefore was deposited during the Toarcian-Oceanic Anoxic Event (T-OAE).

The negative T-CIE can also be seen by the $\delta^{13}\text{C}_{\text{org}}$ values (Fig. 3-3). The most negative one, with a value of -32.4‰ at 898.70 m, is slightly lower than the most negative one from the $\delta^{13}\text{C}_{\text{carb}}$ and clearly in the succession below the «Unterer Stein». The following rapid positive shift is also clearly documented in the organic matter, where the most positive value (-26.9‰) was measured from the sample drilled from the «Oberer Stein» at 897.00 m. The $\delta^{13}\text{C}_{\text{org}}$ values document at the very base of the Rietheim Member a fast shift to negative values, like in BUL1-1 (Wohlwend et al. 2021a), where it was documented in much more detail with several negative shifts similar to the compilation made by Ruebsam & Al-Husseini (2020).

The Rietheim Member is very bituminous and is itself defined by the occurrence of bituminous shale. The TOC as well as the C/N ratio (both Fig. 3-3) limit somehow the range of the member. Both proxies show very increased values in the Rietheim Member. The highest TOC value with 12.3 wt.-% was measured slightly below the «Unterer Stein» at 898.55 m. The average range of

the semi-quantitative TOC content lies between 3.5 and 8.2 wt.-%, whereby the three calcareous beds document lower TOC values less than and equal to 1 wt.-%. The Rietheim Member, as mentioned above, clearly can be assigned as a black shale deposit and those successions below the «Unterer Stein» with the highest TOC were deposited during the T-OAE. 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 below 0.7 wt.-%.

The C/N ratios show the same trend as the TOC with the highest ratios mainly measured contemporaneously with the bituminous lower and middle part of the Rietheim Member (ratios between 23 and 44), compared to the overlying Gross Wolf Member with a much lower C/N ratio (10 – 12). There is just one exception. The C/N ratio calculated from the sample at 892.58 m (ratio: 34.3) would rather belong to the lying Rietheim Member, although reworking cannot be completely ruled out. Such high C/N ratios, measured in the Rietheim Member, are normally rather unusual for marine organic matter, which usually has values between 5 and 8 (e.g. Emerson & Hedges 1988, Meyers 1997) and would therefore pretend that the organic material would be of terrigenous source. However, such high C/N ratios were also reported from mid-Pleistocene sapropels from the Tyrrhenian Basin (Meyers & Bernasconi 2005) which are also clearly produced by marine organic matter. Van Mooy et al. (2002) proposed a model for these very unusual C/N ratios in which they determined from sediment trap studies that suboxic microbial degradation via denitrification preferentially utilises nitrogen-rich amino acids and hence leaves a larger proportion of the nitrogen-poor organic matter components intact than under oxic conditions. C/N values of the surviving organic matter necessarily rise.

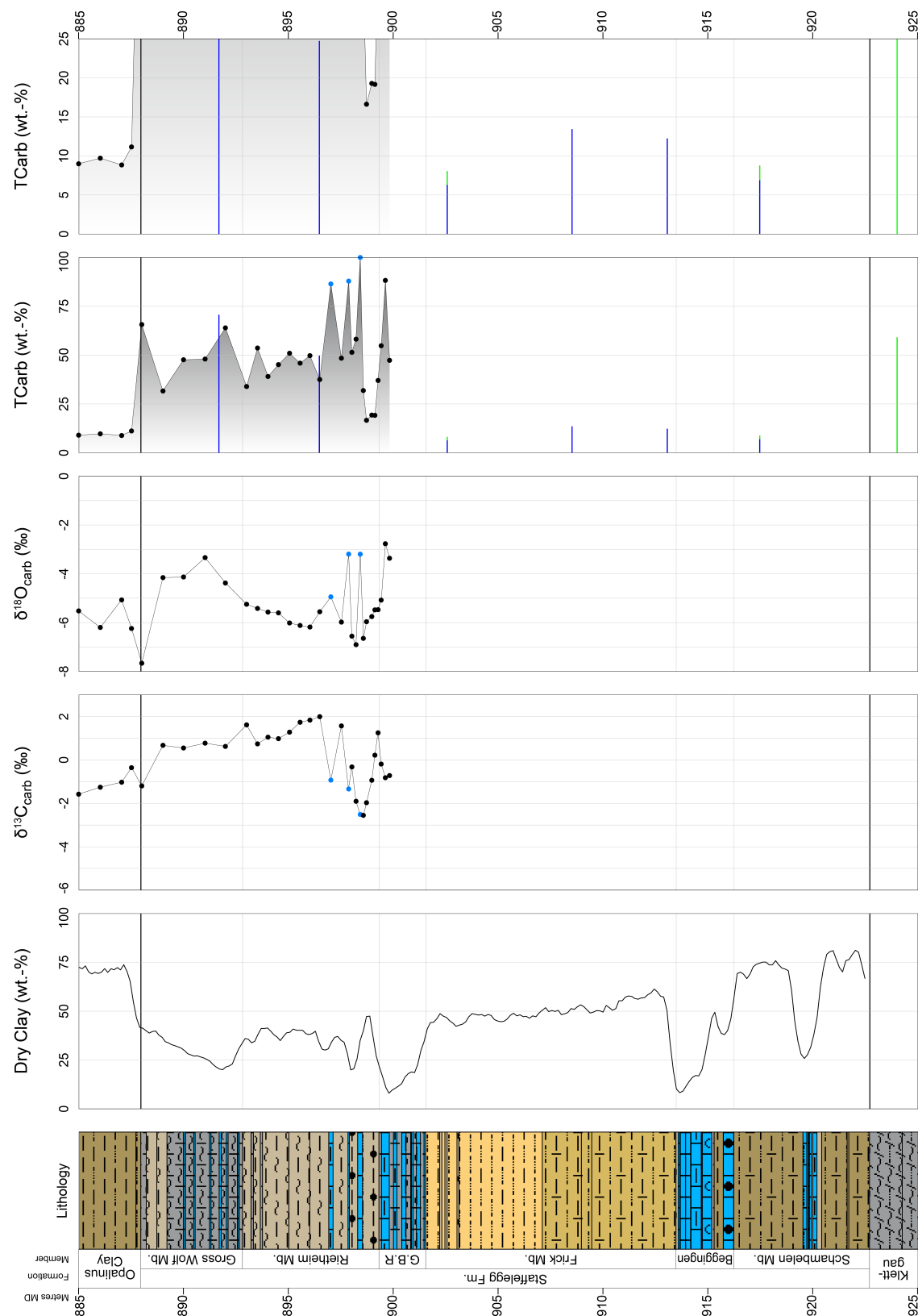


Fig. 3-2: Bulk rock (carbonate) isotopic data from the Lias Group

Geochemical data from 899.80 – 886.00 m, additional explanations and references see text at the beginning of Section 3.4.

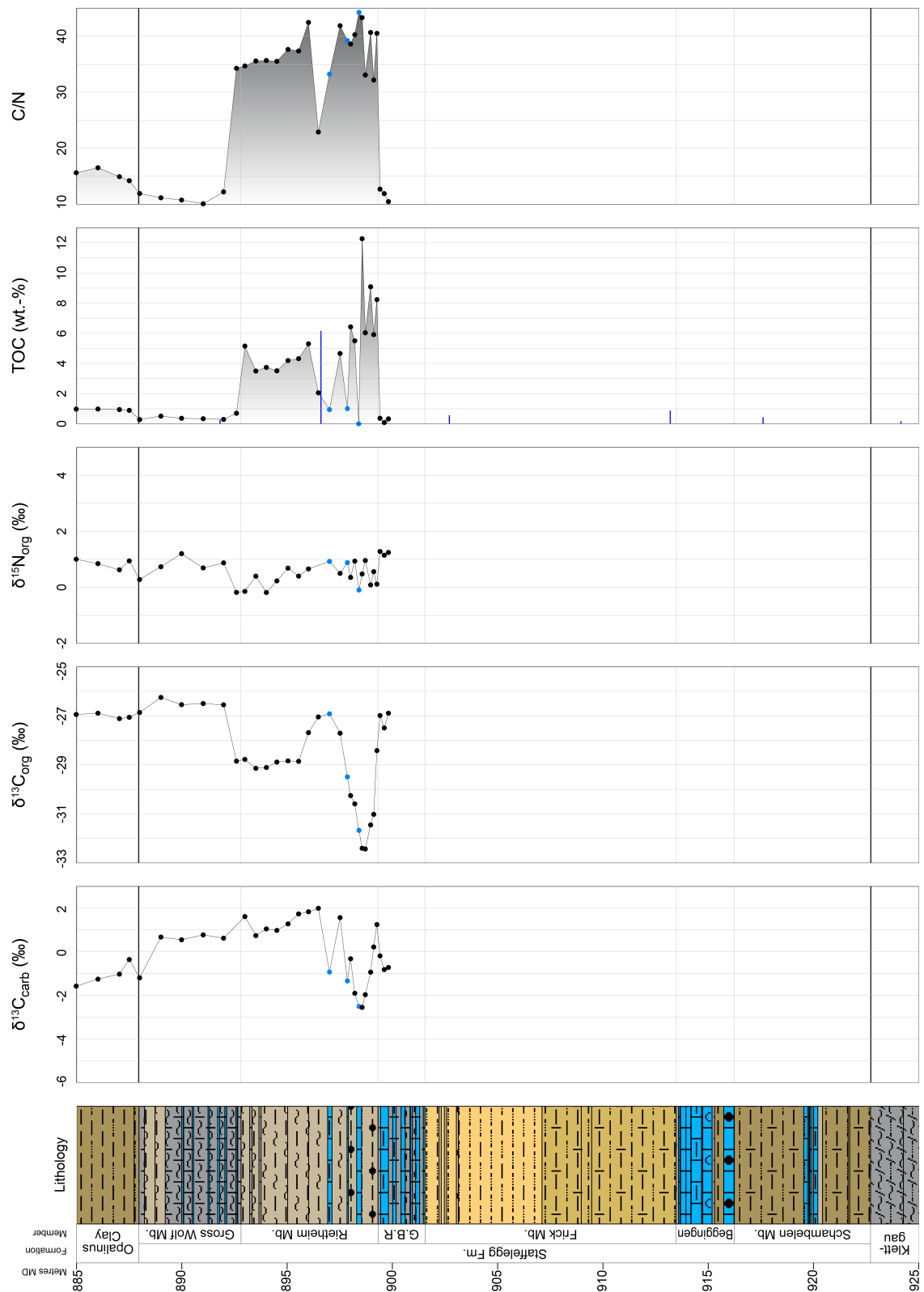


Fig. 3-3: Organic isotopic data from the Lias Group

Geochemical data from 899.80 – 886.00 m, additional explanations and references see text at the beginning of Section 3.4.

Lower part of the Dogger Group – mainly Opalinus Clay

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

The semi-quantitative carbonate content (TCarb) values from the more homogeneous clay mineral-dominated lithologies are rather low and very stable compared to those from the underlying Staffelegg Formation (Fig. 3-4). In the lowermost succession of the Opalinus Clay («Clay-rich sub-unit»: 887.94 – 868.06 m) the average TCarb values decrease from around 12 wt.-% (887.49 m) to values around 6 wt.-% at 869.00 m. Upsection, the TCarb documents a slight increasing trend in the «Mixed clay-silt-carbonate sub-unit» (868.06 – 821.09 m) to values around 13 wt.-% with two higher values around 20 wt.-% (852.00 m and 849.88 m). The trend, to slightly more positive values, stops with a bioclastic calcareous layer (848.43 – 848.22 m; see also Appendix E1). Upsection, the values range between 5 and 12 wt.-% up to the top of the informal «Upper silty sub-unit» (821.09 – 807.34 m). The above hanging «Sub-unit with silty calcareous beds» (807.34 – 779.26 m) documents several trends to increased carbonate contents. Two of them are clearly topped by calcareous beds (794.98 – 794.86 m and 786.37 – 786.30 m). The upper increasing trend documents TCarb values reaching up to 30 wt.-% at 787.00 m slightly below the 7 cm thick firm- to hardground (786.37 – 786.30 m) consisting of encrusted and bored lithoclasts of limestone. In the hanging «Murchisonae-Oolith Formation», three individual successions can be observed when looking at the TCarb contents: a lower one with very variable values reaching up to 79.9 wt.-% in individual bioclastic layers (Appendix E1), a middle one with very low TCarb values between 3.5 and 4.1 wt.-% and an upper one with again higher values reaching the top of the formation. The middle one represents nicely the very monotonous and very argillaceous succession from 775.50 m to 767.86 m.

The above-mentioned uppermost informal «Sub-unit with silty calcareous beds» comprises several calcareous beds. Some of the samples analysed from these are classified as measurements from "hiatus beds" and calcareous concretions. Additional calcareous beds can also be found in the lower part of the Opalinus Clay. They are all illustrated in Fig. 3-4 by thicker light blue lines ending with blue dots marking the TCarb values (see Appendix E1 for data and Section 3.1 for microfacies description). In addition to the blue values, also several septarian nodules were measured, which are illustrated in violet (see Appendix E1 for data) and in Fig. 3-6 also two measurements from macrofossils (crinoid spines) were illustrated with green dots. The calcareous beds (marked in blue) comprise TCarb values that are typical for calcareous marl (50 – 75 wt.-%) and limestone (75 – 100 wt.-%). The septarian nodules (violet) can mainly be found in two specific intervals: the lower one at around 875.15 m and slightly above and the upper one between 796.02 m and 795.01 m. The lower one belongs to a level with typical calcareous concretions and septarian nodules in the «Clay-rich sub-unit», which can be correlated over several boreholes and siting regions (e.g. BUL1-1: Wohlwend et al. 2021a; TRU1-1: Wohlwend et al. 2021b; BOZ1-1: Wohlwend et al. 2022).

The $\delta^{13}\text{C}_{\text{carb}}$ data reveal two negative CIE or negative intervals in the Opalinus Clay (Fig. 3-4): a lower negative CIE in the «Clay-rich sub-unit» and an upper CIE in the «Sub-unit with silty calcareous beds», maybe starting already in the upper part of the «Upper silty sub-unit». The lower negative CIE is represented by a clear decreasing trend, reaching the most negative value (-7.7‰ at 875.00 m) within the horizon with the calcareous concretions and septarian nodules between 875.15 m and 874.22 m. The above following increasing trend, documented in the $\delta^{13}\text{C}_{\text{carb}}$ data, shows a turning point almost coinciding with the transition from the «Mixed clay-silt-carbonate sub-unit» to the hanging «Upper silty sub-unit». There $\delta^{13}\text{C}_{\text{carb}}$ values of 1.0‰ and 1.1‰ are reached with the two samples at 822.00 m and 820.00 m. Trough the «Upper silty sub-

unit» the C-isotope data decrease to values around -1.0‰. In the «Sub-unit with silty calcareous beds», as mentioned above, an upper negative CIE can be observed with the most negative value of -7.0‰ at 795.07 m. The CIE is somehow bounded by two calcareous beds, which are located at: 799.46 – 799.06 m and 794.98 – 794.86 m (*cf.* Dossier III). From 794.97 m to the top of the Opalinus Clay the $\delta^{13}\text{C}_{\text{carb}}$ values show rather stable values, varying around -1.0‰. Crossing the lithological boundary to the hanging «Murchisonae-Oolite Formation», an additional negative CIE can be observed within the very monotonous and argillaceous succession analysed from the same samples with the very low TCarb contents. Upsection, the $\delta^{13}\text{C}_{\text{carb}}$ value increases crossing the lithological boundary to the Wedelsandstein Formation.

The $\delta^{13}\text{C}_{\text{carb}}$ data from the calcareous beds and/or bored and reworked intraclasts document possibly an early diagenetic signal (e.g. Wetzel & Allia 2000). The calcareous concretions and septarian nodules are the only macroscopic features with very negative $\delta^{13}\text{C}_{\text{carb}}$ values (-11.1 to -32.0‰, Appendix E1). However, very fine authigenic calcite was probably also precipitated in the very fine primary porosity of the Opalinus Clay as well as in the middle part of the «Murchisonae-Oolite Formation», which would lead to the more negative $\delta^{13}\text{C}_{\text{carb}}$ values in the lower and upper negative CIE in the Opalinus Clay and the CIE above (see also diagenetic discussion in Wohlwend et al. 2016).

The $\delta^{13}\text{C}_{\text{org}}$ data (Fig. 3-5) show a different picture compared to the $\delta^{13}\text{C}_{\text{carb}}$ values. The curve is relatively stable for the most part. The formation of the Opalinus Clay can be subdivided, based on $\delta^{13}\text{C}_{\text{org}}$ values, into three subintervals: The lowest interval (887.94 m – 871.00 m) can be described from the base of Opalinus Clay and includes the three progressively more negative CIE (-27.1‰ at 887.02 m, -27.3‰ at 880.00 m and -28.3‰ at 873.00 m). The most negative $\delta^{13}\text{C}_{\text{org}}$ value at 873.00 m is 2 m above the most negative $\delta^{13}\text{C}_{\text{carb}}$ value at 875.00 m. As already mentioned above, the most part in the middle (871.00 – 787.00 m) is very stable and documents a slight 0.7‰ increasing trend from around -27.2‰ to values around -26.5‰. The upper interval (786.50 – 779.26 m) is easily observed as the $\delta^{13}\text{C}_{\text{org}}$ data is shifted by 0.7‰ to more positive values. The shift or even jump in the organic C-isotopes happens just below and within the uppermost calcareous bed (786.37 – 786.30 m) in the «Sub-unit with silty calcareous beds». The whole upper part until the top of the Opalinus Clay, as well as into the hanging «Murchisonae-Oolite Formation», shows a positive trend reaching the most positive value with -24.4‰ at 770.00 m. The two measurements at 778.00 m and 777.50 m (open dots in Fig. 3-5) are re-measurements. For the discussion, please see the paragraph in the section "Upper part of the Dogger Group".

The TOC as well as the C/N ratio will be discussed in the same paragraph. Both proxies document rather stable conditions throughout the lower part of the Opalinus Clay up to the top of the «Mixed clay-silt-carbonate sub-unit» at 821.09 m (TOC: ~ 1.0 wt.-%, C/N ratio ~ 15). From 821.09 m upwards, the C/N ratio starts to increase, reaching a peak value of 21.6 at 793.89 m just above the calcareous bed between 794.98 m and 794.86 m. With the same sample at 793.89 m also the TOC reaches a maximum with 1.3 wt.-%. In the upper part of the «Sub-unit with silty calcareous beds» both proxies show similar decreasing trends until the calcareous bed between 786.37 m and 786.30 m. In the «Murchisonae-Oolite Formation» the same three times subdivision, as discussed above by the TCarb data, can be seen with the TOC dataset. The middle part contains slightly higher TOC values close to 1 wt.-% compared to the contents below and above reaching only 0.4 wt.-%.

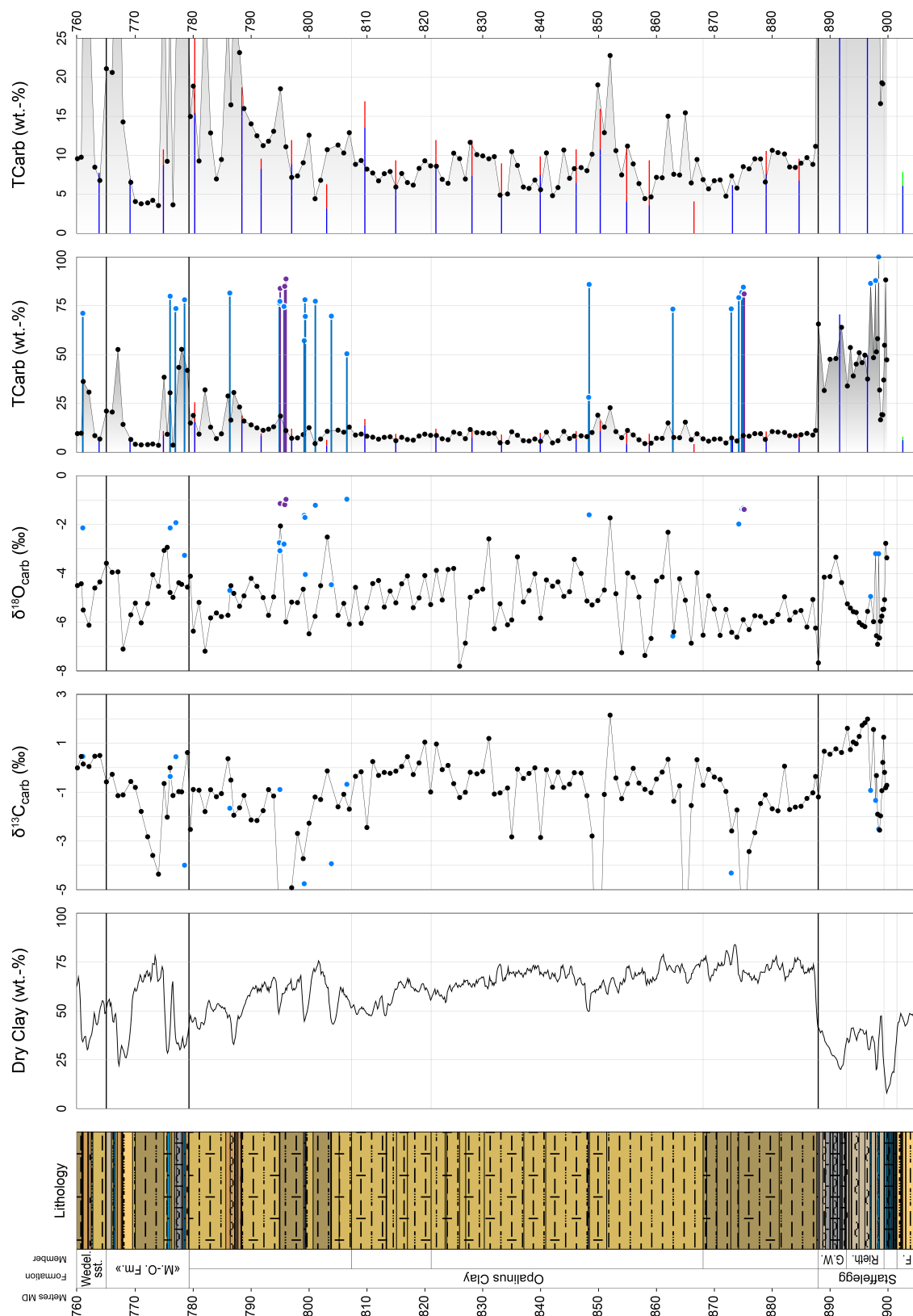


Fig. 3-4: Bulk rock (carb.) isotopic data from the lower Dogger Group – mainly Opalinus Clay
 Geochemical data from 899.80 – 760.00 m, additional explanations and references see text
 at the beginning of Section 3.4.

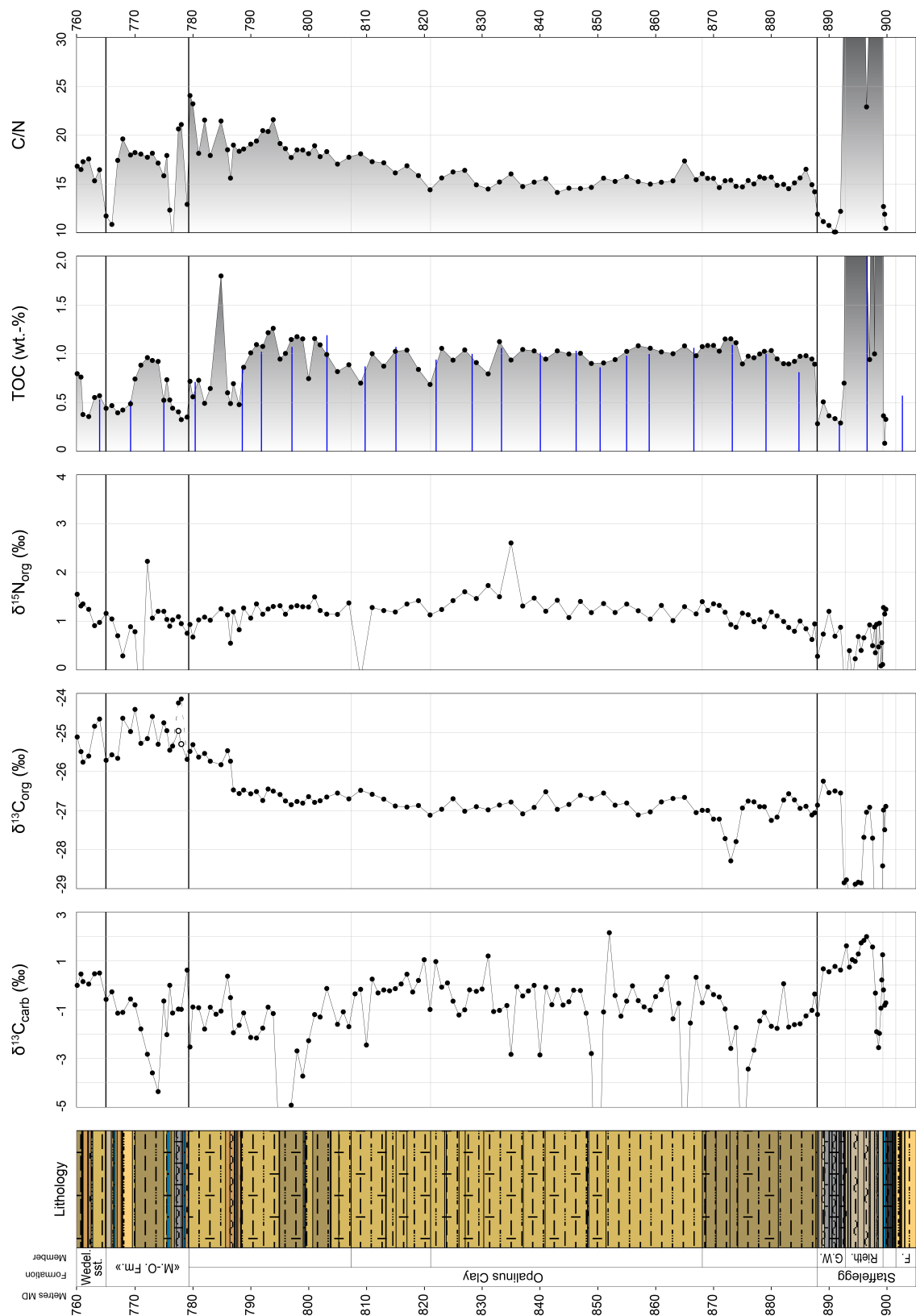


Fig. 3-5: Organic isotopic data from the lower Dogger Group – mainly Opalinus Clay
 Geochemical data from 899.90 – 760.00 m, additional explanations and references see text at the beginning of Section 3.4.

Upper part of the Dogger Group

The following described interval, the upper Dogger Group («Murchisonae-Oolith Formation», Wedelsandstein Formation, «Herrenwis Unit», Variansmergel Formation and «Parkinsoni-Württembergica-Schichten», Wutach Formation as well as the lower part of the Wildegg Formation), covers in time the whole Middle Aalenian to Middle Oxfordian substages (Figs. 3-6 and 3-7).

The semi-quantitative TCarb (Fig. 3-6) represents the alternation of silty claystone, argillaceous to calcareous marl and limestone. However, the TCarb contents are probably slightly underestimated because of the sampling strategy of not sampling every limestone bed (focus on the clay mineral-rich sediments, with an exception for the carbonate-rich «Herrenwis Unit»). Nevertheless, the carbonate content curve reflects the inverse wet clay content curve (*cf.* Dossier X). As mentioned above, the «Murchisonae-Oolith Formation» can be divided into three parts with a middle one represented by the very low TCarb values. The Wedelsandstein Formation, like the drilling in BUL1-1 (Wohlwend et al. 2021a), is showing two increasing trends separated by a hardground at 760.98 – 760.73 m. The overlaying 40.35 m thick «Herrenwis Unit» is very pronounced and can be easily distinguished from the underlying and hanging formations based on TCarb values.

Although the oxygen isotopes data were not discussed until now (too vulnerable to diagenetic overprint in the low-carbonate sediments), the $\delta^{18}\text{O}_{\text{carb}}$ show an interesting feature in the lower «Herrenwis Unit» (742.00 – 729.83 m). This interval is around 3‰ more positive than the hanging intervals. Upsection, there are several trends to more positive $\delta^{18}\text{O}_{\text{carb}}$ values visible. It seems that there are individual stratigraphic intervals that were more prone to diagenetic overprinting.

The $\delta^{13}\text{C}_{\text{carb}}$ data (Figs. 3-6 and 3-7) indicate an increasing trend in the Wedelsandstein Formation, starting already in the upper part of the «Murchisonae-Oolith Formation». With the sample at 754.00 m, the trend is superseded by a more stable interval with a $\delta^{13}\text{C}_{\text{carb}}$ value around 0.8‰ up to the top of the Wedelsandstein Formation. During the «Herrenwis Unit» quite positive values were documented. However, in the lower part a slightly more positive interval can be observed between 734.00 m and 731.00 m with values reaching up to 3.0‰. Upsection, the values decrease to values around 1.5‰ at 714.00 m and reaching again 2.6‰ close to the top of the coral-rich succession. Between the top of the «Herrenwis Unit» (701.65 m) and the top of the iron-oolith rich succession of the Wutach Formation (696.03 m) the $\delta^{13}\text{C}_{\text{carb}}$ values are almost 2‰ lower and stay very stable. The sample taken at 696.15 m (+1.8‰), only 0.12 m below the top of the Wutach Formation, shows already a slightly more positive value, which later becomes much more obvious in the hanging Birmenstorf Member of the Wildegg Formation. The several per mille positive shift to values around +3.2‰ at 694.00 m is typical for the Callovian/Oxfordian boundary and was already documented by Rais et al. (2007) in other locations as well as the Weiach borehole and was for example also documented during this campaign in the BUL1-1 borehole (Wohlwend et al. 2021a). The most positive $\delta^{13}\text{C}_{\text{carb}}$ values were documented in the Middle Oxfordian (Transversarium Zone; see Rais et al. 2007).

The $\delta^{13}\text{C}_{\text{org}}$ data (Fig. 3-7) from the «Murchisonae-Oolith Formation» show an increasing trend, starting already at the uppermost calcareous bed (786.37 – 786.30 m) in the Opalinus Clay. The overall trend has its turning point in the lower part of the Wedelsandstein Formation, followed by a decreasing trend to the top of the formation. The positive and negative trend is interrupted by two smaller negative shifts: One between 767.00 m and 765.00 m, covering the lithological boundary between the «Murchisonae-Oolith Formation» and the Wedelsandstein Formation and a second one slightly above between 762.00 m and 760.66 m. The upper negative shift coincides with the hardground at 760.98 – 760.73 m as already mentioned in connection with the carbonate

content. This hardground is indeed also represented in several other proxies as the $\delta^{18}\text{O}_{\text{carb}}$, TOC and C/N ratio. The $\delta^{13}\text{C}_{\text{org}}$ data from the overlying «Herrenwis Unit» are incomplete because there was not enough material for organic measurements after the decarbonatisation of the limestone-rich succession. Therefore, a description of the only four measurements is not meaningful. Finally, the $\delta^{13}\text{C}_{\text{org}}$ data from the hanging formations of the «Herrenwis Unit» also document the negative trend and the very striking positive shift close to the Callovian/ Oxfordian boundary from -28.8‰ at 697.50 m to -24.3‰ at 695.50 m. The chemostratigraphic data ($\delta^{13}\text{C}_{\text{org}}$ as well as $\delta^{13}\text{C}_{\text{carb}}$) document, with the very large shifts, that the resolution in these very condensed successions is not high enough and that a lot of time is missing in the stratigraphic gaps.

In the lower part of the «Murchisonae-Oolith Formation» two samples (778.00 m and 777.50 m), taken from the very reddish, iron-oolitic and limonitic interval, document strange positive peak values, represented or connected in Fig. 3-7 by a dashed line. Similar strange positive values in the $\delta^{13}\text{C}_{\text{org}}$ data were also analysed during this campaign always in combination with such reddish lithologies (e.g. BOZ1-1; Wohlgend et al. 2022). The questioned samples have been decarbonised a second time for 12 h, but this time at 70 °C. The additional re-measurements document up to 1‰ lower $\delta^{13}\text{C}_{\text{org}}$ values (marked by open data points and connected with solid lines). Therefore, the assumption of incomplete decarbonatisation of ankerite and/or other iron-carbonates thus seems to be confirmed.

The C/N ratio as well as the TOC show less clear trends. The variations in the lithologies are also represented by higher variations throughout the upper part of the Dogger Group. However, remarkable is a clear decreasing trend through the upper part (above the hardground at 760.98 – 760.73 m) of the Wedelsandstein Formation also represented by a decline in the TOC.

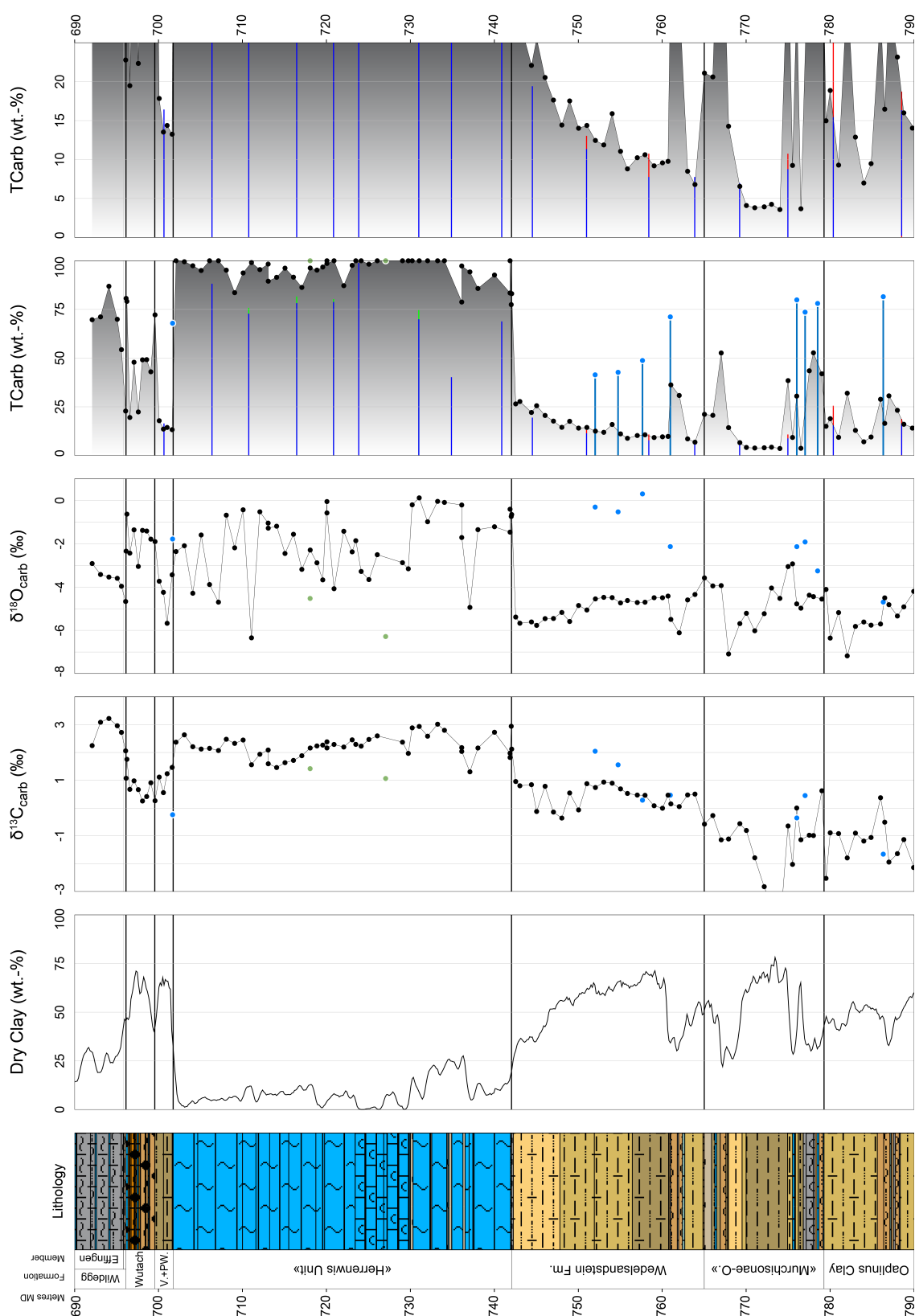


Fig. 3-6: Bulk rock (carbonate) isotopic data from the upper part of the Dogger Group

Geochemical data from 790.00 – 692.00 m, additional explanations and references see text at the beginning of Section 3.4.

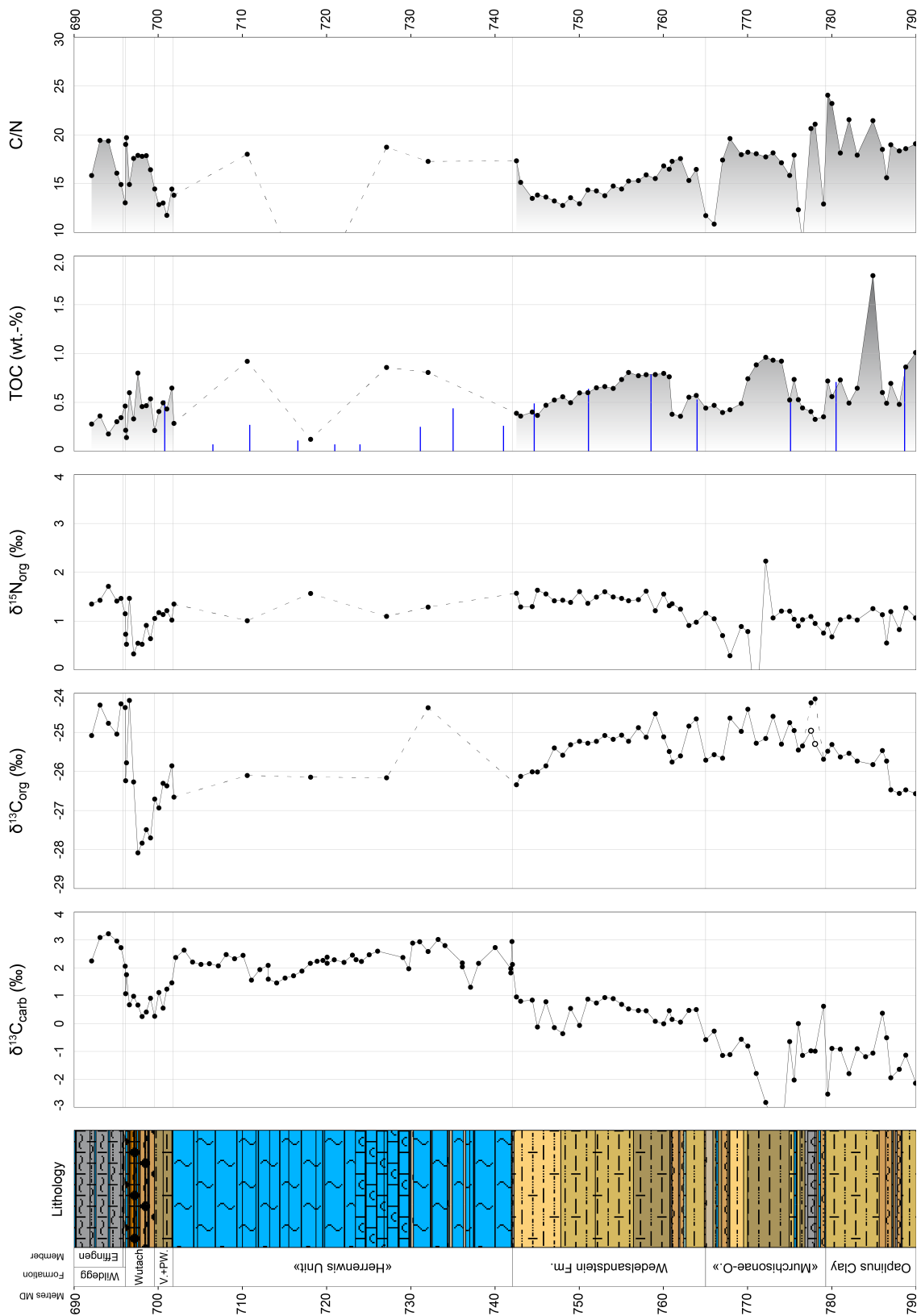


Fig. 3-7: Organic isotopic data from the upper part of the Dogger Group

Geochemical data from 790.00 – 692.00 m, additional explanations and references see text of Section 3.4.

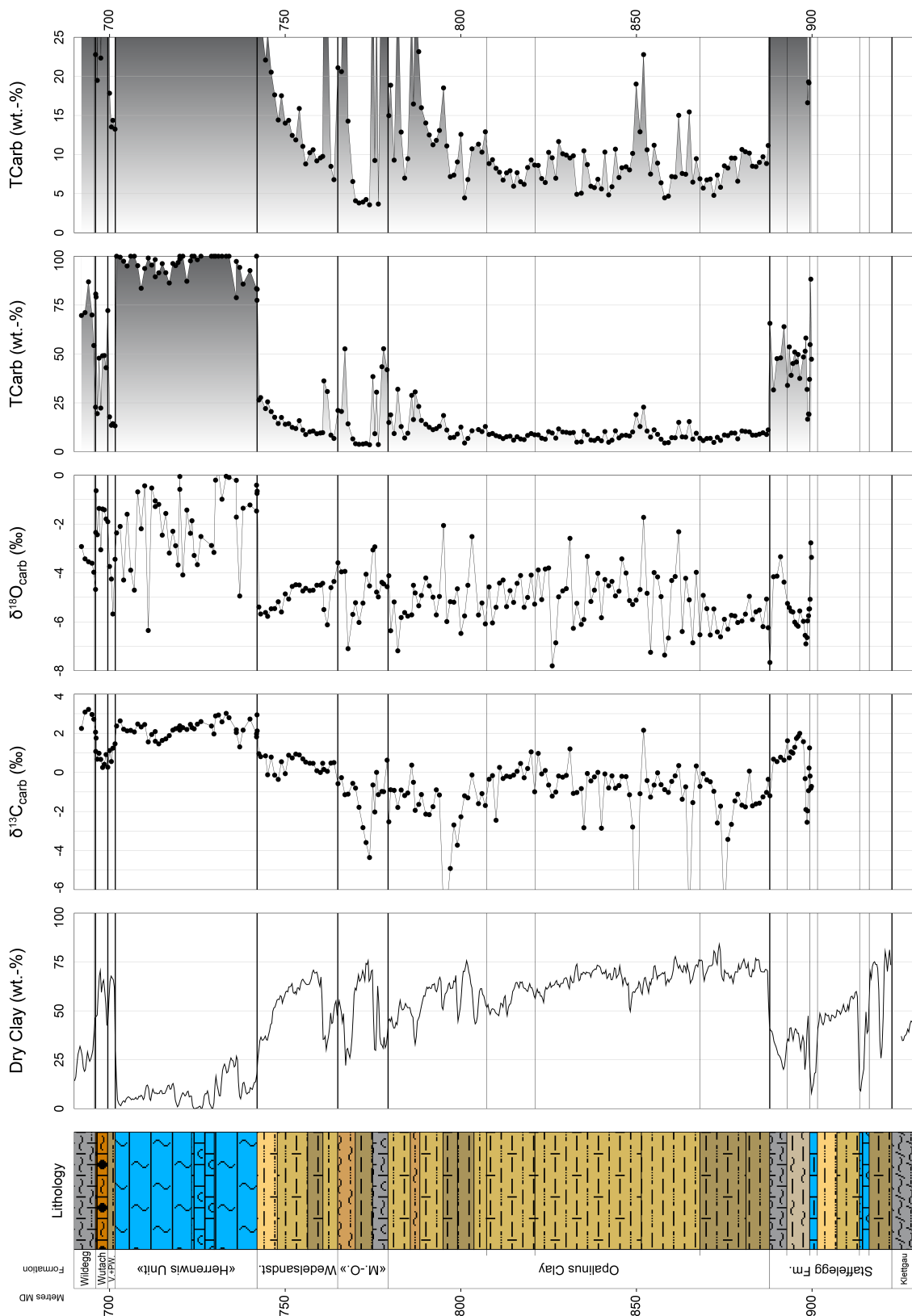


Fig. 3-8: Whole bulk rock (carbonate) isotopic data from STA3-1

Geochemical data from 899.80 – 692.00 m, additional explanations and references see text at the beginning of Section 3.4.

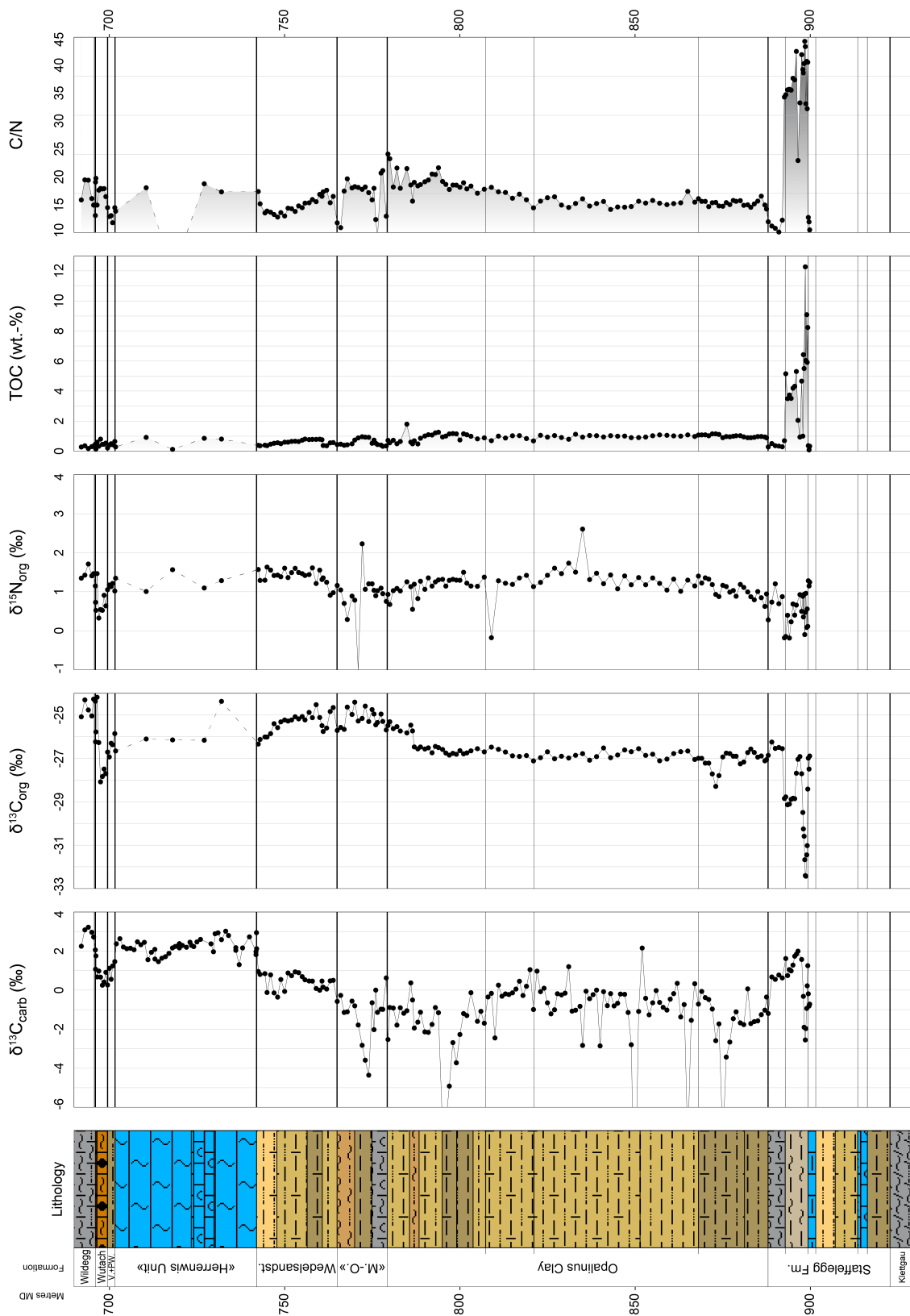


Fig. 3-9: Whole organic isotopic data from STA3-1

Geochemical data from 899.80 – 692.00 m, additional explanations and references see text at the beginning of Section 3.4.

4 Definition of specific lithostratigraphic boundaries

The boundaries between stratigraphical units, as also shown in the stratigraphical logs of the lithostratigraphy report (Dossier III), were mostly defined by using lithological criteria. According to the guidelines on stratigraphical nomenclature of Remane et al. (2005), the definition of lithostratigraphical units should be based, both vertically and horizontally, on lithological variations regardless of their age. In fact, the formation boundaries, as used by Nagra for the ongoing borehole campaign of Stage 3 of the Sectoral Plan for Geological Repositories (Jordan & Deplazes 2019), were not always obvious in the borehole and definitions were difficult to apply, either because of the small core diameter or because of differences in facies. The exact location of some of the formation boundaries caused discussions during core description and the process of quality control. Most of the important data for questionable boundaries were already present before the data-freeze (26.08.2021) and were used for the log descriptions and drawings. In the following paragraphs, the underlying considerations are explained for providing a better understanding of how boundaries were demarcated. We are aware of the fact that several boundaries are no longer based on lithological criteria alone and that chronostratigraphic criteria (ammonite, palyno- and chemostratigraphy) are included in the definitions.

Opalinus Clay (887.94 – 779.26 m)

The *lower boundary* of the Opalinus Clay is set at 887.94 m at the uppermost surface of a slightly bioclastic calcareous marl interval from the underlying Staffelegg Formation, which is covered by claystone (silty, micaceous and slightly calcareous) (*cf.* Dossier III). The lithological boundary is therefore evident above all in the carbonate content (TCarb: Figs. 3-2 and 3-4). The value decreases from 66 wt.-%, measured from the uppermost sample (887.98 m) of the Gross Wolf Member, to values between 9 and 11 wt.-% in the basal Opalinus Clay (Fig. 3-2). The lithological change between the Gross Wolf Member and the Opalinus Clay is also visible in the slight increase in TOC from values < 0.5 wt.-% to values around 1 wt.-% in the Opalinus Clay (Fig. 3-5).

The described ammonites (Section 3.2, Appendices A2 and A3) document, within the resolution of the biostratigraphy, that the lithological boundary coincides with the Toarcian / Aalenian stage boundary. The uppermost ammonite (*Pleydellia ex gr. buckmani*) from the Gross Wolf Member (depth: 888.02 m) yields Aalensis Zone (Torulosum Subzone). The lowermost sampled ammonite from the Opalinus Clay (depth: 874.91 m) can be determined as a *Leioceras ex gr. opalinum* and yields Opalinum Zone (Opalinum Subzone). However, the lowermost provisionally determined *Leioceras* sp. was found at 887.10 m (Appendix A3) and therefore just 0.84 m above the lithological boundary in the Opalinus Clay. The palynosample from 880.18 m also yields Opalinum Zone (Opalinum Subzone).

The *upper boundary* of the Opalinus Clay is set at 779.26 m at the base of a heterogeneous succession of light to medium grey slightly iron-oolitic bioclastic limestone and limonitic and iron-oolitic bioclastic calcareous marl with encrusted iron-oolitic intraclasts (*cf.* Dossier III). The boundary at 779.26 m documents a clear change in lithology, which is evident, for example, in the markedly higher carbonate content (TCarb) and is also supported by the analysis of FMI and GR logs.

In STA3-1 no ammonites were determined from the upper part of the Opalinus Clay. However, the two palynological samples, taken from the uppermost part of the Opalinus Clay at 787.31 m and 786.21 m, document with the occurrence of subspecies of *Nannoceratopsis plegas* and the increase in diversity of *Nannoceratopsis* species in general a typical age close to the top of the

Opalinum Subzone of the Opalinum Zone. The sample at 787.31 m (just above the uppermost calcareous bed) additionally shows, with the abundant occurrence of *Batiacasphaera* sp. A, an assemblage, which is typical for the Bifidatum Subzone of the Opalinum Zone. From the lowermost bioclastic (echinoderm) limestone bed (779.24 m) from the hanging succession a *Leioceras?* sp. was recovered. However, the ammonite is not very indicative. The palynosample taken from the same ammonite sample yields already Murchisonae Zone. This age is also supported by a slightly higher recovered *Staufenia?* sp. at 778.54 m.

The positive chemostratigraphic shift or even jump in the organic C-isotopes, just below and within the uppermost calcareous bed (786.37 – 786.30 m), is typical for the Bifidatum Subzone of the Opalinum Zone (e.g. BUL1-1; Wohlwend et al. 2021a). The additional shift to even more positive $\delta^{13}\text{C}_{\text{org}}$ values at and above the lithological boundary also fits to similar shifts found in the same biostratigraphic intervals. Although, in BUL1-1 the basal succession of the hanging «Murchisonae-Oolith Formation» is very condensed and therefore, the positive shift or trend is more compressed to a peak (Wohlwend et al. 2021a).

«Murchisonae-Oolith Formation» (779.26 – 764.97 m)

The *lower boundary* of the «Murchisonae-Oolith Formation» is set at 779.26 m at the base of a heterogenous succession of light to medium grey slightly iron-oolitic bioclastic limestone and limonitic and iron-oolitic bioclastic calcareous marl with encrusted iron-oolitic intraclasts (*cf.* Dossier III). This succession overlies typical clay-rich sediments from the Opalinus Clay and therefore, documents a clear change in lithology; see above for the detailed discussion about this boundary (upper boundary Opalinus Clay).

The *upper boundary* of the «Murchisonae-Oolith Formation», is defined at the subface of the «Sowerbyi-Oolith», which is per definition (Bloos et al. 2005) the basal bed of the hanging Wedelsandstein Formation (deposited during the Discites Zone). The 15 cm thick bed between 764.97 m and 764.82 m ("Austernbank" *cf.* Dossier III), with large oysters and scattered iron-oolids, seems to correlate with the "Austernpflaster" of Weiach (539.17 – 538.85 m; Matter et al. 1988, Beilage 6.2b and Bläsi et al. 2012). Both event-beds can likely be linked to the «Sowerbyi-Oolith». Therefore, the top of the «Murchisonae-Oolith Formation» is set at 764.97 m.

The lower age of the «Murchisonae-Oolith Formation» is defined by palynomorphs and ammonites as Murchisonae Zone (see discussion above). An additional ammonite from 776.94 m (*Staufenia* ex gr. *staufensis*) yields Bradfordensis Subzone of the Bradfordensis Zone. In the middle and upper part of the formation no other ammonites were found. Therefore, the biostratigraphic interpretation in this succession is based only on palynomorphs. The palynosample, taken with the ammonite at 776.94 m, also yields Bradfordensis Zone. The same ammonite zonation is also assigned to the following two palynosamples (774.96 m and 769.79 m). The uppermost sample at 766.62 m is dated as Concavum Zone to questionably Discites Zone. Only the sample in the hanging part of the possible «Sowerbyi-Oolith» at 764.68 m is clearly younger and is dated as Ovale Zone (Early Bajocian).

Wedelsandstein Formation (764.97 – 742.00 m)

The *lower boundary* of the Wedelsandstein Formation is set at the subface of the 15 cm thick oyster bearing bed (764.97 – 764.82 m), which is believed to correspond to the «Sowerbyi-Oolith» and therefore defines the base of the Wedelsandstein Formation (German Stratigraphic Scheme; Bloos et al. 2005). See more detailed discussion for the boundary above (upper boundary of the «Murchisonae-Oolith Formation»).

The *upper boundary* of the Wedelsandstein Formation is set at 742.00 m at the base of an argillaceous siltstone with the lowermost occurrence of coral fragments and clasts of bioclastic limestone, itself containing coral debris (*cf.* Dossier III). The normally following «Humphriesioolith Formation» in the hanging of the Wedelsandstein Formation was not defined here in STA3-1, as no lithological evidence (neither iron-oids, nor limonitic components) was found for it. In STA3-1, the 22.97 m thick siliciclastic formation is directly overlain by a mainly coralligenous sequence (biohermal limestone) with some intercalated bioclastic limestone intervals. The very calcareous succession was introduced in BUL1-1 by the new informal stratigraphic term «Herrenwis Unit» with an undefined stratigraphic rank.

As already mentioned above (Section 3.4), the Wedelsandstein Formation can be subdivided into a lower increasingly more calcareous interval (764.97 – 760.73 m) including a hardground at the top (760.98 – 760.73 m) and an upper marlier part from 760.73 m to the top at 742.00 m. Both intervals show a nice increase in the TCarb data upsection. The age of the two subintervals and therefore the whole Wedelsandstein Formation was dated by palynomorphs only because no ammonites were found. The lower subinterval until the hardground can be dated as Ovale Zone with two palynosamples (764.68 m and 761.56 m). The upper subinterval was deposited during the Laeviuscula Zone (palynosamples at 760.65 m, 750.42 m and 742.33 m).

«Herrenwis Unit» (742.00 – 701.65 m)

The *lower boundary* of the informal «Herrenwis Unit» is set at 742.00 m at the base of an argillaceous siltstone with the lowermost occurrence of coral fragments and clasts of bioclastic limestone, itself containing coral debris (*cf.* Dossier III). As mentioned just above, the normally following «Humphriesioolith Formation» in the hanging side of the Wedelsandstein Formation was not defined. In STA3-1, as well as in BUL1-1, the following sedimentary succession consists mainly of coral bioherm, reef detritus and crinoidal limestone. This succession corresponds to the new informal «Herrenwis Unit» (introduced in BUL1-1; Jordan et al. 2021).

The *upper boundary* is set at 701.65 m, at the top of the limonitic stromatolitic crust covering the uppermost coral bearing biohermal limestone (platestone). The hardground itself is covered by a 2 cm thick layer of claystone (silty, calcareous), followed by a limestone bed with calcitic and limonitic iron-oids (701.63 – 701.55 m; see also thin section STA3-1-701.59). Both lithological boundaries (*lower* and *upper boundary*) are solely based on lithological criteria.

The age of the «Herrenwis Unit» in STA3-1 is mainly defined by 10 palynomorph samples taken from marlier interlayers and can be divided into three palynological intervals. The succession itself is overlying the Wedelsandstein Formation, which is dated in the uppermost part (742.33 m) to Laeviuscula Zone. The lower interval of the «Herrenwis Unit» (741.99 – 736.02 m) is dated by 5 samples as Sauzei Zone. The middle interval (729.98 – 727.06 m), is interpreted Sauzei to Humphriesianum Zone. The upper interval (714.37 – 705.02 m) is interpreted as Humphriesianum Zone.

The additional four samples (720.09 m, 703.71 m, 701.79 m and 701.66 m) from the stratigraphic succession from the «Herrenwis Unit» were taken to check for possible infilling of younger sediments. At 720.54 m and at 720.09 m, a greyish-green claystone can be observed between corals (*cf.* Dossier II). The latter at 720.09 m was sampled and prepared for palynological analysis. The found assemblage (see Section 3.3) is very different with a mixture of dinoflagellate cyst assemblages of different age. Constraining the age of the sample is difficult. There are a few specimens of taxa that are restricted to the Early Bajocian, but most taxa recorded are typical for a Late Bajocian or somewhat younger age, with some of them having an LAD in the Early Bathonian Zigzag Zone. The sample is interpreted to range from possibly Humphriesianum Zone

to Zigzag Zone, with most constituents indicating Parkinsoni Zone. The claystone, filling the coral space, is clearly showing a younger age than the samples below (727.06 m) and above (714.37 m).

At depth 703.71 m a special greenish slightly bioclastic sediment also appears to fill a former cavity (nicely visible on the planar core picture; cf. Dossier II). The next higher sample at 701.79 m (a greyish, slightly bioclastic marl; cf. Dossier II) again appears to fill a cavity, which may have been formed by dissolution processes of former corals. The top sample at 701.66 m contains the limonitic stromatolitic crust at the top of the succession. All three samples (703.71 m, 701.79 m and 701.66 m) show rich and diverse dinoflagellate cyst assemblages. In all three samples there are some unexpected occurrences that are in conflict with the age suggested by the majority of taxa (see Section 3.3). Based on the majority of taxa recorded, the assemblages in this interval correspond best to the Parkinsoni Zone. Conflicting with this age assignment are the odd occurrences of taxa with an FAD in the Zigzag Zone and of taxa with their main distribution or LADs in the Early Bajocian. The sample 703.71 m, for example, contains among others *Dissilodinium giganteum* and *Hystrichodinium?* sp. indicating an Early Bajocian age as well as a questionable *Ctenidodinium combazii* with its FAD in the Zigzag Zone. The sample at 701.79 m shows even a more diverse assemblage with *Cavatodissilodinium* spp., *Lithodinia* spp. and *Tubotuberella dangeardii* with a FAD in the Zigzag Zone. However, in the sample above at 701.66 m again a dinoflagellate cyst assemblage with the main distribution or LADs in the Early Bajocian is present (*Nannoceratopsis plegas plegas*).

The deposition of the upper part of the coral bearing biohermal limestone seems to have taken place during the Humphriesianum Zone. The end of coral growth seems to coincide with the end of the Humphriesianum Zone. There is no documented younger age from the coral limestone succession. Thereafter, nothing is deposited above it for a long time, which is shown by the limonitic stromatolitic hardground. The sample taken from cavities between corals and possibly in previously dissolved corals at the top document unexpected occurrences of dinoflagellate cysts. Therefore, an infilling seems to happen during the Parkinsoni Zone as well as minor during the Zigzag Zone, or only during the Zigzag Zone with reworking of older sediments mainly from the Parkinsoni Zone as well as from Early Bajocian. Sedimentation in the hanging side of the «Herrenwis Unit» probably resumes in the Zigzag Zone (palynosample at 701.38m). However, the 8 cm thick bed (701.63 – 701.55 m) with calcitic and limonitic iron-ooids, which is below that following palynosample, may still correspond to the «Parkinsoni-Oolith», although an exact dating with ammonites and or palynomorphs is not available. The truncated ammonite from the base of that bed (depth 701.64 m) was not preserved well enough.

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 (26.08.2021). Therefore, the present report complements the lithostratigraphic report of Dossier III for the deep borehole Stadel-3-1. 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 STA3-1 (1'212.35 – 520.56 m)	A-2
Appendix A2:	List of all sampled ammonites from STA3-1 (914.00 – 693.49 m)	A-3
Appendix A3:	List of other provisionally determined conspicuous macrofossils from STA3-1 (920.62 – 693.82 m)	A-4
Appendix A4:	List of all palynological samples from STA3-1 (888.38 – 695.46 m)	A-5

Appendix A1: List of all thin sections from STA3-1 (1'212.35 – 520.56 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
520.54	520.58	520.56	«Felsenkalk» + «Massenkalk»	20.04.2021	STA3-1-520.56-TS
532.78	532.82	532.80	Schwarzbach Fm.	20.04.2021	STA3-1-532.80-TS
652.81	652.85	652.83	Wildeggen Fm.	20.04.2021	STA3-1-652.83-TS
695.98	696.01	696.00	Wildeggen Fm.	07.05.2021	STA3-1-696.00-TS
696.03	696.07	696.05	Wutach Fm.	07.05.2021	STA3-1-696.05-TS
696.08	696.12	696.10	Wutach Fm.	07.05.2021	STA3-1-696.10-TS
701.57	701.61	701.59	«Parkinsoni-Württembergica-Sch.»	26.05.2021	STA3-1-701.59-TS
701.65	701.69	701.67	«Herrenwis Unit»	26.05.2021	STA3-1-701.67-TS
719.46	719.50	719.48	«Herrenwis Unit»	26.05.2021	STA3-1-719.48-TS
723.44	723.48	723.46	«Herrenwis Unit»	26.05.2021	STA3-1-723.46-TS
729.37	729.41	729.39	«Herrenwis Unit»	26.05.2021	STA3-1-729.39-TS
737.02	737.06	737.04	«Herrenwis Unit»	26.05.2021	STA3-1-737.04-TS
741.82	741.86	741.84	«Herrenwis Unit»	26.05.2021	STA3-1-741.84-TS
742.00	742.04	742.02	Wedelsandstein Fm.	26.05.2021	STA3-1-742.02-TS
760.78	760.82	760.80	Wedelsandstein Fm.	11.05.2021	STA3-1-760.80-TS
762.42	762.46	762.44	Wedelsandstein Fm.	11.05.2021	STA3-1-762.44-TS
764.84	764.88	764.86	Wedelsandstein Fm.	11.05.2021	STA3-1-764.86-TS
765.92	765.96	765.94	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-765.94-TS
767.42	767.46	767.44	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-767.44-TS
767.74	767.78	767.76	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-767.76-TS
776.98	777.02	777.00	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-777.00-TS
777.81	777.85	777.83	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-777.83-TS
778.64	778.68	778.66	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-778.66-TS
786.30	786.34	786.32	Opalinus Clay	11.05.2021	STA3-1-786.32-TS
794.93	794.97	794.95	Opalinus Clay	11.05.2021	STA3-1-794.95-TS
799.34	799.38	799.36	Opalinus Clay	18.05.2021	STA3-1-799.36-TS
803.83	803.87	803.85	Opalinus Clay	18.05.2021	STA3-1-803.85-TS
848.28	848.32	848.30	Opalinus Clay	18.05.2021	STA3-1-848.30-TS
872.90	872.94	872.92	Opalinus Clay	18.05.2021	STA3-1-872.92-TS
914.75	914.79	914.77	Staffellegg Fm.	18.05.2021	STA3-1-914.77-TS
915.81	915.85	915.83	Staffellegg Fm.	18.05.2021	STA3-1-915.83-TS
935.25	935.29	935.27	Klettgau Fm.	20.07.2021	STA3-1-935.27-TS
936.40	936.43	936.42	Klettgau Fm.	20.07.2021	STA3-1-936.42-TS
938.00	938.04	938.02	Klettgau Fm.	20.07.2021	STA3-1-938.02-TS
944.43	944.47	944.45	Klettgau Fm.	20.07.2021	STA3-1-944.45-TS
946.87	946.90	946.88	Klettgau Fm.	20.07.2021	STA3-1-946.88-TS
950.63	950.67	950.65	Klettgau Fm.	20.07.2021	STA3-1-950.65-TS
954.77	954.80	954.79	Bänkerjoch Fm.	06.07.2021	STA3-1-954.79-TS
964.42	964.45	964.44	Bänkerjoch Fm.	06.07.2021	STA3-1-964.44-TS
983.70	983.73	983.72	Bänkerjoch Fm.	06.07.2021	STA3-1-983.72-TS
999.10	999.13	999.12	Bänkerjoch Fm.	06.07.2021	STA3-1-999.12-TS
1'008.94	1'008.97	1'008.96	Bänkerjoch Fm.	06.07.2021	STA3-1-1008.96-TS
1'018.97	1'019.00	1'018.99	Bänkerjoch Fm.	06.07.2021	STA3-1-1018.99-TS
1'039.76	1'039.80	1'039.78	Schinzach Fm.	20.07.2021	STA3-1-1039.78-TS
1'047.74	1'047.78	1'047.76	Schinzach Fm.	20.07.2021	STA3-1-1047.76-TS
1'095.80	1'095.84	1'095.82	Schinzach Fm.	20.07.2021	STA3-1-1095.82-TS
1'107.35	1'107.39	1'107.37	Zeglingen Fm.	20.07.2021	STA3-1-1107.37-TS
1'212.33	1'212.37	1'212.35	Kaiseraugst Fm.	22.07.2021	STA3-1-1212.35-TS

Appendix A2: List of all sampled ammonites from STA3-1 (914.00 – 693.49 m)

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

Top [m]	Bottom [m]	Sample depth [m]	Formation	Retrieval date [dd.mm.yyyy]	Sample ID
693.46	693.49	693.49	Wildegge Fm.	07.05.2021	STA3-1-693.49-BS(MF)
694.82	694.84	694.82	Wildegge Fm.	07.05.2021	STA3-1-694.82-BS(MF)
696.27	696.32	696.29	Wutach Fm.	07.05.2021	STA3-1-696.29-BS(MF)
696.33	696.39	696.35	Wutach Fm.	07.05.2021	STA3-1-696.36-BS(MF)
698.32	698.355	698.35	Wutach Fm.	07.05.2021	STA3-1-698.34-BS(MF)
701.61	701.64	701.64	«Parkinsoni-Württemb.-Sch.»	26.05.2021	STA3-1-701.64-BS(MF)
776.92	776.96	776.94	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-776.94-BS(MF)
777.68	777.72	777.72	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-777.70-BS(MF)
778.52	778.56	778.55	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-778.54-BS(MF)
779.22	779.26	779.24	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-779.24-BS(MF)
871.56	871.59	871.56	Opalinus Clay	11.05.2021	STA3-1-871.56-BS(MF)
874.89	874.91	874.91	Opalinus Clay	11.05.2021	STA3-1-874.91-BS(MF)
887.99	888.02	888.02	Staffelegg Fm.	18.05.2021	STA3-1-888.02-BS(MF)
888.36	888.39	888.36	Staffelegg Fm.	18.05.2021	STA3-1-888.36-BS(MF)
889.09	889.12	889.12	Staffelegg Fm.	18.05.2021	STA3-1-889.12-BS(MF)
892.72	892.77	892.74	Staffelegg Fm.	18.05.2021	STA3-1-892.74-BS(MF)
913.97	914.05	914.00	Staffelegg Fm.	18.05.2021	STA3-1-914.00-BS(MF)

Appendix A3: List of other provisionally determined conspicuous macrofossils from STA3-1 (920.62 – 693.82 m)

Top [m]	Bottom [m]	Fossil	Determination (provisional)
693.82		Ammonite	<i>Glochiceras</i> sp.
695.42		Ammonite	<i>Perisphinctes</i> sp.
695.69		Fragments of Ammonites	<i>Perisphinctes</i> sp., <i>Taramelliceras</i> sp.
695.79		Ammonite	<i>Euaspidoceras</i> sp.
696.13		Brachiopode	<i>Aulacothyris</i> sp.
728.55		Bivalve	<i>Trichites</i> sp.
761.12		Oyster	indet.
764.98		Oysters	<i>Gryphaea</i> sp.
777.93		Ammonite	indet.
778.05		Ammonite	indet.
795.28		Belemnite	Belemnite indet.
798.60		Belemnite	Belemnite indet.
843.76		Fragment of Ammonite	<i>Leioceras</i> sp.
871.14		Ammonite	<i>Leioceras subglabrum</i>
879.30		Ammonite	<i>Leioceras</i> sp.
887.10		Ammonite	<i>Leioceras</i> sp.
888.18		Ammonite	Ammonite indet.
888.22		Ammonite	<i>Pleydellia</i> sp.
888.40		Ammonite	<i>Pleydellia</i> ex gr. <i>aalensis</i>
888.96		Ammonite	<i>Pleydellia</i> sp.
895.41		Bivalve	<i>Pseudomytiloides dubius</i>
899.81		Ammonite	<i>Amaltheus</i> sp. ?
920.62		Wood	indet.

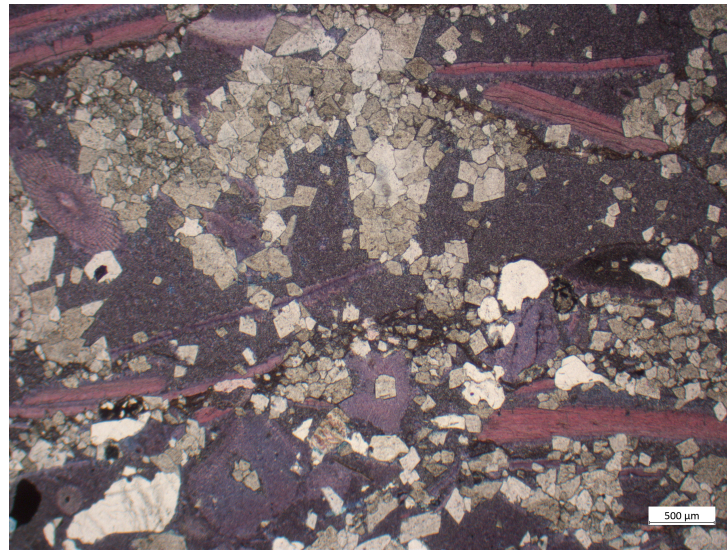
Appendix A4: List of all palynological samples from STA3-1 (888.38 – 695.46 m)

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
695.45	695.47	695.46	Wildegge Fm.	07.05.2021	STA3-1-695.46-BS(PA)
695.98	696.01	696.00	Wildegge Fm.	07.05.2021	STA3-1-696.00-BS(PA)
696.08	696.12	696.10	Wutach Fm.	07.05.2021	STA3-1-696.10-BS(PA)
696.27	696.32	696.29	Wutach Fm.	07.05.2021	STA3-1-696.29-BS(PA)
699.21	699.23	699.22	Wutach Fm.	07.05.2021	STA3-1-699.22-BS(PA)
699.73	699.75	699.74	Variansmergel Fm.	07.05.2021	STA3-1-699.74-BS(PA)
701.37	701.39	701.38	Variansmergel Fm.	07.05.2021	STA3-1-701.38-BS(PA)
701.63	701.65	701.64	«Parkinsoni-Württemb.-Sch.»	26.05.2021	STA3-1-701.64-BS(PA)
701.65	701.66	701.66	«Herrenwis Unit»	03.06.2021	STA3-1-701.66-BS(PA)
701.78	701.80	701.79	«Herrenwis Unit»	03.06.2021	STA3-1-701.79-BS(PA)
703.70	703.72	703.71	«Herrenwis Unit»	03.06.2021	STA3-1-703.71-BS(PA)
705.00	705.03	705.02	«Herrenwis Unit»	18.05.2021	STA3-1-705.02-BS(PA)
708.22	708.24	708.23	«Herrenwis Unit»	18.05.2021	STA3-1-708.23-BS(PA)
714.36	714.38	714.37	«Herrenwis Unit»	18.05.2021	STA3-1-714.37-BS(PA)
720.08	720.10	720.09	«Herrenwis Unit»	03.06.2021	STA3-1-720.09-BS(PA)
727.04	727.07	727.06	«Herrenwis Unit»	18.05.2021	STA3-1-727.06-BS(PA)
729.96	729.99	729.98	«Herrenwis Unit»	03.06.2021	STA3-1-729.98-BS(PA)
736.00	736.04	736.02	«Herrenwis Unit»	18.05.2021	STA3-1-736.02-BS(PA)
736.04	736.07	736.06	«Herrenwis Unit»	18.05.2021	STA3-1-736.06-BS(PA)
736.47	736.50	736.49	«Herrenwis Unit»	03.06.2021	STA3-1-736.49-BS(PA)
741.40	741.42	741.41	«Herrenwis Unit»	18.05.2021	STA3-1-741.41-BS(PA)
741.98	742.00	741.99	«Herrenwis Unit»	03.06.2021	STA3-1-741.99-BS(PA)
742.32	742.34	742.33	Wedelsandstein Fm.	18.05.2021	STA3-1-742.33-BS(PA)
750.41	750.43	750.42	Wedelsandstein Fm.	11.05.2021	STA3-1-750.42-BS(PA)
760.64	760.66	760.65	Wedelsandstein Fm.	11.05.2021	STA3-1-760.65-BS(PA)
761.55	761.57	761.56	Wedelsandstein Fm.	11.05.2021	STA3-1-761.56-BS(PA)
764.67	764.69	764.68	Wedelsandstein Fm.	11.05.2021	STA3-1-764.68-BS(PA)
766.61	766.63	766.62	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-766.62-BS(PA)
769.78	769.80	769.79	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-769.79-BS(PA)
774.94	774.97	774.96	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-774.96-BS(PA)
776.92	776.96	776.94	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-776.94-BS(PA)
779.22	779.26	779.24	«Murchisonae-Oolith Fm.»	11.05.2021	STA3-1-779.24-BS(PA)
786.20	786.22	786.21	Opalinus Clay	11.05.2021	STA3-1-786.21-BS(PA)
787.30	787.32	787.31	Opalinus Clay	11.05.2021	STA3-1-787.31-BS(PA)
796.26	796.28	796.27	Opalinus Clay	18.05.2021	STA3-1-796.27-BS(PA)
820.32	820.34	820.33	Opalinus Clay	18.05.2021	STA3-1-820.33-BS(PA)
839.99	840.01	840.00	Opalinus Clay	18.05.2021	STA3-1-840.00-BS(PA)
860.02	860.04	860.03	Opalinus Clay	18.05.2021	STA3-1-860.03-BS(PA)
880.17	880.19	880.18	Opalinus Clay	18.05.2021	STA3-1-880.18-BS(PA)
888.36	888.39	888.38	Staffellegg Fm.	18.05.2021	STA3-1-888.38-BS(PA)

Appendix B: Photos microfacies

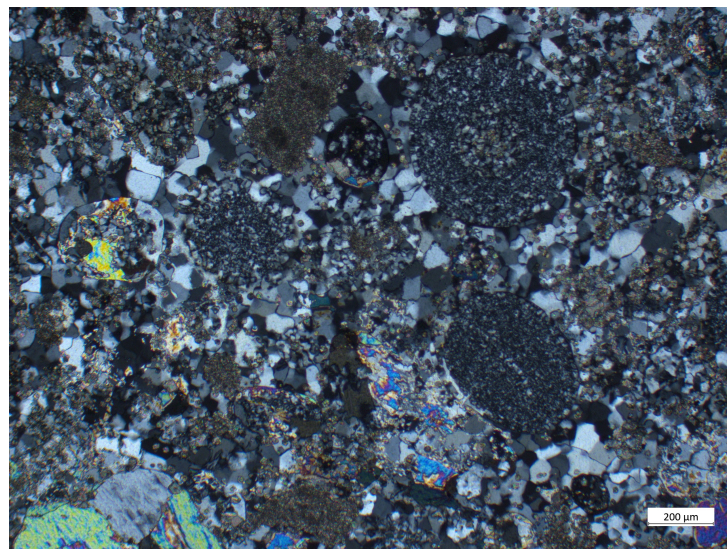
Fig. B-1:	Thin section STA3-1-1212.35, Kaiseraugst Fm.	B-2
Fig. B-2:	Thin section STA3-1-1107.37, Zeglingen Fm.	B-2
Fig. B-3:	Thin section STA3-1-1047.76, Schinznach Fm.	B-2
Fig. B-4:	Thin section STA3-1-1018.99, Bänkerjoch Fm.	B-3
Fig. B-5:	Thin section STA3-1-983.72, Bänkerjoch Fm.	B-3
Fig. B-6:	Thin section STA3-1-964.44, Bänkerjoch Fm.	B-3
Fig. B-7:	Thin section STA3-1-848.30, Opalinus Clay	B-4
Fig. B-8:	Thin section STA3-1-803.85, Opalinus Clay	B-4
Fig. B-9:	Thin section STA3-1-799.36, Opalinus Clay	B-4
Fig. B-10:	Thin section STA3-1-794.95, Opalinus Clay	B-5
Fig. B-11:	Thin section STA3-1-786.32, Opalinus Clay	B-5
Fig. B-12:	Thin section STA3-1-777.00, «Murchisonae-Oolith Fm.»	B-5
Fig. B-13:	Thin section STA3-1-767.76, «Murchisonae-Oolith Fm.»	B-6
Fig. B-14:	Thin section STA3-1-764.68, Wedelsandstein Fm.	B-6
Fig. B-15:	Thin section STA3-1-723.46, «Herrenwis Unit»	B-6
Fig. B-16:	Thin section STA3-1-723.46, «Herrenwis Unit»	B-7
Fig. B-17:	Thin section STA3-1-719.48, «Herrenwis Unit»	B-7
Fig. B-18:	Thin section STA3-1-701.67, «Herrenwis Unit»	B-7
Fig. B-19:	Thin section STA3-1-701.67, «Herrenwis Unit»	B-8
Fig. B-20:	Thin section STA3-1-701.59, «Parkinsoni-Württembergica-Sch.» (most probably «Parkinsoni-Oolith»)	B-8
Fig. B-21:	Thin section STA3-1-696.10, Wutach Fm.	B-8

**Fig. B-1:**

Biotrititic limestone (dolomitic): bivalves (red) in a microsparitic matrix (violet) with dolomite rhombohedrons, arranged in clusters and scattered (light beige to white) and quartz grains (white)

Thin section photo,
TS stained for calcite = red

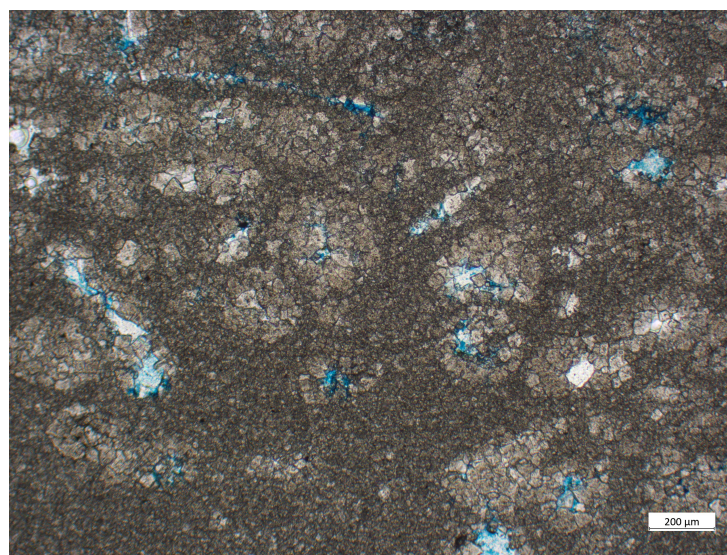
STA3-1-1212.35
Kaiseraugst Fm.

**Fig. B-2:**

Siliceous oolite: Ooids, consisting of fine-crystalline quartz (chalcedon) (grey), replacing primary calcite, and authigenic quartz cement (grey), as well as few anhydrite crystals (coloured)

Thin section photo, crossed nicols

STA3-1-1107.37
Zeglingen Fm.

**Fig. B-3:**

Dolomitic oolite (oolitic dolostone): dolomite replaces components (ooids and bivalves) as well as micrite matrix, and generates some porosity (bluish coloured glue within pores)

Thin section photo

STA3-1-1047.76
Schinznach Fm.

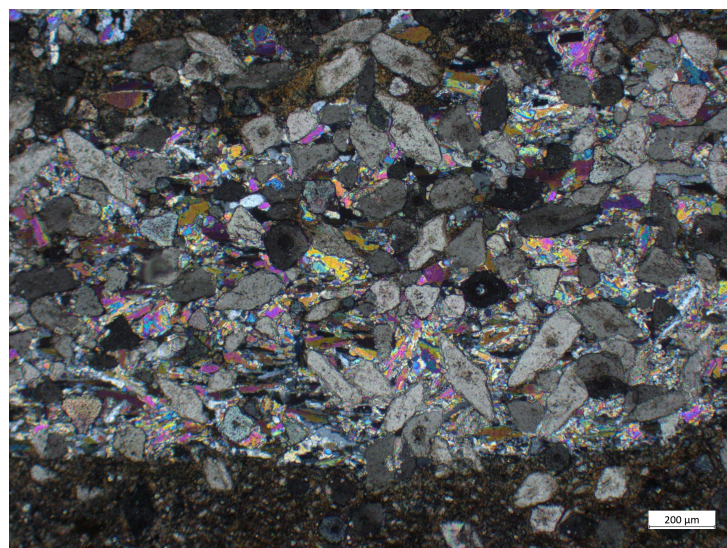
Selected photos of microfacies from Kaiseraugst Fm., Zeglingen Fm. and Schinznach Fm.

**Fig. B-4:**

Laminated limestone, consisting of rosettes (spheres) of calcite, pseudomorphs after twinned gypsum crystals

Thin section photo, crossed nicols

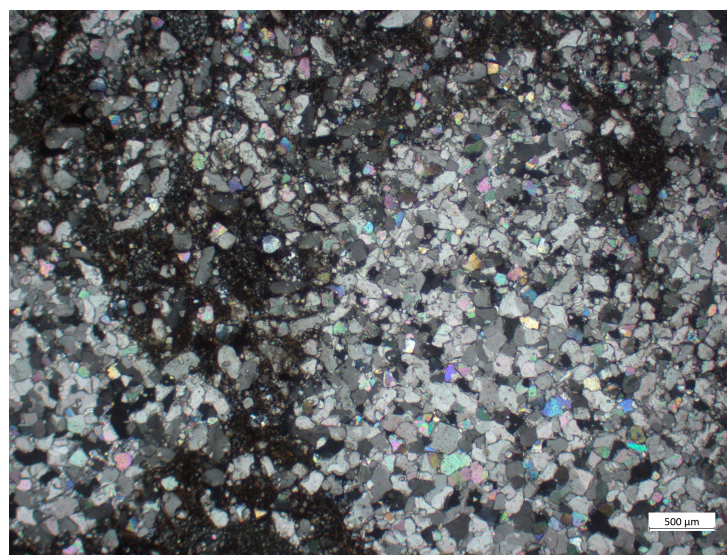
STA3-1-1018.99
Bänkerjoch Fm.

**Fig. B-5:**

Laminated dolomitic marl, consisting of elongated dolomite rhombohedrons, pseudomorph after single twinned gypsum crystals, with few anhydrite crystals (coloured) and claystone layers

Thin section photo, crossed nicols

STA3-1-983.72
Bänkerjoch Fm.

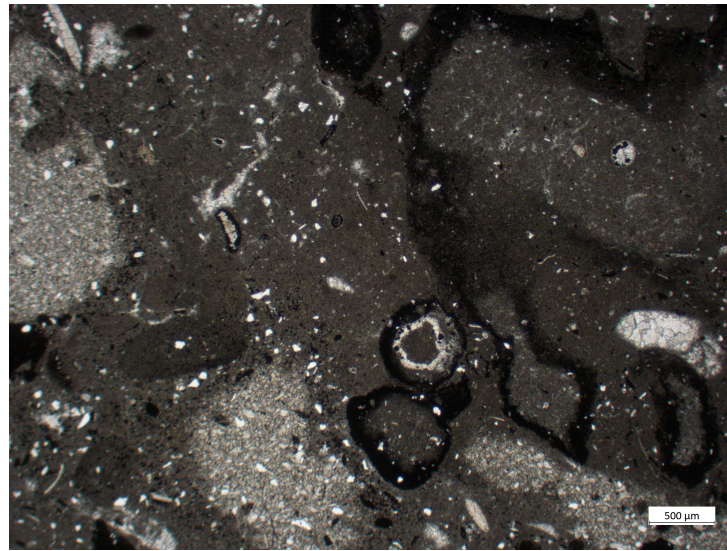
**Fig. B-6:**

Dolomite nodules, composed of small rhombohedral dolomite crystals and few anhydrite crystals; the nodules are embedded in a clay matrix

Thin section photo, crossed nicols

STA3-1-964.44
Bänkerjoch Fm.

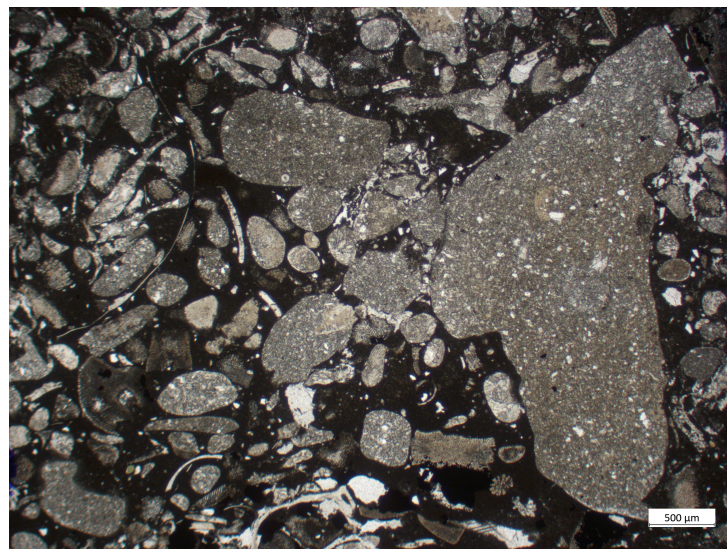
Selected photos of microfacies from Bänkerjoch Fm.

**Fig. B-7:**

"Hiatus bed" consisting of different nodules (few of "stellate calcite", few with pyrite rims) "grown" during diagenesis, as well as some quartz grains, bioclasts and clay matrix

Thin section photo

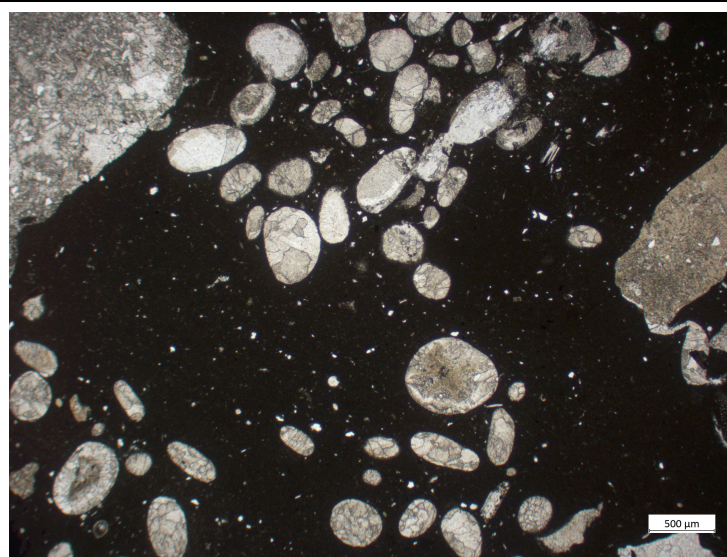
STA3-1-848.30
Opalinus Clay

**Fig. B-8:**

"Hiatus bed" (bioclastic limestone with nodules): Different diagenetic nodules, intraclasts, bioclasts and sideritic clay matrix

Thin section photo

STA3-1-803.85
Opalinus Clay

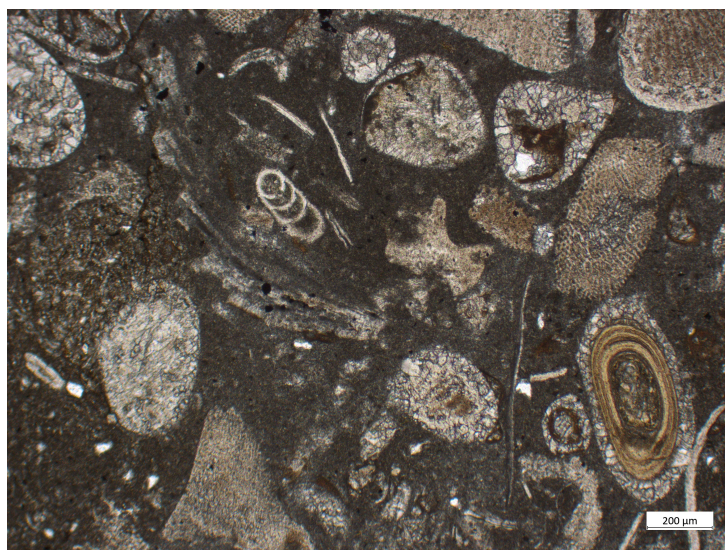
**Fig. B-9:**

Hardground:
Nodule with calcitic iron-ooids embedded in a clay matrix. The nodule also contains iron-stromatolitic flasers

Thin section photo

STA3-1-799.36
Opalinus Clay

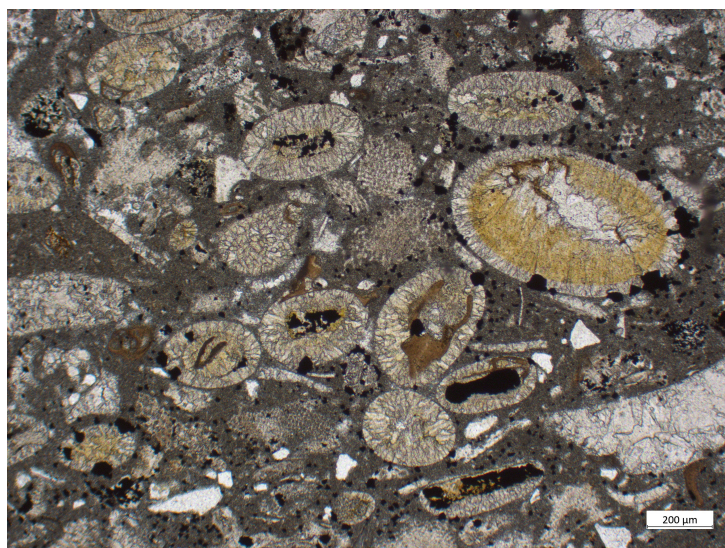
Selected photos of microfacies from Opalinus Clay

**Fig. B-10:**

Hardground: nodule with an iron-oid, some calcitic iron-oids and biogene components. The nodule is embedded in a silty, bioclastic, sideritic matrix with "stellate calcite"

Thin section photo

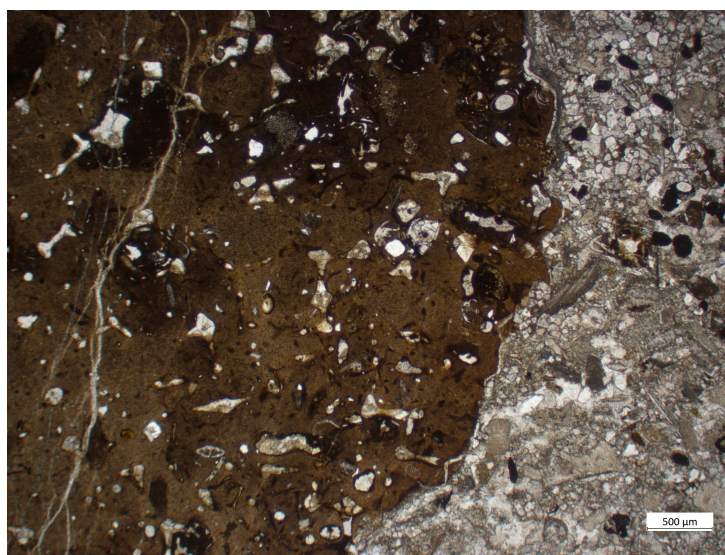
STA3-1-794.95
Opalinus Clay

**Fig. B-11:**

Hardground: bioclastic limestone (iron-oolitic); most of the iron-oids are, partly or totally, replaced by calcite or the original iron-oid has been compressed by the growing cement rim

Thin section photo

STA3-1-786.32
Opalinus Clay

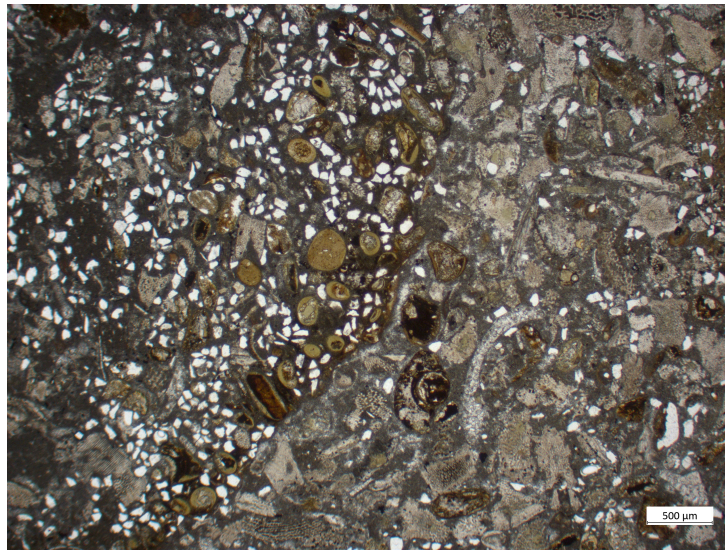
**Fig. B-12:**

Big limonitic sponge as component of a bioclastic limestone (iron-oolitic, sandy)

Thin section photo

STA3-1-777.00
«Murchisonae-Oolith Fm.»

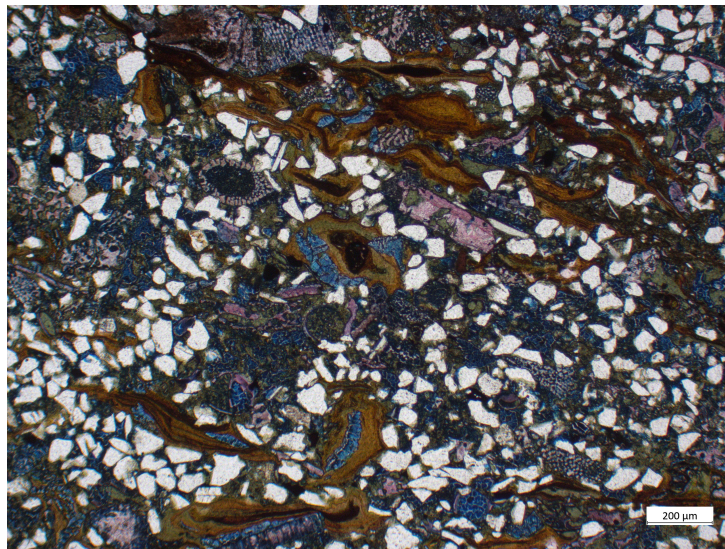
Selected photos of microfacies from Opalinus Clay and «Murchisonae-Oolith Fm.»

**Fig. B-13:**

On the left side limestone (sandy, bioclastic, iron-oolitic) as an intraclast in a bioclastic limestone (right side)

Thin section photo

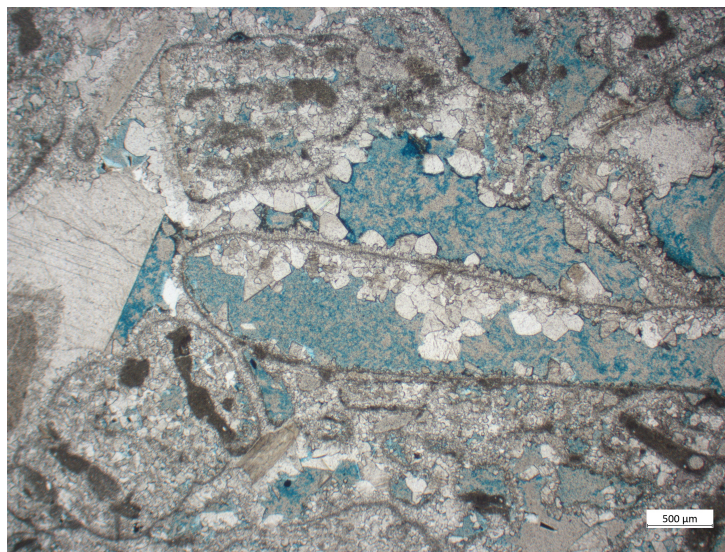
STA3-1-767.76
«Murchisonae-Oolith Fm.»

**Fig. B-14:**

Compressed iron-oids and iron-stromatolitic flasers in a bioclastic limestone (sandy)

Thin section photo
TS stained for calcite = red

STA3-1-764.68
Wedelsandstein Fm.

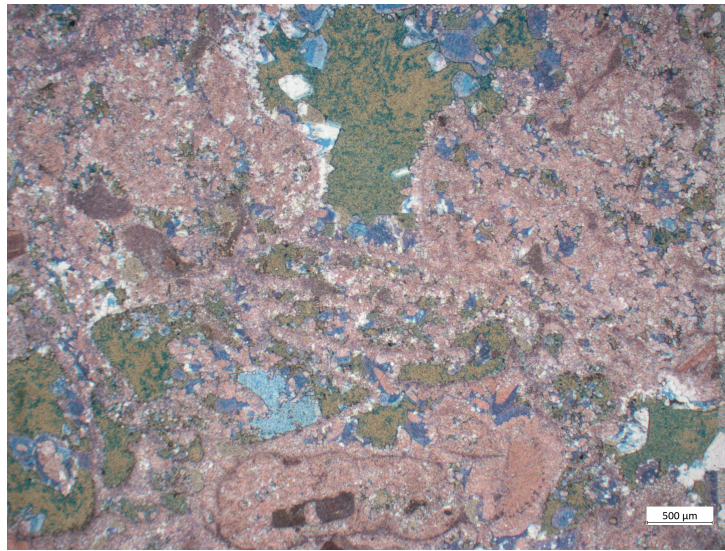
**Fig. B-15:**

Very porous bioclastic limestone, composed of coral- and bivalves-clasts. Both species are leached or partly leached, then – beginning at the rims – cemented, but only a part; so porosity remains (filled with blue coloured glue)

Thin section photo

STA3-1-723.46
«Herrenwis Unit»

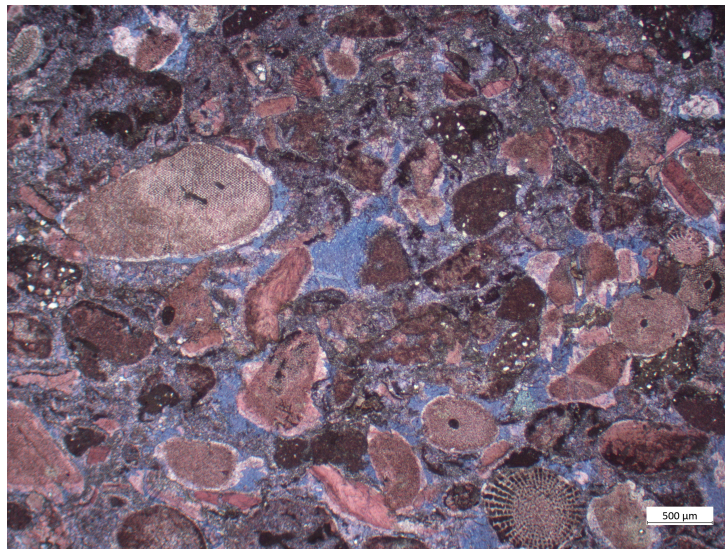
Selected photos of microfacies from «Murch.-Ool. Fm.», Wedelsand. Fm. and «Herrenwis Unit»

**Fig. B-16:**

Beautiful calcite cement crystals in the leached bivalves and corals: fine fibrous calcites on the rims and bigger to the centres; remaining porosity = brown glue

Thin section photo
TS stained for calcite = red

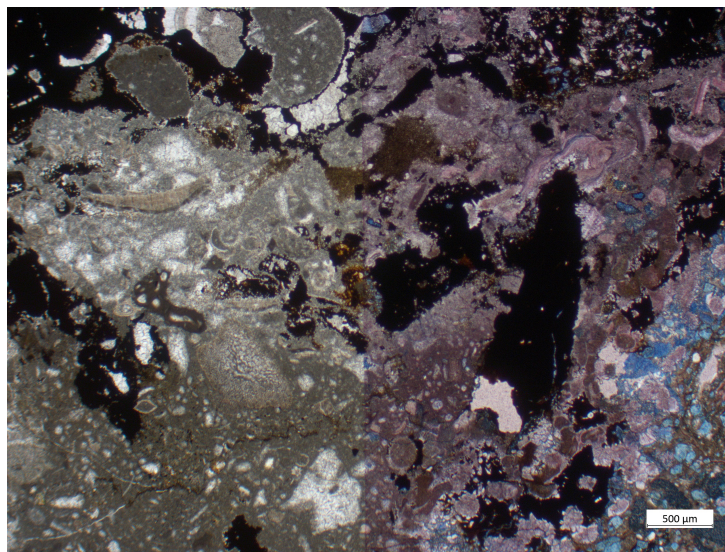
STA3-1-723.46 (same sample as above
«Herrenwis Unit»

**Fig. B-17:**

Bioclastic limestone: consisting mainly of echinoderm skeletal elements and microsparitic matrix

Thin section photo
TS stained for calcite=red

STA3-1-719.48
«Herrenwis Unit»

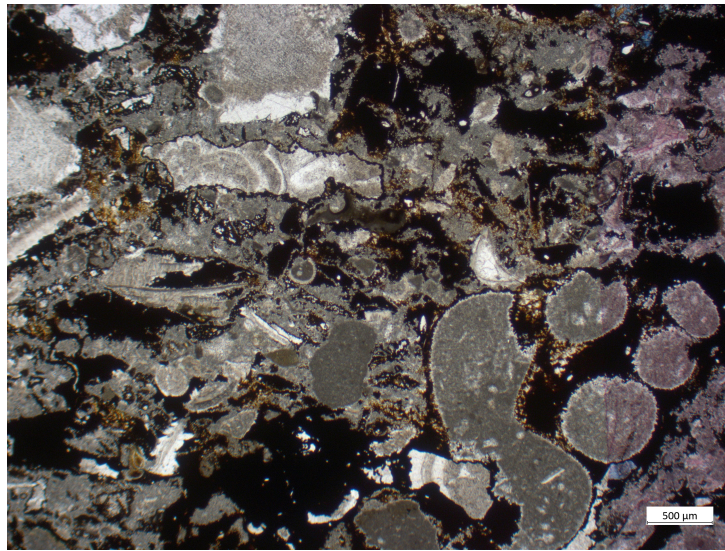
**Fig. B-18:**

Hardground: limonitic sediment and limonitic crust (uppermost part) on top of the coral bearing biohermal limestone (right bottom corner)

Thin section photo
TS stained for calcite = red (right half)

STA3-1-701.67
«Herrenwis Unit»

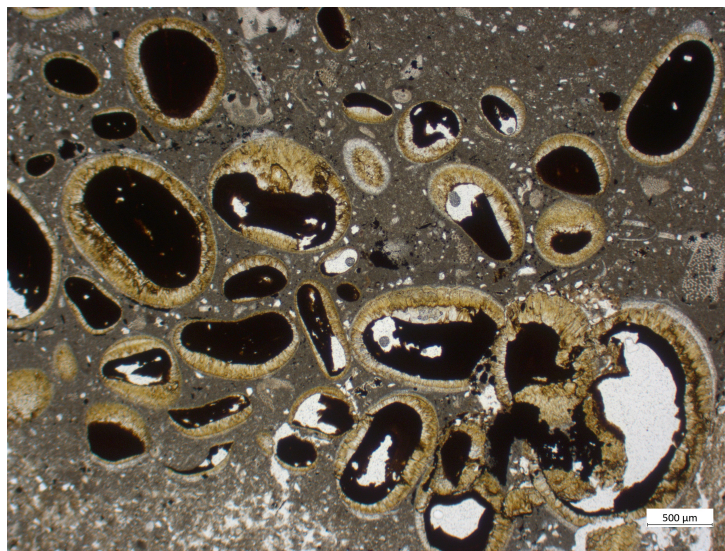
Selected photos of microfacies from «Herrenwis Unit»

**Fig. B-19:**

Detail of Fig. B-18:
bioclastic limestone
(limonitic), composed of
echinoderm skeletal
elements, clasts of bivalves
and corals and a gastropod
(right bottom corner)

Thin section photo

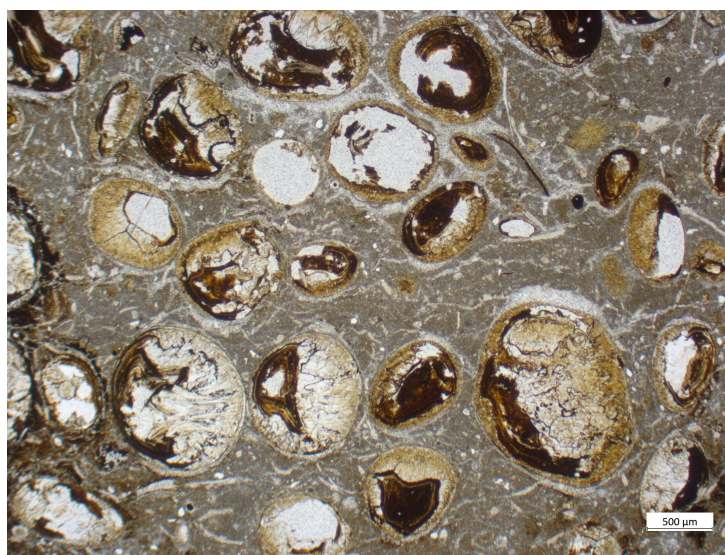
STA3-1-701.67
«Herrenwis Unit»

**Fig. B-20:**

Iron-oolite: iron-oolids with
limonitic cores and calcite
cement rims, and micrite
matrix; partly leached by
pressure-solution

Thin section photo
(white = holes, broke out
during thin-section prep.)

STA3-1-701.59
«Parkinsoni-
Württembergica-Sch.»
(most probably «Parkinsoni-
Oolith»)

**Fig. B-21:**

Iron-oolite: iron-oolids, partly
replaced by calcite,
sedimented with micrite
matrix

Thin section photo
(white = holes, broke out
during thin-section prep.)

STA3-1-696.10
Wutach Fm.

Selected photos of microfacies from «Herrenwis Unit», «Park.-Württ.-Sch.» and Wutach Fm.

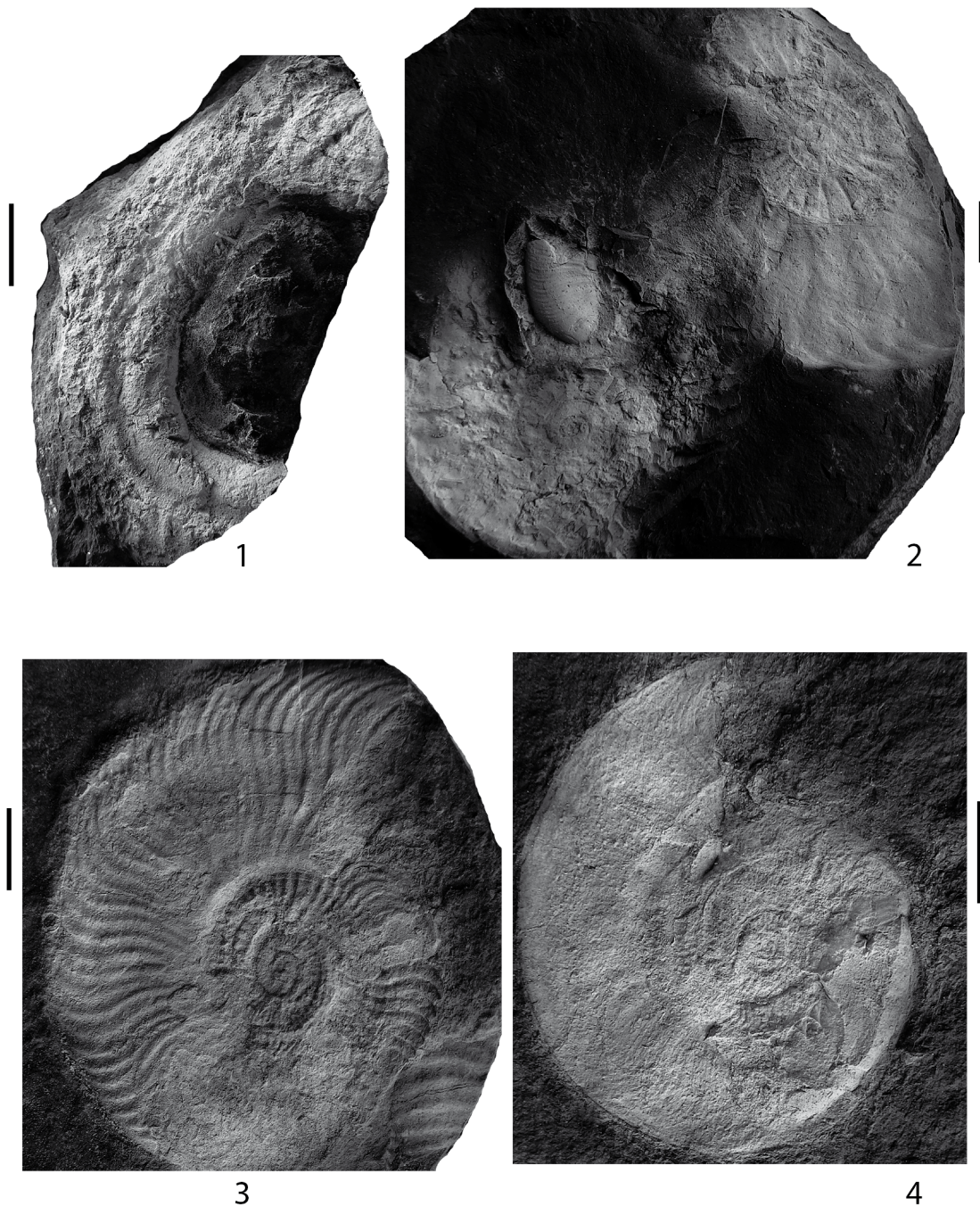
Appendix C: Plates of ammonites

Plate I:	STA3-1 (892.74 – 888.02 m).....	C-3
Plate II:	STA3-1 (874.91 – 776.94 m).....	C-5
Plate III:	STA3-1 (698.34 – 693.49 m).....	C-7

Plate I STA3-1 (892.74 – 888.02 m)

- Fig. 1: *Hildoceras* sp., depth: 892.74 m, Staffelegg Fm. (Gross Wolf Mb.), Variabilis Zone.
- Fig. 2: *Cotteswoldia* sp., three specimens, depth: 889.12 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, probably Aalensis Subzone.
- Fig. 3: *Cotteswoldia* ex gr. *lotharingica* (Branco, 1879) or *C. pseudolotharingica* (Maubeuge, 1950), depth: 888.36 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, Torulosum Subzone.
- Fig. 4: *Pleydellia* ex gr. *buckmani* (Maubeuge, 1947), depth: 888.02 m, Staffelegg Fm. (Gross Wolf Mb.), Aalensis Zone, Torulosum Subzone.

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



1cm

Plate II STA3-1 (874.91 – 776.94 m)

- Fig. 1: *Leioceras* ex gr. *opalinum* (Reinecke, 1818), microconch, depth: 874.91 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 2: *Leioceras* ex gr. *opalinum* (Reinecke, 1818), microconch, depth: 871.56 m, Opalinus Clay, Opalinum Zone, Opalinum Subzone.
- Fig. 3: *Staufenia*? sp., depth 778.54 m, «Murchisonae-Oolith Fm.», Murchisonae Zone ?
- Figs. 4a, 4b: *Staufenia* ex gr. *staufensis* (Oppel, 1856), depth: 776.94 m, «Murchisonae-Oolith Fm.», Bradfordensis Zone, Bradfordensis Subzone. Fig. 4a: lateral view, Fig. 4b: cross section.

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



Plate II: STA3-1 (874.91 – 776.94 m)

Plate III STA3-1 (698.34 – 693.49 m)

Figs. 1a, 1b: *Oecotraustes* sp., depth: 698.34 m, Wutach Fm., Bathonian. Fig. 1a: lateral view, Fig. 1b: cross section.

Figs. 2a, 2b: *Macrocephalites* sp., depth: 696.29 m, Wutach Fm., probably Early Callovian. Fig. 2a: lateral view, Fig. 2b: cross section.

Fig. 3: *Perisphinctes* sp., microconch, depth: 694.82 m, Wildegg Fm. (Effingen Mb.), Transversarium to Early Bifurcatus Zone.

Fig. 4: *Taramelliceras* ex gr. *dentostriatum* (Quenstedt, 1887), macroconch, depth: 693.49 m, Wildegg Fm. (Effingen Mb.), Transversarium Zone, Luciaeformis Subzone.

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

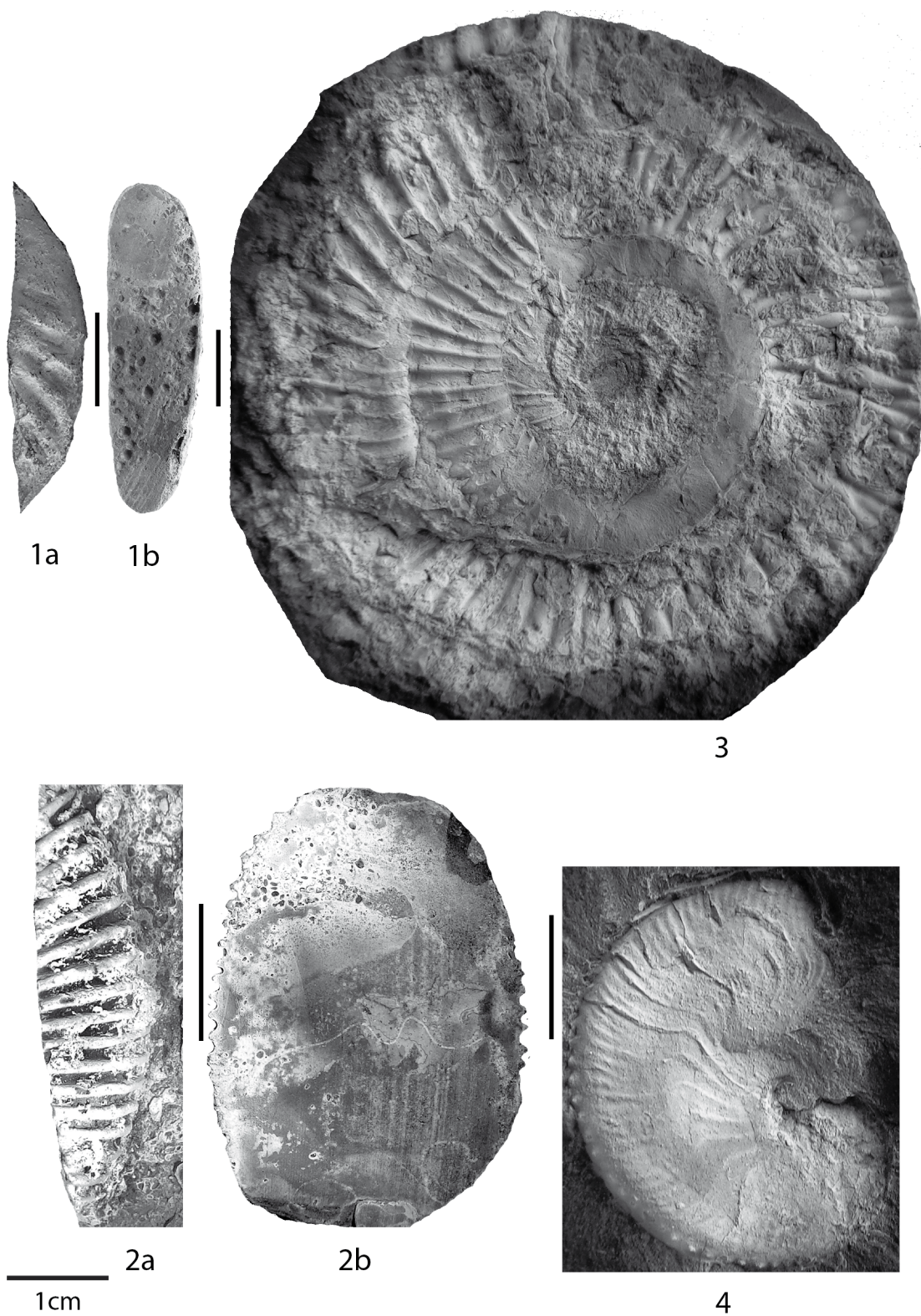


Plate III: STA3-1 (698.34 – 693.49 m)

Appendix D: Palynostratigraphy

Appendix D1: Range Chart: Quantitative stratigraphic distribution of Middle Jurassic palynomorphs in the Stadel-3-1 borehole

Appendix D2: Depth/Age plot: Stadel-3-1 borehole

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

Appendix E: Chemostratigraphy

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

Data are discussed in Section 3.4 and partly illustrated in Fig. 3-4 (part of the data points lie outside the presented scale for the $\delta^{13}\text{C}_{\text{carb}}$): HB: drilled from a "hiatus bed" (for definition of HB see Section 2.1), CC: drilled from a calcareous concretion, SC: drilled from a sideritic concretion or nodule, SN: drilled from a septarian nodule, MF: drilled from macrofossil, TS: drilled directly from thin section sample (see microfacies description in Section 3.1); The driftwood sample at 700.90 m (marked by an asterisk) is an organic measurement ($\delta^{13}\text{C}_{\text{org}}$).

Depth [m]	Description of sample		TS	$\delta^{13}\text{C}_{\text{carb}}$ [‰ VPDB]	$\delta^{18}\text{O}_{\text{carb}}$ [‰ VPDB]	Carbonate [wt.-%]
700.90	driftwood (organic sample) (8 cm)	MF		-22.45*		
701.59	iron-oolite, calcareous		×	-0.24	-1.78	67.9
717.99	echinoid spine	MF		1.42	-4.53	100.0
727.00	echinoid spine	MF		1.06	-6.29	100.0
751.97	sideritic concretion	SC		2.04	-0.31	41.4
754.71	sideritic concretion	SC		1.55	-0.53	42.7
757.61	sideritic concretion	SC		0.28	0.30	48.8
760.93	sandy limestone, bioclastic			0.46	-2.14	71.2
776.01	bioclastic limestone			-0.36	-2.14	79.9
777.00	bioclastic limestone, iron-oolitic		×	0.45	-1.92	73.6
778.50	sandy limestone, bioclastic			-3.99	-3.26	78.1
786.32	bioclastic limestone, iron-oolitic		×	-1.66	-4.70	81.5
794.87	calcareous nodule	CC		-19.39	-2.74	76.3
794.97	bioclastic limestone (argillaceous)		×	-0.89	-3.07	77.3
795.01	septarian nodule	SN		-7.29	-1.14	83.9
795.03	calcite vein from the same SN	SN		-3.06	-6.77	100.0
795.68	calcareous concretion	CC		-20.73	-2.80	74.6
795.80	septarian nodule	SN		-20.69	-1.18	85.0
796.02	septarian nodule	SN		-16.38	-0.97	88.7
796.02	calcite vein from the same SN	SN		-2.44	-8.12	100.0
799.17	calcareous marl			-4.75	-1.63	57.1
799.30	micrite with calcitic or iron-oolids?			-5.60	-1.71	78.1
799.36	limestone, iron-oolitic		×	-5.60	-4.05	69.6
801.08	calcareous nodule	CC		-19.71	-1.21	77.4
803.85	bioclastic limestone		×	-3.93	-4.46	69.7
806.53	sideritic concretion	SC		-0.68	-0.96	50.4
848.30	nodular, calcareous and sideritic bed	CC	×	-6.97	-8.84	28.1
848.38	calcareous concretion	CC		-30.04	-1.60	85.9
862.84	calcareous concretion	CC		-11.08	-6.57	73.3
872.92	"cone-in-cone" calcite horizon	HB		-4.31	-10.38	73.4
874.22	calcareous concretion	CC		-19.65	-1.98	79.2
874.75	calcareous concretion	CC		-30.89	-1.35	81.9
875.02	calcareous concretion	CC		-31.51	-1.33	84.5
875.15	septarian nodule with ammonite	SN		-31.96	-1.38	81.1
887.98	nodular layer (Top Gross Wolf Mb.)			-1.20	-7.66	65.7
890.50	nodular layer (limestone)			1.13	-1.89	95.0
892.58	nodular layer (Base Gross Wolf Mb.)			0.84	-2.74	89.7

(continued)

Depth [m]	Description of sample		TS
897.00	«Oberer Stein» (Rietheim Mb.)		
897.85	«Homog. Kalkbank» (Rietheim Mb.)		
898.40	«Unterer Stein» (Rietheim Mb.)		

$\delta^{13}\text{C}_{\text{carb}}$ [‰ VPDB]	$\delta^{18}\text{O}_{\text{carb}}$ [‰ VPDB]	Carbonate [wt.-%]
-0.93	-4.94	86.5
-1.34	-3.19	87.9
-2.51	-3.20	100.0