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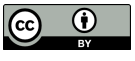

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Total Organic Carbon Evaluation Using Geophysical Well-Logs in Lorraine Coal Basin (NE France).

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Abstract

The Lorraine Coal Basin, recognized as the most promising coal bed methane basin in France, holds significance for the energy transition after more than a century of coal mining until 2004 and renewed interest in oil and gas exploration in the 80s and 90s. New data from an ongoing exploration campaign within this basin rise new opportunities in the assessment of gas resources. In the scope of this evaluation the determination of Total Organic Carbon (TOC) content using well-log data is a necessary step. The study employs a methodology encompassing Schmoker's method, ΔlogR, and multivariate regression, focusing on two reference boreholes. While TOC calculations techniques are usually developed for marine shale deposits, an adaptation to highly heterogeneous fluviatile deposits is presented. Schmoker's method provides the most accurate TOC values, consistent with Rock-Eval data. However, the ΔlogR method underestimates TOC values, particularly for coal lithologies, for which logarithmic equations are proposed for proportional corrections. Moreover, new equations based on multivariate regression of gamma-ray, sonic, and

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resistivity logs are developed for TOC estimation. Schmoker's method proves to be the most reliable with available density logs in the Lorraine Coal Basin. Alternatively, the modified ΔlogR equations or those derived from the multivariate regression of gamma-ray, sonic, and resistivity logs can be used. These new equations represent an alternative approach and identify new possibilities for estimating TOC in hetereogenous coaly formations. Based on TOC, lithologies of the investigated sedimentary series are classified from lean to fair source-rocks for shaly lithologies to excellent for the coal layer.

Keywords

Total Organic Carbon, Lorraine Carboniferous Basin, Coal Bed Methane, Well log, Δ log R, Schmoker Method

Résumé – Evaluation des teneurs en carbone organique total par les diagraphies dans le bassin carbonifère lorrain. Le bassin carbonifère lorrain, reconnu comme l'un des bassins les plus prometteurs en France pour ses ressources en gaz de charbon (Coal Bed Methane - CBM), revêt une importance particulière pour la transition énergétique après plus d'un siècle d'exploitation charbonnière achevée en 2004 et un regain d'intérêt pour l'exploration pétrolière et gazière dans les années 1980 et 1990. De nouvelles données issues d'une campagne d'exploration en cours dans ce bassin facilitent l'évaluation des ressources gazières piégées dans les dépôts sédimentaires. Cette évaluation est réalisée en déterminant le Carbone Organique Total (COT) le long des puits, à l'aide des données diagraphiques. Plusieurs méthodes dans la littérature décrivent l'utilisation de la diagraphie dans le contexte des séquences marines, mais peu d'études se concentrent sur leur utilisation dans le cadre des dépôts continentaux. L'étude emploie une méthodologie englobant la méthode de Schmoker, la méthode Δ log R, et la régression multivariable, se concentrant sur deux

forages de référence : Fols 1A et Dbl S1. La méthode de Schmoker fournit les valeurs de COT les plus précises, cohérentes avec les données Rock-Eval. Cependant, la méthode ΔlogR sous-estime les valeurs de COT, en particulier pour les lithologies charbonneuses, pour lesquelles des équations logarithmiques sont proposées afin de corriger ces estimations. De plus, de nouvelles équations basées sur la régression multivariable des logs gamma-ray, soniques et de résistivité sont développées pour l'estimation du COT. La méthode de Schmoker s'avère être la plus fiable avec les logs de densité disponibles dans le bassin houiller lorrain. Alternativement, les équations ΔlogR modifiées ou celles dérivées de la régression multivariable des logs gamma-ray, soniques et de résistivité peuvent être utilisées. Ces nouvelles équations peuvent constituer une approche innovante et ouvrir des pistes à explorer pour estimer le TOC dans les niveaux riches en matière organique. Sur la base du COT, les lithologies des séries sédimentaires étudiées peuvent être classées de roches mères pauvres à moyennes pour les lithologies argileuses, et excellentes pour les couches de charbon.

Mots clés

Carbone organique total, Bassin carbonifère lorrain, Gaz de charbon, Diagraphie, Δ log R, Méthode de Schmoker.

1. Introduction

After more than a century of coal exploitation until 2004 and exploration for oil and gas during the 80s-90s, renewed interest in evaluating of the gas reserves of the Lorraine Carboniferous basin has emerged in recent years (Gunzburger, 2019). Currently, the Lorraine Basin is undergoing a new investigation, with recent drillings providing both core and well log data. Previous studies described the coal seams distribution (Donsimoni, 1981), the organic geochemistry of coal and

kerogen-bearing strata (Fleck, 2001), reconstructed the burial history of the basin, and evaluated gas generation (Izart *et al*., 2016). However, until recently no attempt was made to quantitatively evaluate the gas generation potential of the basin as part of the assessment of the ultimate gas reserves.

The Total Organic Carbon content (TOC) is a key parameter to assess the gas potential of sedimentary strata (Passey *et al*., 1990). While major coal strata are well characterized in the Lorraine basin wells, the quantitative estimation of the abundance of kerogen present in surrounding rock facies (clay, siltstone, sandstone, and conglomerate) has never been evaluated in a continuous manner along the formations, as previous studies (Fleck, 2001) relied on sampling approaches that did not capture the full complexity. Yet, the calculation of the total gas generation potential of the Carboniferous deposits requires the appraisal of all organic matter-containing facies.

TOC measurements in the laboratory may be performed by carbon analyzers (Van Krevelen, 1993) or Rock-Eval pyrolysis (Espitalié *et al.*, 1985) applied to core samples and drilling cuts. However, these laboratory measurements are time-consuming and the TOC data is discontinuously determined along the sedimentary profiles. To overcome this drawback, methods involving well-logging methods have been developed to assess TOC contents.

Well-logging techniques have greatly enhanced the exploration of Coalbed Methane (CBM) reservoirs by providing workflows to evaluate coal quality, and reservoir parameters such as fracture density, permeability, and gas content (Morin, 2005; Chatterjee and Paul, 2013; Meng *et al*., 2013; Sutton *et al*., 2014; Ghosh *et al*., 2016; Su *et al*., 2018).

The systematic determination of the TOC content of sedimentary logs by such methods has however mostly been developed for marine petroleum source rocks (Nixon, 1973; Meissner, 1987; Meyer and Nederlof, 1984; Mendelzon and Toksoz, 1985; Mann and Muller, 1986,1988; Passey *et al*., 1990 ; Bessereau *et al*., 1991;Schwarzkopf., 1992).

Schmoker (1979, 1981) first published a method to calculate TOC content from density and gamma-Ray logs. Schmoker (1979) proposed a linear relationship between TOC and the formation density log in shales. Generally, shale mineral matrix density presents an average value of 2.7 g/cm^3 while matrix density values for organic matter are approximately 1.1 g/cm^3. The occurrence of organic carbon vastly influences the formation bulk density and hereafter TOC is calculated from density logs. Meyer and Nederlof (1984) and Mendelzon and Toksoz (1985) used a combination of density, sonic slowness, and electrical resistivity logs to calculate Total Organic Carbon (TOC) for characterizing petroleum systems. They explained that source rocks are characterized by their low density, low sonic slowness, and high electrical resistivity. To improve TOC assessment, Passey *et al*. (1990) proposed to use a combination of well-logs and developed the ΔlogR technique, which consists of the overlay of porosity (sonic, density, neutron) with resistivity logs. In organic matter-rich sediments, the two geophysical signals exhibit distinct characteristics, and the magnitude of their separation is primarily proportional to TOC, with additional influence from the thermal maturity of the formation (including the presence of oil and gas). Consequently, utilization charts have been developed based on vitrinite reflectance to account for these factors. This method has limitations in terms of accuracy for interwell correlation, as the ΔlogR technique requires the arbitrary selection of a baseline, which varies significantly from well to well due to lithological variations (Yu *et al*., 2017; Wang, 2022) and thermal maturity of kerogen (Sun *et al*., 2013). In fact, the thermal maturity of the formations intersected by the wells can

influence the porosity, which is susceptible to measurement by density, sonic, and resistivity logs, thereby leading to variations in the log readings between wells.

In shale and coal, the ΔlogR method requires calibration as it tends to underestimate the Total Organic Carbon content in these formations (Sondergeld *et al*., 2010).To address this, alternative approaches are proposed to determine correction coefficients in organic-rich layers (Sondergeld *et al*., 2010). Additionally, the inclusion of other well logs, such as natural gamma spectroscopy, is proposed by Li and Zhang (2023).

Bessereau *et al.* (1991) introduced the CARBOLOG method, which utilizes Sonic slowness and resistivity well logs taking into account the composition of rock, including matrix, water, clay, and organic matter. The method defines the CARBOLOG diagram, where the square root of resistivity is plotted against sonic slowness.

Moreover, statistical methods, such as multivariate analyses, are employed to predict TOC, demonstrating good correlations between density logs and the predicted TOC (Zhang and Xu, 2016; Nyakilla *et al*., 2022). However, the generalization of these models is not possible for all continental shales and coal due to weak linear correlations with log curves (Hu *et al*., 2016; Wang *et al*., 2017). Currently, the most advanced method for calculating Total Organic Carbon (TOC) utilizing well-log data is the application of machine learning algorithms (Huang and Williamson, 1996; Kamali and Mirshady, 2004; Amiri Bakhtiar *et al*., 2011; Khoshnoodkia *et al*., 2011; Alizadeh *et al*., 2012; Cranganu and Dimitrijevic , 2016; Bolandi *et al*., 2017; Mahmoud *et al*., 2017, 2019; Nezhad *et al*., 2018; Wang *et al*., 2018; Zhu *et al*., 2018; Elkatatny, 2019; Zhao, 2019; Goliatt and Saporetti, 2023; Zhu *et al*., 2023; Wood, 2023). However, there is currently no standardized algorithm established for the computation of TOC from well logs. This limitation can

be primarily attributed to the heterogeneity of lithological formations (Chan *et al*., 2022). Passey *et al*. (1990) had already noted that TOC values obtained using their approach were unreliable for organic matter-rich layers with thicknesses less than 1 meter. However, a significant challenge arises from the complexity of sedimentary successions, particularly in continental detrital deposits. This is the case for instance for the fluvial facies which are dominant in the Lorraine Carboniferous Basin and characterized by hundreds of fining upward depositional sequences (conglomerate to sandstone, silt, clay, and coal seams). Therefore, this study aims to calculate Total Organic Carbon (TOC) using well logs across all fluvial-lacustrine sedimentary facies, contributing to the gas reserve calculations.

2. Geological setting

The Lorraine Carboniferous Basin, located in North-East France, is about 200 km long and 80 km wide. It extends into the German Saar-Nahe Basin where strata outcrop (Schäfer, 2011) (Fig. 1). In the French part, the basin is bounded to the north by the Metz-Hunsrück Fault, a major SW-NE trending thrust fault belonging to Variscan orogeny (Henk, 1993; Schäfer, 2005, Hemelsdaël et al., 2023), to the south by the gravity anomaly between Sarrebourg and Gironcourt and to the west by La Marne Fault (Donsimoni, 1981; Izart *et al*., 2016). It is an intermountain basin (Courel et al., 1986; Donsimoni, 1981; Hemelsdaël et al., 2023) that developed during the Hercynian orogeny and therefore contains no marine sediments (Schäfer, 1989, 2005, 2011). More precisely, the Lorraine Carboniferous basin developed during the compression phase and late collapse phase of the Variscan belt. The main part of the sedimentary filling consists of up to 8 km of Westphalian-Stephanian detrital sediments covered by Permian and Mesozoic deposits of about 500 m thickness on average (Pruvost, 1934; Donsimoni, 1981; Barrabé and Feys, 1965; Izart *et al*., 2016).

In this study, well logs investigated stratigraphical interval is comprised between the top of Westphalian C to top Westphalian D. Those regional lithostratigraphical and biostratigraphical subdivisions can be correlated to the international chronostratigraphical chart (Gradstein *et al.*, 2020), and assigned to Middle and Late Pennsylvanian stages, thanks to the datings of zircons from the volcanic tuffs of the Saar and Lorraine basins (Izart *et al.*, 2025). These authors dated the Westphalian B/Westphalian C boundary (313.82 Ma), the mid-part of the Westphalian C (313.24 Ma), the Westphalian D top (307.95 Ma) and the Early Stephanian (304.49 Ma), and proposed a correlation with the other regional substages from the Western European coal basins. The Westphalian B corresponds to the Duckmantian regional substage, the Westphalian C to the Bolsovian, the Westphalian D to the Asturian, and the Early Stephanian to the upper part of the Cantabrian and Barruelian. The marine global stages corresponding to these local substages are respectively the Moscovian and the Kasimovian, assigned to the Middle and Late Pennsylvanian.

At the basin scale, the sedimentary deposits are subdivided into two major series which were defined essentially by palynological and paleobotanical data in galleries and boreholes (Pruvost, 1934; Laveine, 1974; Alpern *et al.*, 1969; Termier, 1923; Merry, 1967; (Izart *et al.*, 2025): i) The Westphalian series displaying approximately 4 km of accumulated deposits with about a hundred coal beds. Their thickness varies from a few centimeters to a maximum of 25 meters exceptionally, with an average of four to five meters. ii) The Stephanian series of about 1.1 km of deposits containing four major coal layers.

Coal layers are interstratified within all grain size siliciclastic series with variable thicknesses of conglomerates, sandstones, siltstones, and claystones. Deposits show differential preservation due to the development of recurrent erosional surfaces.

A wide spectrum of different continental environments (figs. 2 and 3), studied by Izart *et al.* (2005) for the Westphalian C and Allouti (2024) for the Westphalian D, can be highlighted, with from source to sink restricted to that intermountain context, alluvial fans, braided rivers, meandering rivers, anastomosed rivers with more or less preserved floodplains, and finally delta-lakes where sediment storage become permanent due to provided suitable accommodation. River systems were interconnected to well-developed lowland swamps and lakes organized in variable continuous areas with rich and diversified plant life indued high organic productivity (Pruvost, 1934; Donsimoni, 1981; Fleck *et al*., 2001; Izart *et al*., 2005). Higher proportion of floodplain deposits give appropriate conditions to more widespread distribution of coal. Moreover, organic-rich swamps were to show rapid rate of organic growth and accumulation outpaces clastic sedimentation. This kind of sedimentological evolution and stratigraphical organization is typical of depositional environments for Carboniferous coal-bearing strata (McCabe, 1985; Diessel, 1992; Thomas, 2002). The high frequency sequences reported in the figures 2 and 3 were determined by Allouti (2024) and their durations (close to 20 ka, precession-scale) were calculated by Izart *et al.* (2025, their Fig. 5) thanks to the Bayesian method.

3. Materials and Methods

3.1. Data availability

3.1.1. Studied wells and core samples

The study is focused on two boreholes, Folschviller (Fols 1A) and Diebling (Dbl S1), which were drilled by La Française de l'Energie company and penetrated the top of the Carboniferous units (Figs. 1, 2 and 3). Fols 1A reached Westphalian D in the (690-1303 m TVD interval), while Dbl S1 drilled through Westphalian D (875-1265 mTVD interval) and Westphalian C (1265-1440 m TVD

interval). Detailed lithologies, depositional environments as well as stratigraphic sequences are synthesized in Figures 2 and 3. Thirty-seven samples were collected from these boreholes, including coals and shaly coals, claystones, siltstones, and sandstones.

3.1.2. Organic petrography and Rock-Eval analysis

The rock and coal samples were crushed, sieved (<180 µm mesh), and analyzed by Rock-Eval pyrolysis at the Institut des Sciences de la Terre d'Orléans (ISTO) (France) (analytical procedure described in Le Meur *et al.* (2021).The major parameters considered were TOC (wt%) and Tmax (°C). Organic petrography and vitrinite reflectance measurements were assessed by EGS-exploration (Switzerland).

3.1.3. Well logs data

The well logs are presented in Log Ascii Standard (LAS) format for both the boreholes Fols 1A and Dbl S1. Data were imported into Techlog© Schlumberger software and then exported to Microsoft Excel© to evaluate TOC using ΔlogR and Schmoker methods. Gamma-Ray, Sonic, and Density Logs are used to determine shale volume, total porosity, and lithological interpretation. TOC computation involves Sonic, Density, and Resistivity Logs. The caliper is also available for both wells to control potential washout/breakout detected by borehole diameter widening in some coal layers.

3.2 Methods of Calculating Total Organic Carbon Using Well-Logs

3.2.1. Well Log Responses for Characterizing Coal Deposits

Various methods for identifying and characterizing coal layers and organic-rich strata in subsurface rock units, including gamma-ray, density, resistivity, sonic slowness, and caliper measurements are described in the literature (Seidle, 2011; Keskinsezer *et al*., 2019; Thomas, 2002).

The gamma-ray method involves measuring the intensity of naturally occurring gamma rays. Coal layers typically exhibit low gamma ray values, whereas clayey formations present high values. Also, gamma ray values are lower in lithologies such as sandstones and conglomerates (Hollub and Schafer, 1992; Karacan, 2009; Seidle, 2011; Keskinsezer *et al*., 2019). Therefore, this tool cannot be used alone to identify organic-rich sediments.

In regards to the use of density logs, coal and organic-rich strata typically exhibit lower density values compared to other lithologies (*Mavor et al*., 1994; Zhou and Esterle, 2008; Keskinsezer *et al*., 2019).

In terms of resistivity, coal layers exhibit higher values, but only when the water content is low (Keskinsezer *et al*., 2019). The resistivity of coal is dependent on its rank, with lignite and anthracite displaying very low resistivity and subbituminous and bituminous coal displaying a range from low to high resistivity values (Mavor *et al*., 1994; Thomas, 2002). In addition, resistivity may be influenced by factors such as water saturation and salinity as well as quantity of clay or conductive minerals like pyrite (Sondergeld *et al*., 2010) and must therefore be combined with other tools to determine the organic matter content of strata.

Sonic logs are valuable tools for identifying coal layers (Rider and Kennedey, 2011; Seidle, 2011). The sonic wave transit time in coal range generally between those of sandstone and shale. However, anthracite coal, with a transit time of approximately 90 μs/ft, exhibits a response closely resembling that of shale, making accurate discrimination more challenging. While sonic logs are useful in

assessing coal quality, their application to coal gas reservoir engineering is limited by certain constraints such as breakout and washout. Nonetheless, sonic logs combined with the previously mentioned tools may serve as indicators of organic matter content (Passey *et al*., 1990; Meyer and Nederlof, 1984).

The caliper log is used for measuring the diameter of the borehole and serves as an effective quality control for other wireline logs, including density, gamma-ray, and sonic logs. By applying this tool, errors in the identification of coal layers caused by unusually low formation density and gamma ray responses across severe washouts can be prevented. It should be noted that while washout is often considered an indicator of permeability, as well as an indicator of coal mechanical friability (Thomas, 2002).

3.2.2. Schmoker Method

Schmoker (1979) developed a method for estimating TOC contents of Appalachian Devonian marine shale using a density log RHOb. Schmoker and Hester (1983) suggested that TOC has a positive linear correlation with the reciprocal of bulk density:

$$\mathrm{TOC} = \frac{A}{\mathrm{RHOb}} - \mathrm{B} \tag{1}$$

Schmoker (1979, 1981) considered the rock is composed of mineral matrix, interstitial pores, pyrite, and organic matter. In this case, the formation bulk density is a function of fractional densities and volumes of these four components. The volume of pyrite was assumed to increase linearly with the organic matter content because the decomposition of organic matter generates reducing conditions that promote pyrite formation in anoxic environments. For this reason, pyrite

was treated as a separate component from the matrix. The values of A and B in equation (1) are calculated by incorporating density values for pyrite, organic matter, and matrix at 5.0, 1.01, and 2.69 g/cm^3, respectively.

$$\mathrm{TOC} = \frac{154.497}{\mathrm{RHOb}} - 57.261 \tag{2}$$

3.2.3. ΔlogR Method

Passey *et al.* (1990) proposed ΔlogR method for estimating TOC content from well-log data. Currently, the ΔlogR is a widely used method for marine clay series. The ΔlogR technique requires the superposition of resistivity with porosities logs (sonic slowness ΔT, density RHOb or neutron porosity Φn; in equations 3, 4 and 5) and the availability of organic matter maturity data (e.g. vitrinite reflectance). The integration of sonic slowness and resistivity logs facilitates the identification of a baseline cutoff. A distinct separation between the two curves indicates the presence of source rock zones, while the overlap of the curves signifies non-source rock intervals. (Fig. 4).

$$\Delta \log \mathrm{R} = \log_{10}\left(\frac{\mathrm{R}}{\mathrm{R}_{\mathrm{Baseline}}}\right) + 0.02 * (\Delta \mathrm{t} - \Delta \mathrm{t}_{\mathrm{Baseline}}) \tag{3}$$

$$\Delta \log \mathrm{R} = \log_{10}\left(\frac{\mathrm{R}}{\mathrm{R}_{\mathrm{Baseline}}}\right) + 4 * (\phi \mathrm{t} - \phi \mathrm{t}_{\mathrm{Baseline}}) \tag{4}$$

$$\Delta \log \mathrm{R} = \log_{10}\left(\frac{\mathrm{R}}{\mathrm{R}_{\mathrm{Baseline}}}\right) - 2{,}5 * (\mathrm{RHOb} - \mathrm{RHOb}_{\mathrm{Baseline}}) \tag{5}$$

In this study, equation (3) is used to calculate Δ log R. The amount of organic carbon is directly proportional to Δ log R, consequently, TOC can be calculated using equation (6).

$$TOC = \Delta \log R * 10^{(2.297 - 0.1688 * LOM)} \quad (6)$$

If the Level of Maturity (LOM) is known, the ΔlogR separation of different lithologies using well logs data can be used to estimate the TOC. LOM is a scale of organic matter thermal evolution applicable to fine-grained sedimentary rocks proposed by Hood *et al*. (1975). LOM values were estimated from vitrinite reflectance (%Ro) values using equation (7).

$$LOM = 0.0989 \times Ro^5 - 2.1587 \times Ro^4 + 12.392 \times Ro^3 - 29.032 \times Ro^2 + 32.53 \times Ro - 3.0338 \quad (7)$$

Thermal maturity values for the Westphalian D formation in the Lorraine Carboniferous Basin, Fols 1A and Dbl S1 wells are available in Table 1. The equation for LOM was determined from digitalization of the % Ro correlation table established by Hood *et al*. (1975).

4. Results

4.1. TOC calculation using Schmoker

The widely used TOC calculation method proposed by Schmoker (1979, 1981) is represented by equation (2) with constants A and B of 154.497 and 57.261 respectively. These values are not always suitable for any well and may thus be adjusted for our reference wells Fols 1A and Dbl S1. These constants are typically gauged from the linear regression of TOC Rock-Eval and density log (Schmoker and Hester, 1983; Yu *et al*., 2017).

In the case of the Fols 1A borehole the crossplots of the TOC Rock-Eval versus 1/density and TOC Schmoker versus TOC Rock-Eval (Fig. 5a and b) reveal a linear relationship that closely matches with equation (2) with acceptable correlation coefficients. In this case, correction of A and B may not be applied.

In the case of the borehole Dbl S1, the same graphs show significant deviations (Fig. 5) revealing that the A and B parameters of the original Schmoker method induce an underestimation of TOC values. Consequently, constants A and B are changed to 256.02 and 100.4 respectively for the Dbl S1 borehole (Fig. 5a; Eq. 8).

$$\mathrm{TOC} = \frac{256.02}{\mathrm{RHOb}} - 100.4 \tag{8}$$

Figure 5b shows the relationship obtained between Rock-Eval TOC and TOC calculated using the adapted Schmoker equation. The TOC values are calculated using the Schmoker relationship, and are used as a reference for the other developed relationship.

4.2. TOC calculation using Δ log R

Continuous sonic and resistivity logs are available for the Fols 1A and Dbl S1 boreholes. Prior to overlaying the curves, appropriate scaling is necessary to ensure that each resistivity cycle corresponds to 50 µs/ft. Following scaling, the curves require baseline definition. Baseline resistivity and sonic values are established at 150 ohm.m and 65 µs/ft for the Fols 1A well and 100 ohm.m and 80 µs/ft for the Dbl S1 well (Tab. 2 and Fig. 4). Equation (3) is then used to calculate the ΔlogR separation in this study (Fig. 4), which enables the estimation of TOC using equation (6).

For Fols 1A and Dbl S1 wells, TOC values were calculated by applying the ΔlogR method and equal to 8 wt% for coal layers. These values are approximately ten-fold lower than the TOC values obtained from Rock-Eval analysis, which range from 20 to 75 wt% in Fols 1A and 10 to 85 wt% in Dbl S1, with maximum values of 75 and 85 wt%, respectively. For shaly lithologies, mean TOC values are 0.5 wt% in both wells, which is lower than the values obtained from Rock-Eval analysis in Fols 1A (7 wt% TOC on average) and Dbl S1 (3 wt% on average) (Track 2 in Figs. 6 and 7 respectively).

4.3. TOC calculation using Modified ΔlogR Method

4.3.1. TOC Schmoker vs. TOC ΔlogR evaluation

The Schmoker and calibrated Schmoker methods as defined above allow to calculate TOC values in good agreement with Rock Eval data measured on the various lithologies (coal, shaly coals, coaly shales, sandstones, conglomerates) present in our wells (Figs. 6 and 7). The Schmoker method may then be considered as the most appropriate for our study. In contrast, the ΔlogR method tends to underestimate TOC values for coaly and shaly lithologies. Cross-plot analyses using TOC Schmoker/ TOC ΔlogR versus geophysical parameters (Sonic slowness, bulk density, and resistivity) are tested. Only the cross-plot using sonic slowness showed a consistent trend (Fig. 8a) in which values greater than 80 µs/ft and 100 µs/ft for Fols 1A and Dbl S1 respectively represented a logarithmic trend with a convergence limit of 10. The consideration of bulk density (color scale (Fig. 8a)) shows that these points correspond to low-density values related to coal and coaly facies. Changes in density values from 1.7 to 2.3 g/cm^3 correspond to increasing shale volume on carbonaceous lithologies. All data points showing sonic slowness values lower than 70 µs/ft and

high density (more than 2.3 g/cm^3) are related to non-source rock formations (sandstones and conglomerates) and displayed no correlation with sonic slowness.

The cut-off values of 80 µs/ft and 100 µs/ft were applied to select shale, shaly coal, and coal from figure 8a. For coaly lithologies, the minimum sonic slowness value is 80 µs/ft for Fols 1A and 100 µs/ft for Dbl S1, while the maximum value is 140 µs/ft for Fols 1A and 160 µs/ft for Dbl S1. The analysis of the data reveals a logarithmic increase in the ratio in relation to sonic slowness, ranging from 0.1 to 10 as shown in figure 8b. Equations (9) and (10) represent this relationship for Fols 1A and Dbl S1 wells, respectively.

$$(\text{TOC Schmoker})/(\text{TOC } \Delta \log R) = 19.15 * \ln(\Delta T) - 83.48 \quad (9)$$

$$(\text{TOC Schmoker})/(\text{TOC } \Delta \log R) = 23.298 * \ln(\Delta T) - 101 \quad (10)$$

Therefore, to mitigate the discrepancy between TOC values calculated by ΔlogR and measured by Rock-Eval, equations (11) and (12) are applied as sonic slowness filters to wells Fols 1A and Dbl S1 respectively. Proportional corrections are thus applied to shaly and coaly lithologies while values for non-source rock formations are left unaltered.

$$\text{TOC} = \Delta \log R * 10^{(2.297 - 0.1688 * \text{LOM})} * (19.15 * \ln(\Delta T) - 83.48) \quad (11)$$

$$\text{TOC} = \Delta \log R * 10^{(2.297 - 0.1688 * \text{LOM})} * (23.298 * \ln(\Delta T) - 103.48 \quad (12)$$

Figure 6 (track 8) and 6 (track 6) show the consistency between assessed and measured TOC values once the corrections are applied. The box plot (Fig. 9) for the Fols 1A borehole shows that upon

application of the logarithmic factor to the ΔlogR method, 50 % of coal sample points analyzed exhibit TOC ranging from 30 wt% to 60 wt%. Also, 50 % of shaly lithology sample points analyzed exhibit an average TOC amount ranging from 3 wt% to 6 wt%. Similarly, after correction of the ΔlogR method via the logarithmic factor, the box plot for the Dbl S1 borehole (Fig. 9) indicates that 50 % of coal sample points analyzed exhibit a TOC amount ranging from 20 wt% to 70 wt%, with 50 % of shaly lithology sample points analyzed exhibiting an average TOC amount ranging from 3 wt% to 6 wt%.

4.3.2. "Δ. log R separation" and TOC calibration

In the method proposed by Passey *et al*. (1990), the relationship between TOC values and the separation ΔlogR is given by equation (6), which requires the consideration of LOM (Level of Organic Maturity, a factor proportional to vitrinite reflectance) (Hood *et al*., 1975). The results for our sample sets (LOM=10.12 -10.65; %Ro = 0.84 to 0.96 and TOC as determined by Rock-Eval) are consistent with ΔlogR method for facies with TOC lower than 10 wt%. However, for TOC greater than 10 wt%, the data points fall outside the range, indicating that equation (6) may not be appropriate for coaly facies (Fig. 10). These findings have important implications for the interpretation of well-log data, as they suggest that the linear LOM trends proposed by Passey *et al.* (1990) may not apply for coaly facies. Therefore, alternative equations may be proposed for TOC determination in coal-rich deposits. Two approaches are used to calibrate TOC values over a large range: i) Rock-Eval TOC (using the depth average where the sample was taken) and ii) TOC calculated using the method by Schmoker (1979, 1981) as validated previously vs Δ log R.

In figure 11 (borehole Fols 1A), two correlation equations may be derived from Rock-Eval TOC vs Δ log R, a polynomial (Eq. 13) (red solid line) and an exponential (Eq. 14) (red dashed line).

When considering TOC calculated after Schmoker (1979, 1981) and $\Delta \log R$, a polynomial (Eq. 15) (blue solid line) and an exponential (Eq. 16) (blue dashed line) are derived.

$$TOC = 22.117 * \Delta \log R^2 + 6.997 * \Delta \log R \quad (13)$$

$$TOC = e^{2.6136 * \Delta \log R} \quad (14)$$

$$TOC = 16.262 * \Delta \log R^2 + 6.5631 * \Delta logR \quad (15)$$

$$TOC = e^{2.4374 * \Delta \log R} \quad (16)$$

In Fig. 12 (borehole Dbl S1), a correlation between Rock-Eval TOC and ΔlogR results in a polynomial (Eq. 17) (red solid line). Correlation between Schmoker TOC and ΔlogR leads to a polynomial (Eq. 18) (blue solid line).

$$TOC = -8.5903 * \Delta \log R^2 + 64.702 * \Delta \log R - 12.655 \quad (17)$$

$$TOC = -3.2901 * \Delta \log R^2 + 45.123 * \Delta logR - 2.4875 \quad (18)$$

4.4. TOC calculation using Multivariate Regression

As the density log is not always available for all the wells of our basin, it is interesting to further explore the relationship between calculated TOC using Schmoker (1979, 1981) and various borehole logs. Therefore, we conducted multivariate regression analyses using gamma ray (GR), sonic (Δt), and resistivity (R) logs in regard to TOC as determined by the Schmoker method

validated by TOC Rock-Eval. Based on a total of 8785 measurements for Fols 1A and 6381 measurements for Dbl S1, the multivariable regression analysis led to the following equations:

$$\text{Fols 1A: TOC} = 0.73 * \Delta t - 0.065 * GR + 0.02 * R - 46.29 \quad (19)$$

$$\text{Dbl S1: TOC} = 0.82 * \Delta t - 0.066 * GR + 0.02 * R - 64.15 \quad (20)$$

With determination coefficient R2 of 0.82 and 0.73 respectively. This indicates a strong relationship between TOC and the geophysical variables (gamma ray, sonic, and resistivity logs) for both boreholes (Fig. 6 Track 7 and Fig. 7 Track 5).

5. Discussion

The analysis of logs signals in Fols 1A and Dbl S1 boreholes revealed discrepancies in the equations used to calculate TOC primarily due to sonic slowness value deviations of 20 µs/ft between the two boreholes. Fols 1A exhibits less dispersion around correlation curves and a higher correlation coefficient compared to Dbl S1. The divergence stems from contrasting sediment composition. The siltites, sandstones, and conglomerates from the Fols 1A borehole are litharenites rich in pseudo-detrital matrix with abundant micritic siderite cementation, while those from Dbl S1 are of better sorting (mineralogical and grain sized based sorting) with low pseudo-detrital matrix contribution and far lessauthigenic siderite. The predominant types of cement are later diagenetic phases such as dickite and illite. Furthermore, the burial history of the two boreholes varies. Fols 1A experienced greater burial and compaction due to its structural position on the flank of a syncline) compared to Dbl S1, which is positioned on the hinge zone of an anticline.

The application of the Schmoker method on this case study well-log data leads to TOC values that are consistent with those obtained from Rock-Eval measurements on rock samples. The Schmoker equation for TOC calculations considers the contribution of organic matter, pyrite, interstitial porosity, and rock matrix as variables. Schmoker (1979, 1981) demonstrated a proportional relationship between the abundance of organic matter and pyrite and integrated this into equation (1). Yet, his study was based on claystone deposited in the marine environment. It is well known that in the anoxic sulfate-rich marine waters, organic matter is a substrate for the growth of sulfate-reducing bacteria communities which generate reduced sulfur. In the presence of detrital minerals, reduced iron is combined with sulfur to produce iron sulfide, hence the relationship observed by Schmoker (1979, 1981). In this case study, sediments were deposited in a fluvial-lacustrine system without connection to the marine environment (Donsimoni, 1981; Izart *et al.*, 2005; Fleck *et al.*, 2001) and therefore poor in sulfate. As a consequence, the coal layer present is lean in pyrite.

As considered by Schmoker (1979, 1981), porosity may be considered as constant for a given facies (marine claystone in his study cases) and thus may not influence TOC calculation. In the present case study, regarding the diversity of facies from coal to conglomerate, the influence of porosity changes may be questioned. Conglomerate aside, the studied facies present porosities up to 5% for coaly facies and values lower than 10% for sandstones, siltstones, and claystones. Calculations applied to our most porous facies (tight sandstones) led to lean to no TOC contents, consistent with Rock-Eval measurements. This might indicate that bulk density may not be highly influenced solely by porosity. In this case, porosity changes between our facies may be considered negligible. It may also be noted that all rock facies contain the same type of mineralogy (only grain size classes change) (*Hering et al.*, 1976; Fleck, 2001), with densities ranging from 2.57 g/cm^3 for sandstones to 2.7 g/cm^3 for claystone. Well-log density of our coal varies between 1.1 g/cm^3 and 1.8 g/cm^3.

The density contrast between organic matter and sandstones as well as siltstones may thus be considered as similar. In regards to the above-mentioned considerations, the changes in the bulk density well-log signal may then be essentially a function of kerogen content. This might explain why the Schmoker method may be efficient in the calculation of the TOC in the present case study.

The presence of pyrite significantly impacts well-log responses, particularly in terms of density and electrical resistivity, thereby influencing interpretations and calculations based on these parameters, such as the determination of Total Organic Carbon (TOC) using methods like the Schmoker or ΔlogR techniques. Studies by Clavier *et al*. (1976), Kennedy (2004), and Jiang *et al*. (2018) have extensively documented these effects.

Pyrite is distinct from other components of organic-rich rocks due to its very low resistivity and high density. In claystone layers deposited in marine environments, the presence of pyrite can affect log signals and, consequently, TOC calculations. To address this, new methods have been developed to correct for pyrite influence in clay-rich samples. Jiang *et al*. (2018) incorporated pyrite volume considerations into their updated equation based on density to improve accuracy.

In this study, 20 sandstone samples, 14 claystone and siltstone samples, 17 shaly coal samples, and 36 coal samples were analyzed using X-ray diffraction (XRD) and petrographic methods. The pyrite content in these samples is very low, averaging 0.50% in clays and siltstones, 0.8% in carbonaceous clays, approximately 1% in clayey coals, and nearly 0% in coals (Fig. 13). This low pyrite content reflects the fluvial-lacustrine depositional environment, which is isolated from marine settings and therefore lacks sulfate, resulting in kerogen that is low in pyrite. This suggests that the Schmoker method is well adapted and needs some adjustment of the coefficients A and B to provide accurate values for TOC Rock-Eval measurements (Section 4.1).

437 However, Section 4.2 demonstrates that the ΔlogR method results in a tenfold underestimation of
438 TOC compared to Rock-Eval measurements on our samples. Kennedy (2004) noted that pyrite
439 effects on electric resistivity tools are significant, as at concentrations above a few per cent, pyrite
440 can reduce formation electric resistivity. Sondergeld *et al*. (2010) explain that pyrite in organic-
441 rich intervals can substantially affect TOC evaluation due to its conductive nature, which reduces
442 rock resistivity and decreases Δ log R. Sondergeld *et al*. (2010) applied a correction factor of 4 to
443 their TOC calculations for marine shales.

444 Within LCB samples analyzed here, the maximum pyrite content reaches 1 % (Fig. 13), which
445 might partially affect the underestimation of TOC but does not fully explain the tenfold discrepancy
446 observed. This suggests that other factors, such as water saturation, may also perturb resistivity
447 signals, as discussed below.

448 Passey *et al*. (1990) suggest that the presence of coal intervals induces a significant resistivity
449 deflection compared to adjacent intervals such as sandstones, siltstones, and shales. Indeed,
450 Telford *et al.* (1990) measured high resistivity values ranging from 0.6×10^5 to 1×10^5 Ohm.m on
451 dry bituminous coal samples. This may account for ΔlogR values in accordance with high TOC of
452 coaly intervals. However, the resistivity increase observed in the well-logs here is not as strong as
453 expected.

454 Figure 14 recalls the data presented in Figure 10 with the addition of TOC vs ΔlogR data obtained
455 for sub-bituminous and bituminous coal from the literature. The dark shaded area is relative to dry
456 coal samples for which ΔlogR values are calculated using Equation (3) with sonic slowness of 150
457 µs/ft (maximum observed in our well-log data for coal layers), resistivity values for dry coal
458 (McCabe and Tholey.,1945; Telford *et al*., 1990), (Tab. 3) versus TOC data chosen from literature

for pure coals of various rank (Mastalerz *et al*., 2011) (Tab. 3). These values once positioned in Figure 14 suggest the true relationship that ΔlogR and TOC should have for dry coal layers. The blue shaded area is relative to wet coal samples for which ΔlogR values are similarly calculated, but using resistivity for wet coal from literature (Tab. 3). These values illustrate the ΔlogR and TOC for wet coal seams. It is noteworthy that these results do align with the TOC vs ΔlogR relationship of our wells and sample sets. This implies that the water saturation of our coal-rich layers significantly influences the calculations. Indeed, the presence of moisture decreases resistivity (McCabe and Tholey., 1945; Keskinsezer *et al*., 2019) and hence the TOC vs ΔlogR relationship presents a greater slope than for dry coal. This slope approaches that observed for TOC values obtained by Rock-Eval measurements, completed by TOC values calculated using the method by Schmoker (1979, 1981). This suggests that the ΔlogR values calculated from our well log data is strongly underestimated because it is influenced by the presence of formation water in coal beds. Indeed, in Fols 1A and Dbl S1 wells, resistivity values for coal beds are only 300 to 400 Ohm.m while a dense fracture network is observed (Privalov *et al*., 2022).

In figure 14, the light gray shaded area represents TOC values calculated for dry (dark shaded area) and wet coal (blue shaded area) using equation (6) with a LOM of 10.6. In all cases, TOC is strongly underestimated for TOC>10% (as observed for figure 6, track 1, 14, and 15). This suggests that the calibration equation proposed by Passey *et al*. (1990) for marine shale to determine TOC from resistivity data may not be valid for coal layers. As suggested earlier, our calibration equations (Figs. 11 and 12) may be used for other wells to overcome this problem. However, a more thorough approach would be to measure laboratory resistivity and sonic slowness of dry and water-saturated samples for major coaly lithologies and establish the relationship to Rock-Eval TOC to propose a new ΔlogR vs. TOC equation.

The observation that moisture decreases resistivity has been demonstrated by McCabe and Tholey (1945) and Keskinsezer *et al*. (2019). In Table 4, resistivity data for dry coal samples were compiled from references such as McCabe and Tholey (1945) and Telford *et al*. (1990), covering various coal ranks. Additional data were sourced from laboratory measurements (McCabe and Tholey.,1945)), where samples were saturated with water for 24 hours. These measurements reveal that resistivity decreases significantly upon water saturation, mirroring the conditions in water-saturated coal seams. In this study, the analysis was extended by calculating the ΔlogR separation under both dry and wet conditions. The results show that the separation decreases when samples are wet, comparable to what occurs in situ within water-saturated coal seams. Consequently, TOC values calculated under wet conditions using the original ΔlogR method were significantly underestimated compared to expected values reported by Mastalerz *et al*. (2011) for similar coal ranks. Figure 14 illustrates the relationship between expected TOC values and ΔlogR measurements for wet samples. The data points align more closely with results obtained from the corrected equations proposed in this study. This finding highlights the importance of conducting sonic and resistivity measurements under varying moisture conditions. To improve TOC estimates, laboratory testing is recommended to measure ΔlogR separation and TOC (via Rock-Eval) for coal samples of different ranks under wet conditions. Developing new, tailored equations that relate ΔlogR separation (between sonic and resistivity logs) to TOC would enhance accuracy, particularly for values exceeding 10 wt%, and provide a more reliable model derived from laboratory data.

Kenomore *et al*. (2017) explained that in shale reservoirs, when the formation's porosity is less than 3–4%, resistivity increases significantly due to the absence of electrically conductive fluids. Consequently, the ΔlogR separation can be very high and should not be used under such conditions. In this case study, the matrix porosity appears to be less than 4%, which places the coal layers

505 within this category where resistivity is expected to increase. However, in coalbed methane (CBM)
506 reservoirs, the effective porosity is predominantly defined by the fracture porosity within the cleat
507 system. This cleat porosity can significantly counteract the impact of low matrix porosity, as the
508 fractures are often filled with water, which dramatically reduces resistivity. This phenomenon
509 underscores a key aspect of the unconventional nature of these CBM reservoirs-Source Rock,

510 Tables 4 and 5 present the determination coefficient and the Root Mean Squared Error (RMSE)
511 calculated for each of the proposed TOC calculation equations using well log data of Fols 1A and
512 Dbl S1 wells. Figures 6 and 7 present in yellow the difference between TOC calculated using the
513 different equations proposed and values obtained by using the equation based on Schmoker (1979,
514 1981). RMSE allows to rank of the proposed equations to calculate TOC as follows: i) modified
515 ΔlogR (Eqs. 11 and 12) ii) multivariate analysis (Eqs. 19 and 20) iii) TOC ΔlogR equation
516 calibrated with Rock-Eval and calculated TOC using the method by Schmoker (1979, 1981). (Eqs.
517 13 and 18).

518 **6. Conclusion**

519 In the literature, TOC determination using well-logs is most commonly applied to quite
520 homogenous marine shale deposits. Our objective was to adapt such techniques to the very
521 heterogeneous fluviatile deposits in two reference wells of the Carboniferous Lorraine basin. We
522 therefore focused on Schmoker's method (1978, 1979), ΔlogR (Passey et al. 1990) and multivariate
523 regression analysis in accordance to the well-log data available. Continuous TOC determination
524 profiles were obtained despite the complexity of facies changes. The average TOC content in the
525 shales of Fols 1A Well ranges from 3.5 wt % to 4.5 wt %, while for coal layers, it ranges from 40
526 wt % to 50 wt %. In Dbl S1 Well, the average TOC content in shales varies from 4.8 wt % to 6.2

wt %, while in coal layers, it ranges from 30 wt % to 45 wt %. Accordingly, quality assessment based on TOC (Kenomore *et al*., 2017), source rocks range from very good for shaly lithologies to excellent for coal layers.

The Schmoker method lead to best results but can only be used when density logs are available. In the case only resistivity and sonic data are accessible, a proposed modified ΔlogR equations was utilized as the original ΔlogR method tends to significantly underestimate values for coaly lithologies. Alternatively, if gamma ray, sonic, and resistivity data are present, the use of the derived equations from the multivariate regression analysis is recommended. This combination of available well-log data in this basin, along with additional Rock-Eval and petrophysical data from core samples, can serve as the basis for future studies employing machine learning applications that reduce error and increase the precision of TOC predictions in the Lorraine Basin and could be further tested on other coal-rich basins.

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Figures

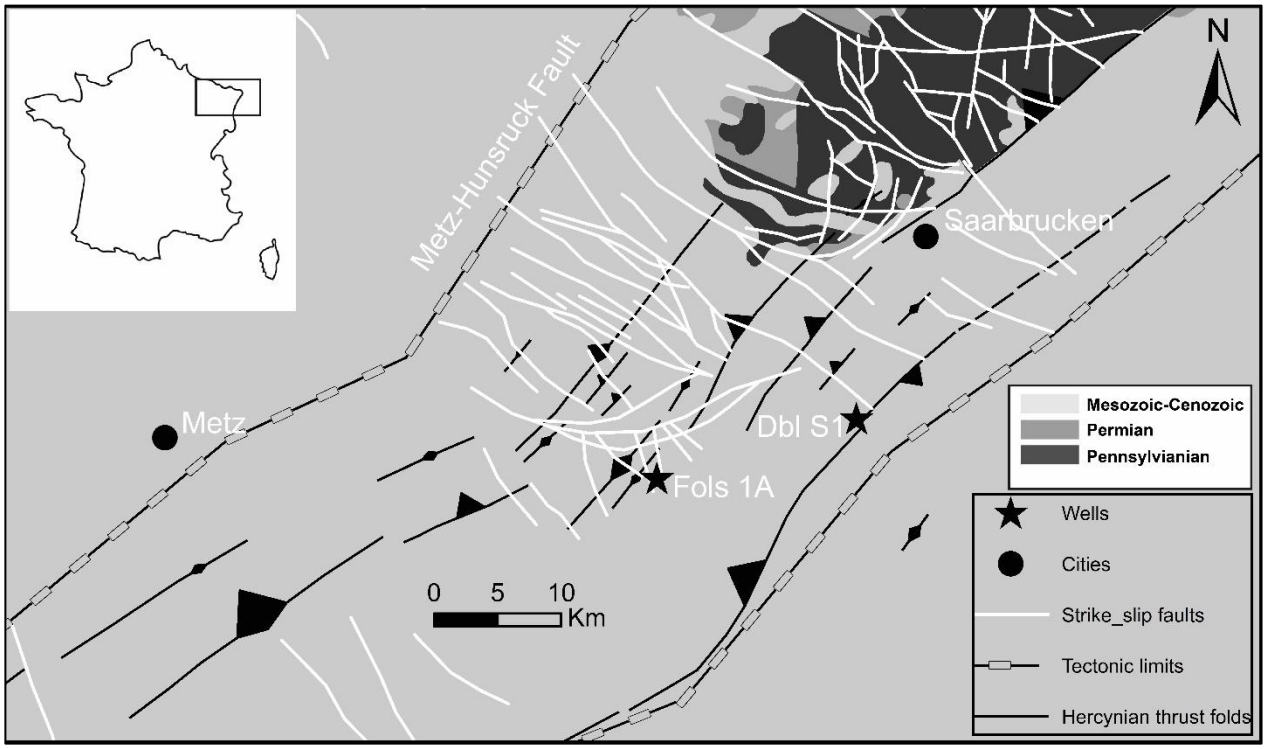
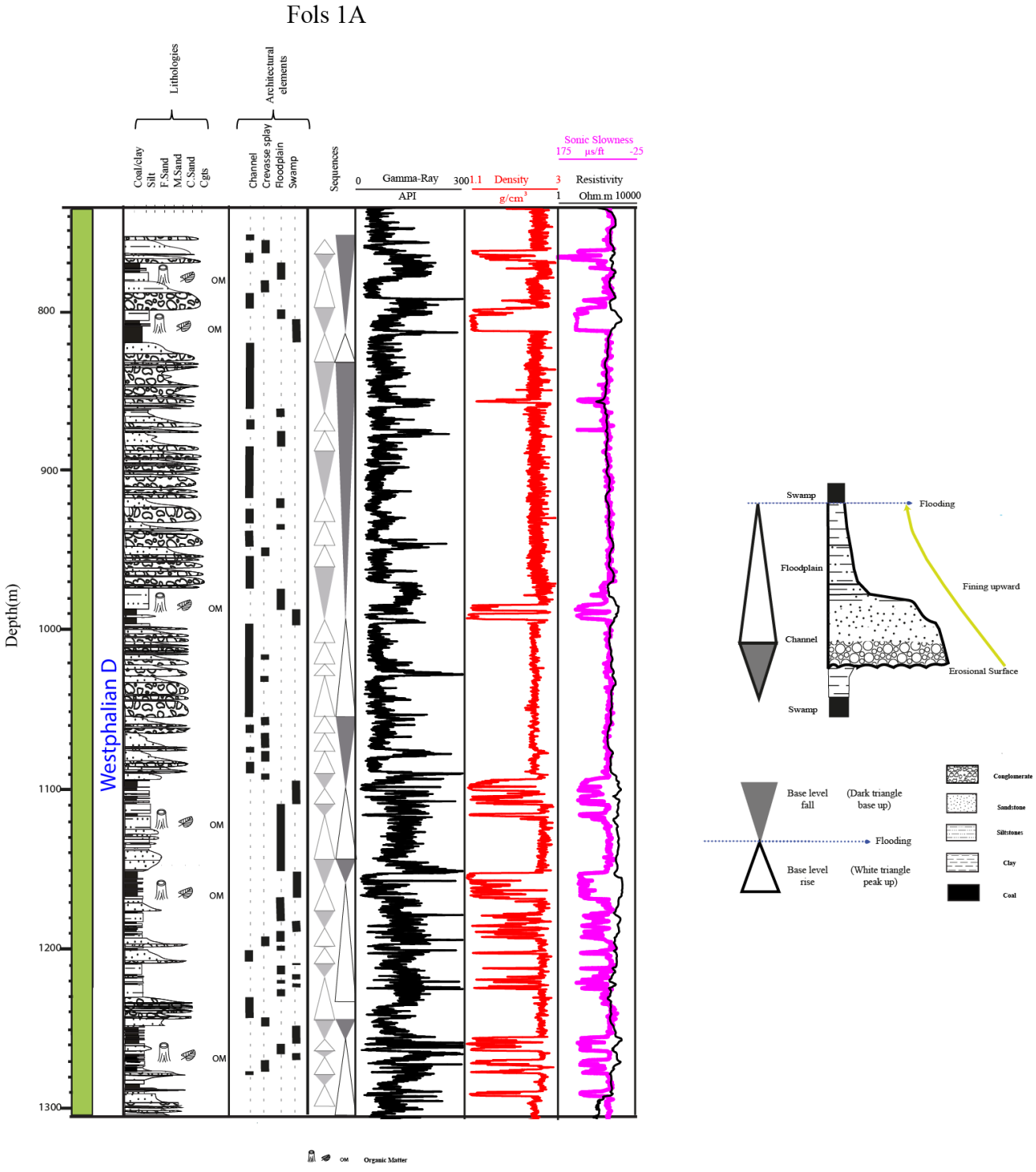
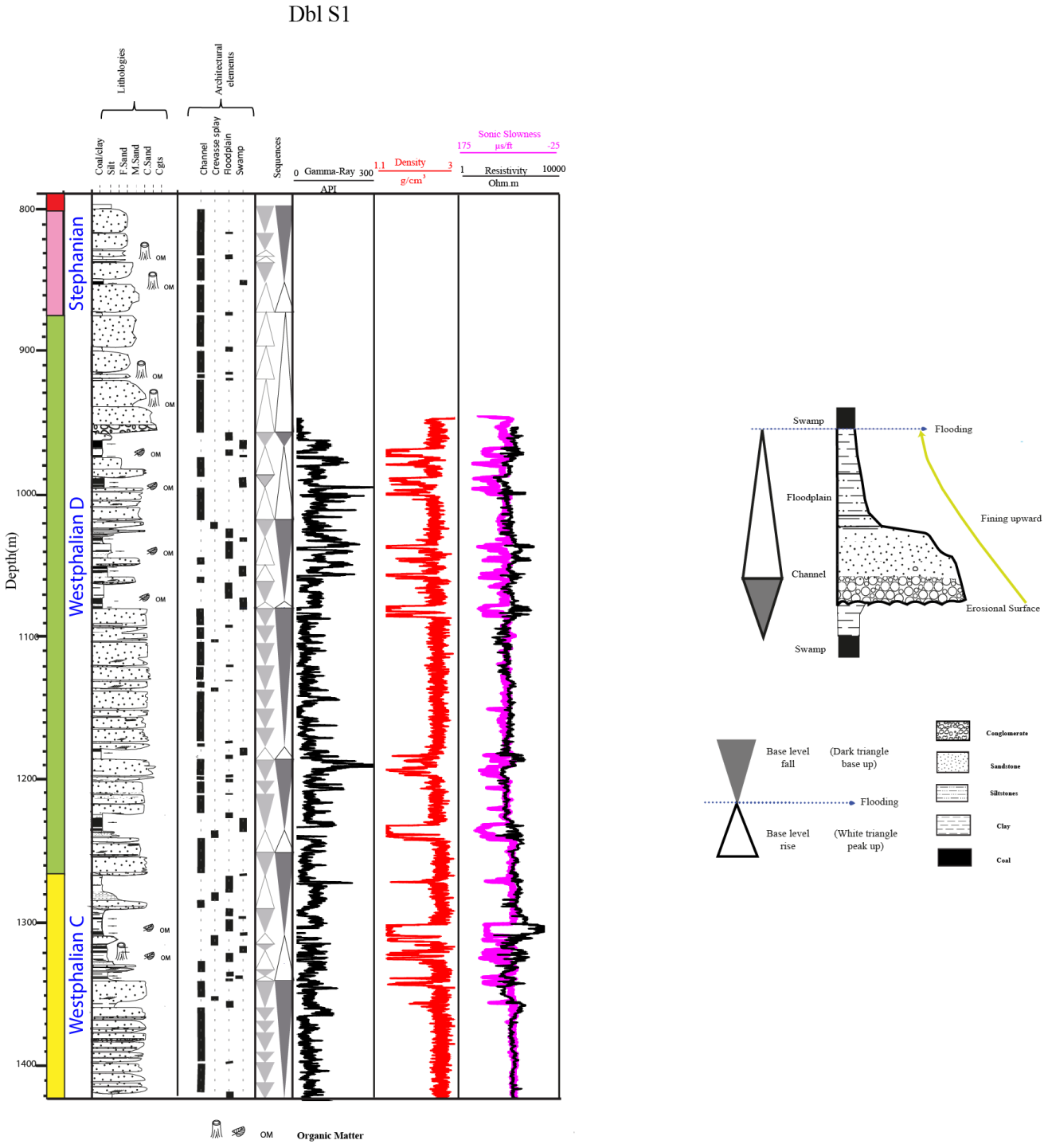


Fig. 1: Simplified geological map of the Saar-Lorraine Basin showing the location of Folschviller (Fols 1A) and Diebling (Dbl S1) boreholes. The Carboniferous Basin is accessed by both boreholes at depths of 700 and 600 meters, respectively. Permian and Carboniferous outcrop in Germany. Modified after Pruvost (1934), Donsimoni (1981), Schäfer (2011) and Izart *et al.* (2016).



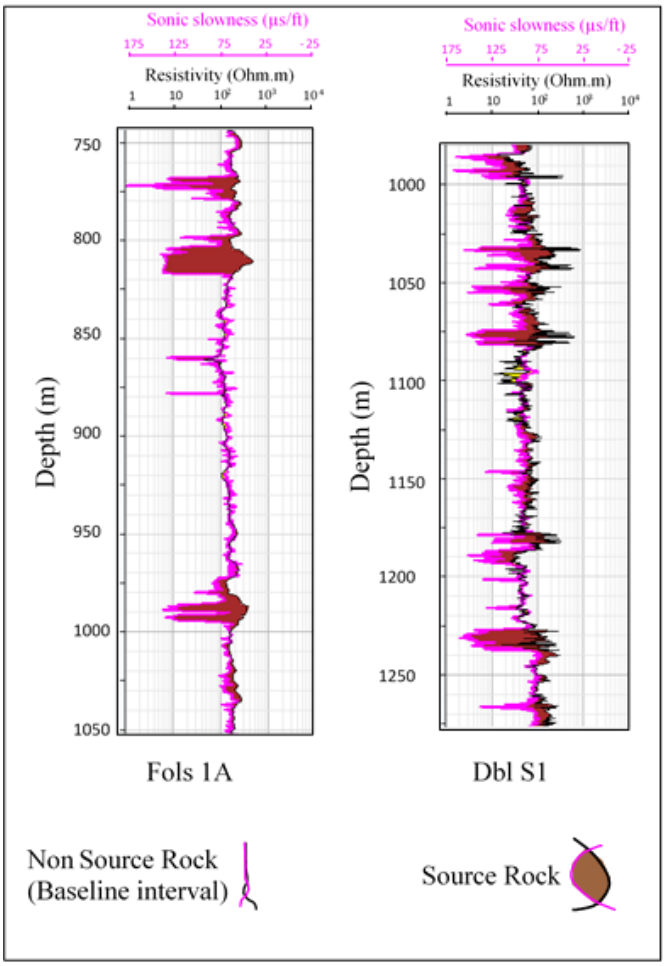
775

776 **Fig. 2:** Sedimentary logs of Folschviller (Fols 1A) well presenting lithological succession,
777 corresponding depositional environments, architectural element log and sedimentary sequences
778 representative of the Lorraine Carboniferous basin. Data based on well-logs and core analysis.



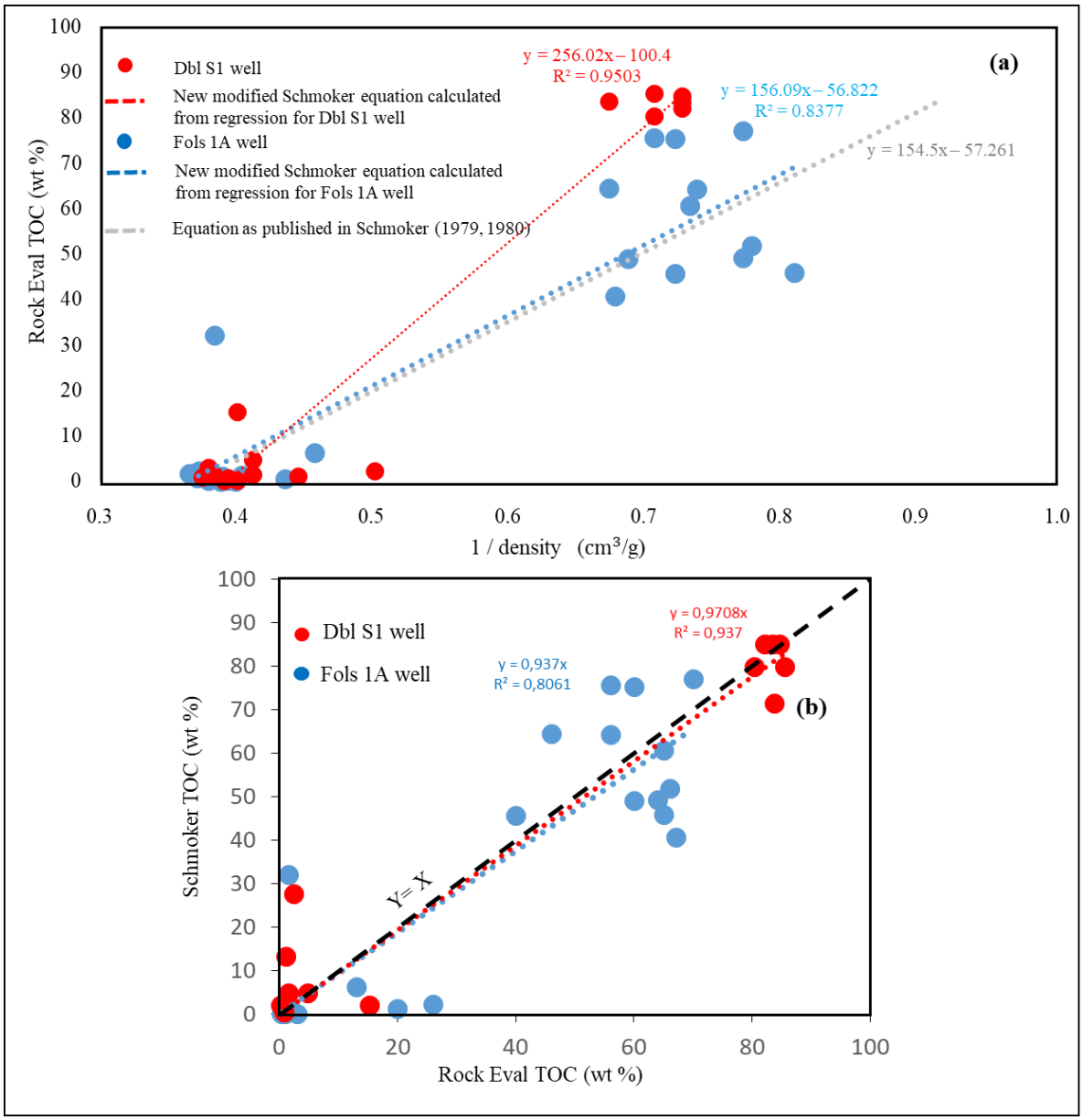
779

780 **Fig. 3:** Sedimentary logs of Diebling (Dbl S1) well presenting lithological succession,
781 corresponding depositional environments, architectural element log and sedimentary sequences
782 representative of the Lorraine Carboniferous basin. Data based on well-logs and core analysis.



783

784 **Fig. 4:** Sonic/Resistivity Overlay is showing ΔlogR separation in the coal rich intervals for Fols 1A
785 and Dbls1 wells. The relative scaling and resistivity curves correspond to a 50 µs/ft increment,
786 representing one decade of resistivity.



787

788 **Fig. 5:** Calibration of TOC by Schmoker (1979, 1981): (a) Linear relationship among Rock Eval
789 TOC (wt%) and 1/density (cc/g) in Fols 1A and Dbl S1 wells as calibrated by the method published
790 by Schmoker (1979,1981); (b) Comparison of Rock Eval TOC with TOC calculated using the
791 equation published by Schmoker for Fols 1A and proposed modified equation for calibration of
792 Dbl S1 wells.

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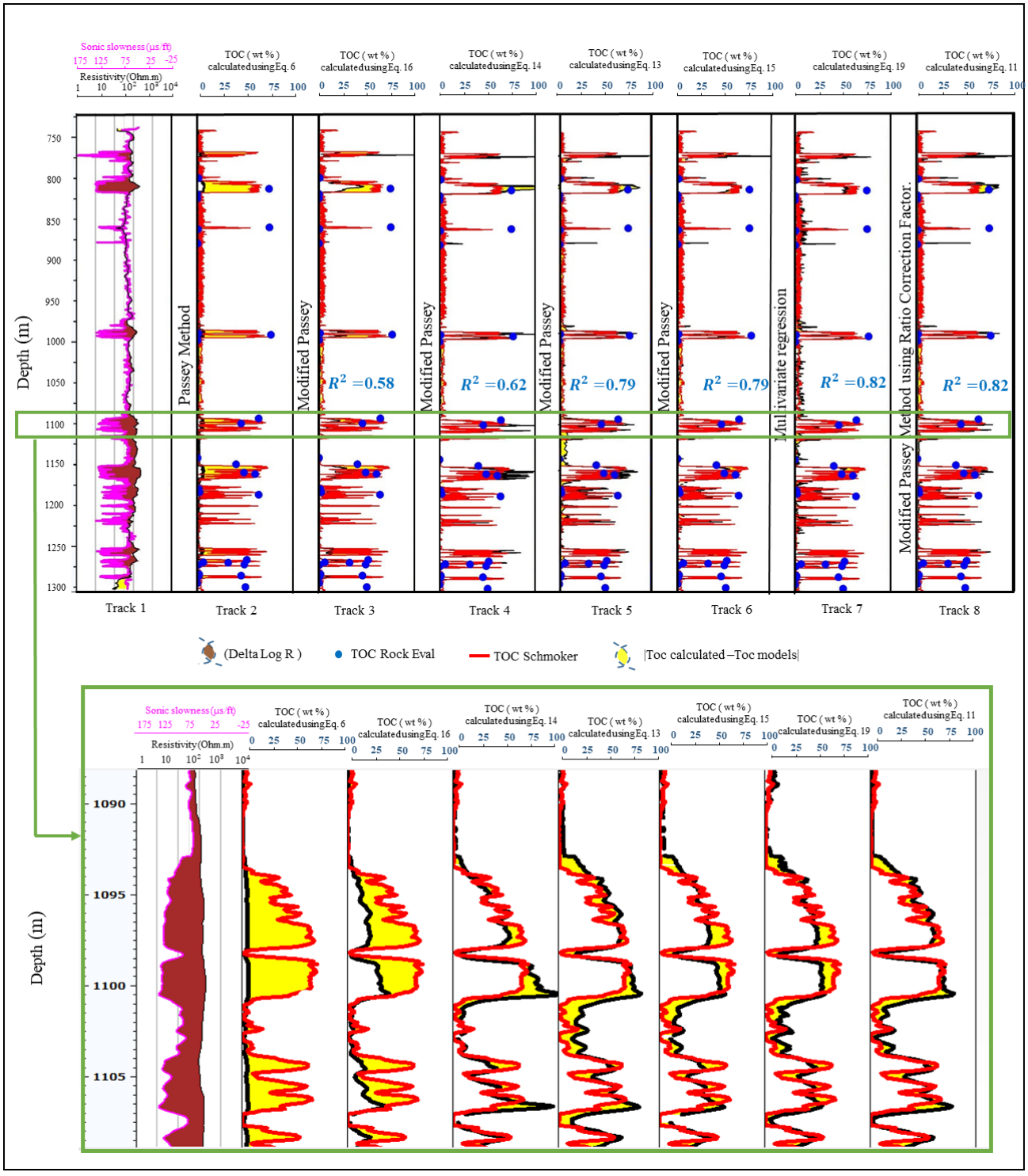
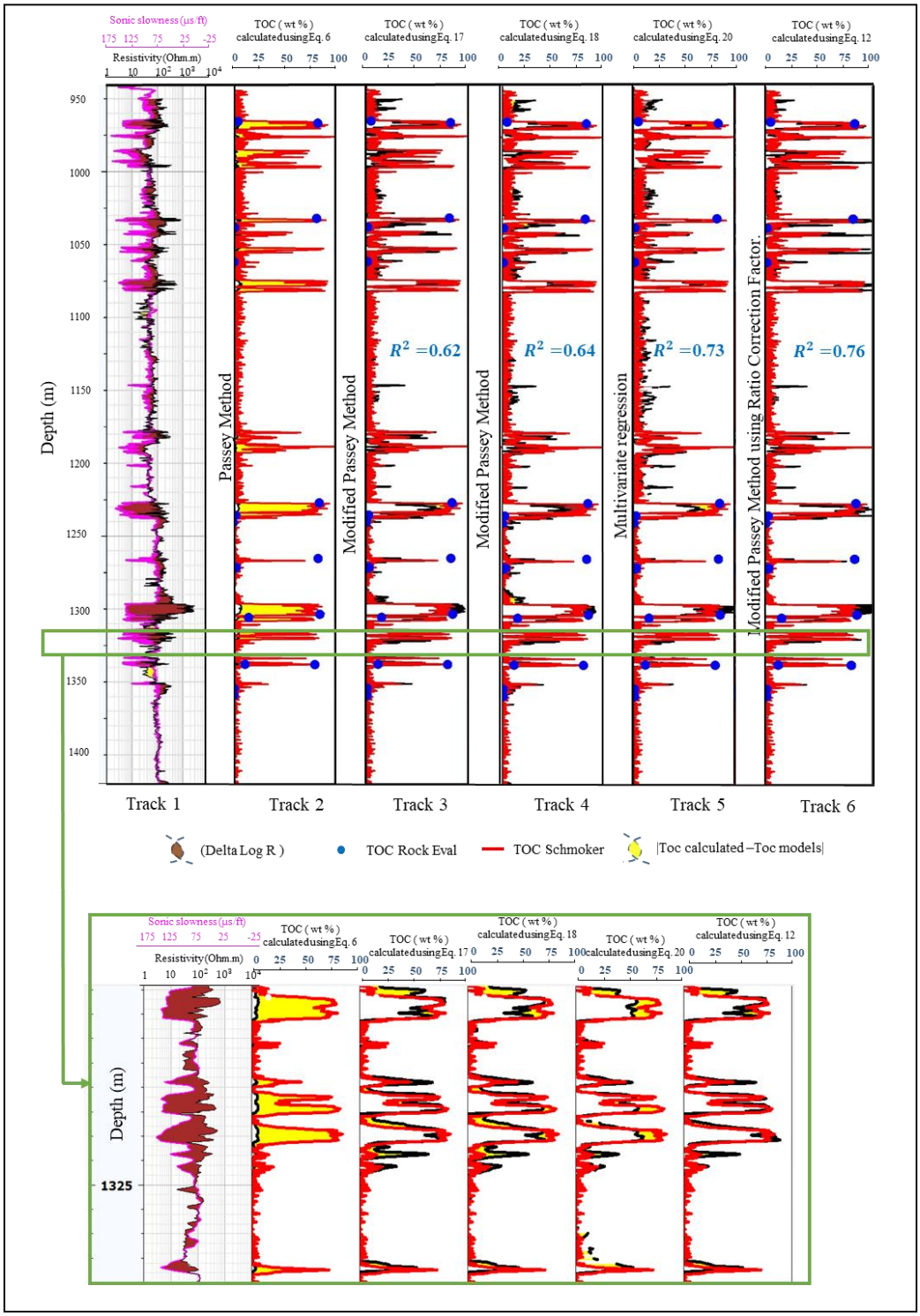


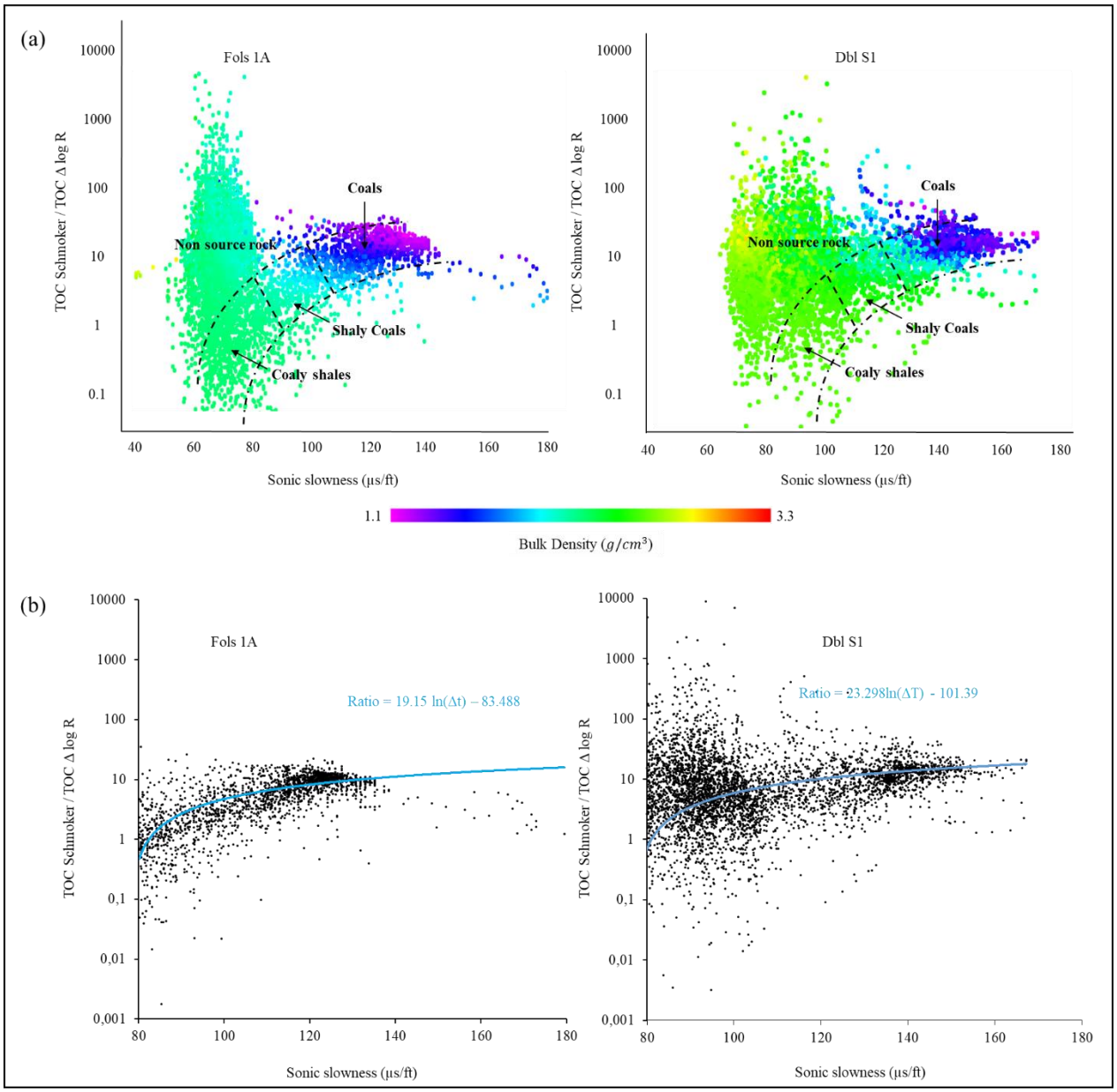
Fig. 6: Assessment of Total Organic Carbon (TOC) in Fols 1A well using different calculation methods based on well log data.



799

800 **Fig. 7:** Assessment of total organic carbon (TOC in wt%) in Dbl S1 well using different calculation

801 methods based on well log data.

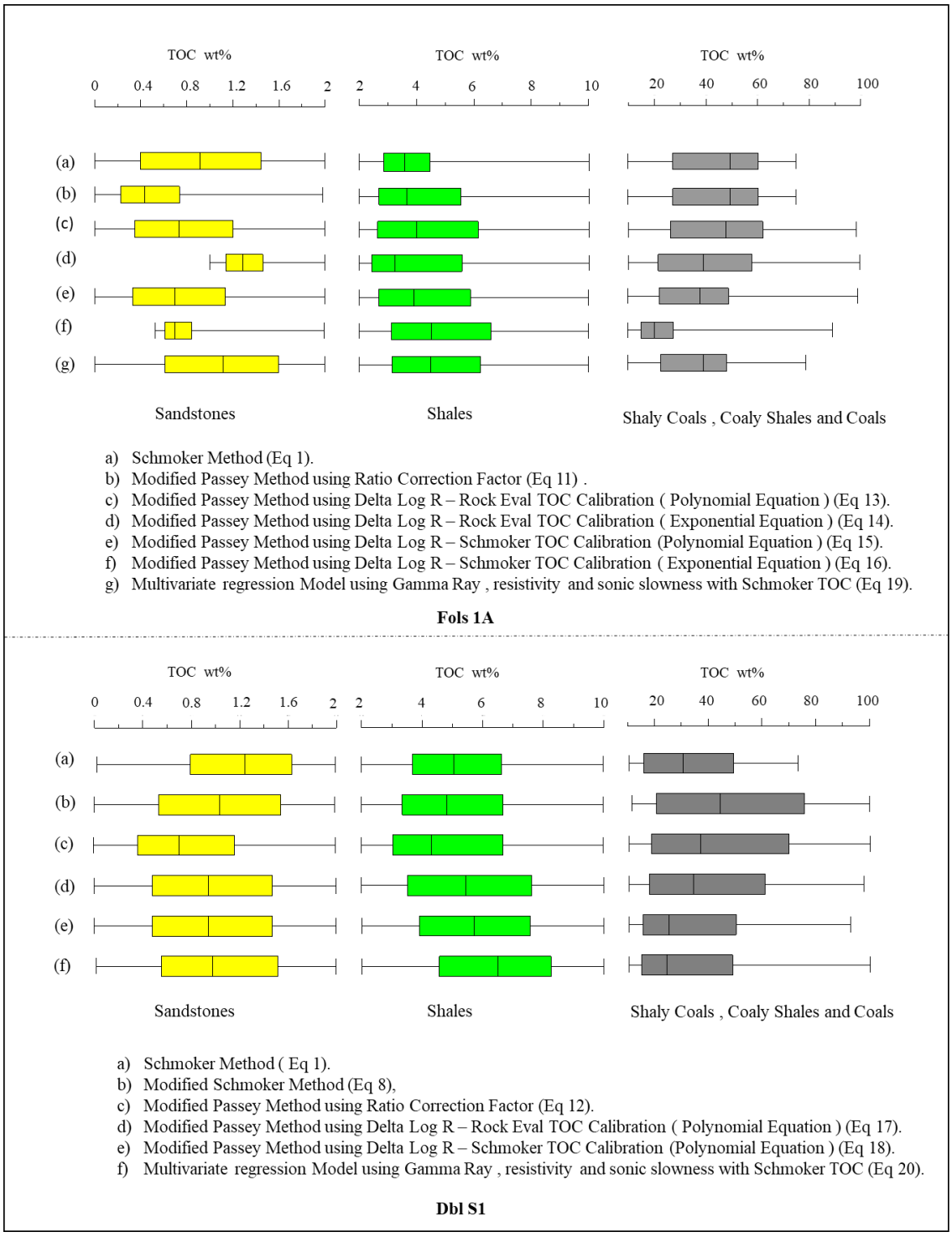


802

803 **Fig. 8:** Calculated TOC ratio using Schmoker and Delta log R methods in Fols 1A and Dbl S1

804 wells: (a) as a function of Sonic Slowness and bulk density: in color code for all lithologies, (b) as

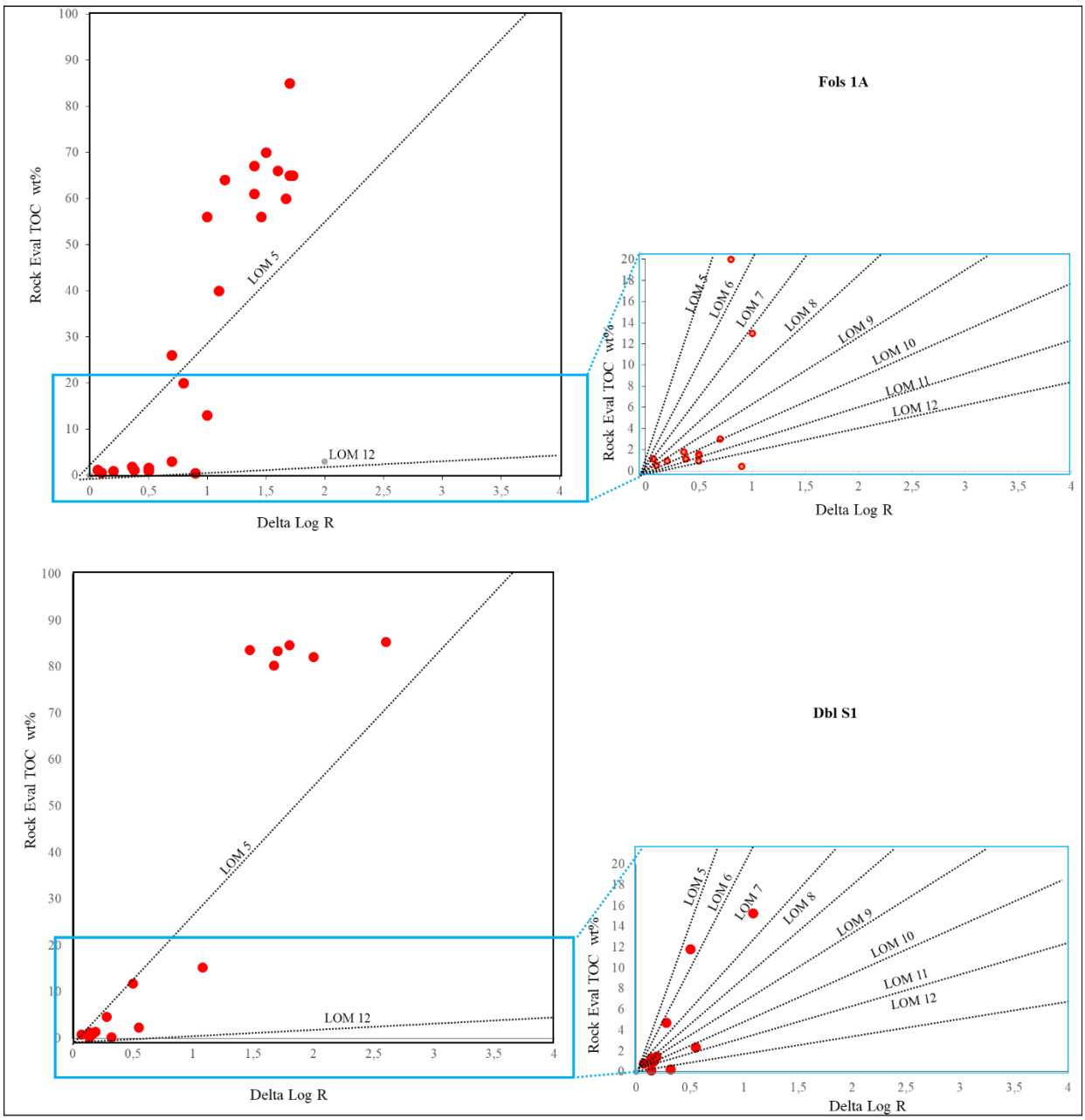
805 a function of Sonic Slowness only for coaly lithologies.



806

807 **Fig. 9:** Assessment of total organic carbon (TOC in wt%) in Fols 1A and Dbl S1 wells using

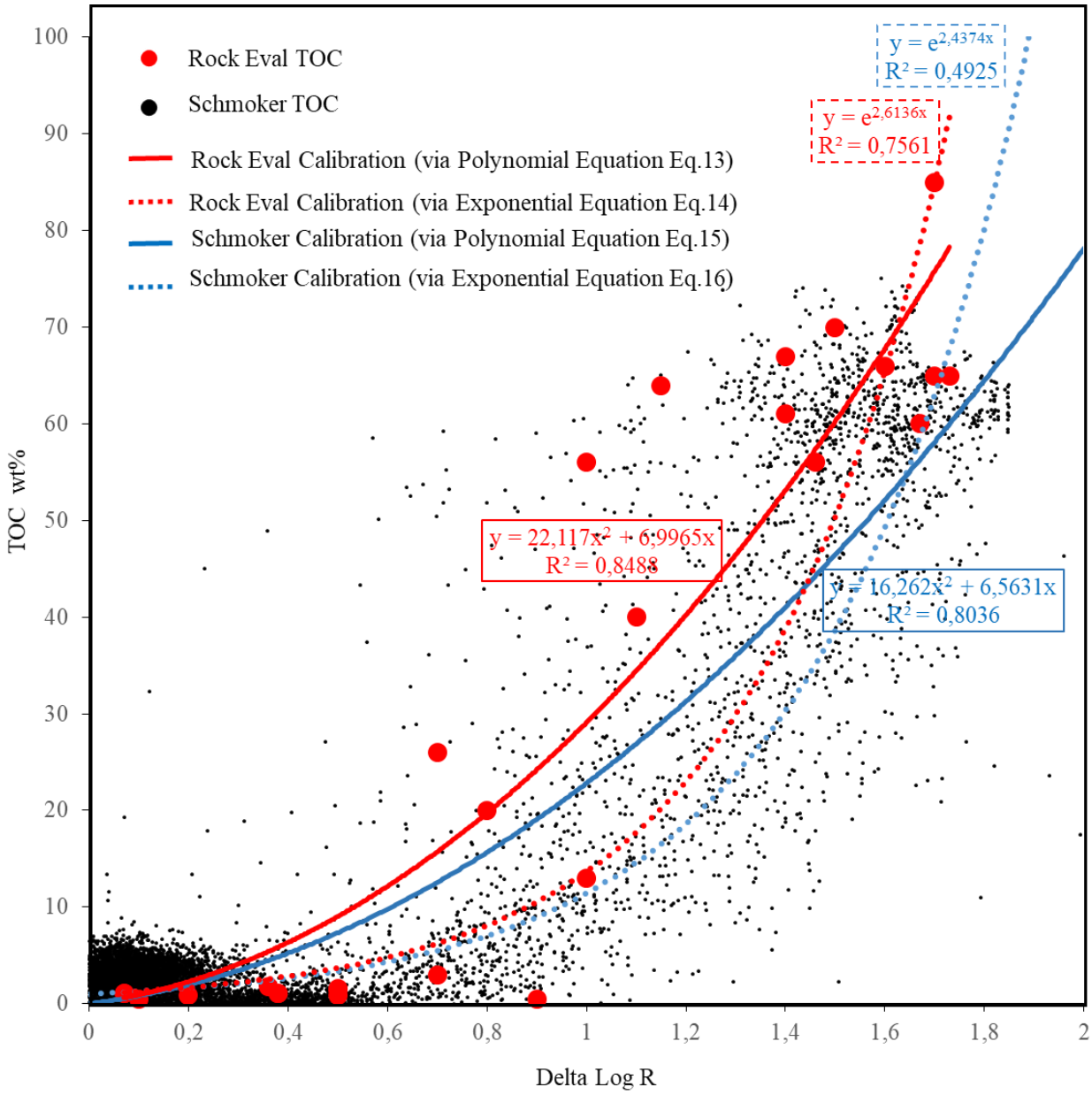
808 different calculation methods based on well log data as box plot analysis.



809

810 **Fig. 10:** Examining the Relationship between TOC (wt%) values and Delta log R using the diagram

811 of Passey *et al*. (1990) for Fols1A and Dbl S1 wells.



812

813 **Fig. 11:** Correlation equations between Rock-Eval measurements (red dots) and calculated using

814 Schmoker (1979, 1981) (black dots) TOC (wt%) versus delta log R (Passey *et al.*, 1990) for

815 Fols 1A well using different calibration equations.

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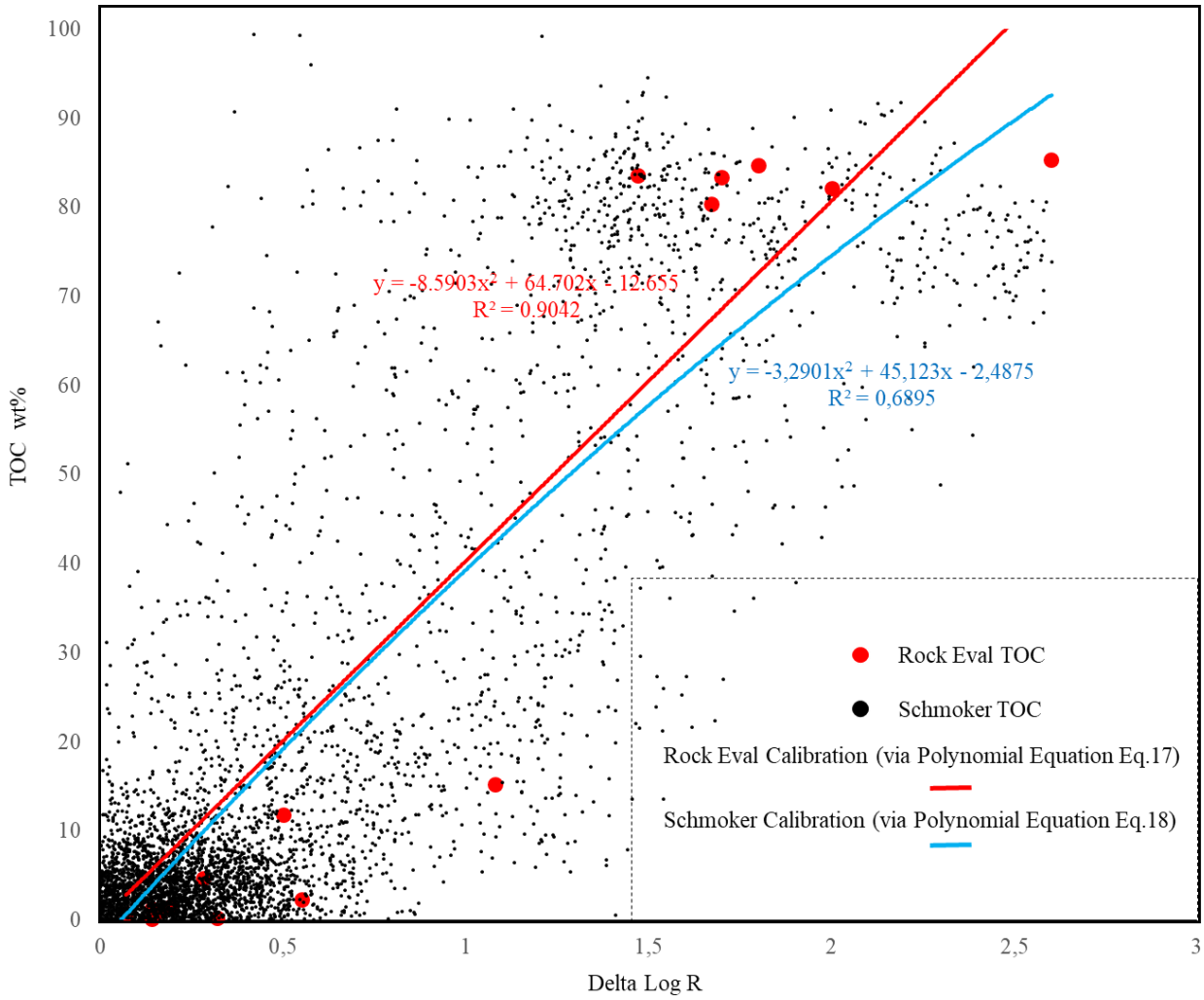

817

818 **Fig. 12:** Correlation equations between Rock-Eval measurements (red dots) and calculated using

819 Schmoker (1979, 1981) (black dots) TOC (wt%) versus Delta log R (Passey *et al.*, 1990) for

820 DBL S1 well using different calibration equations.

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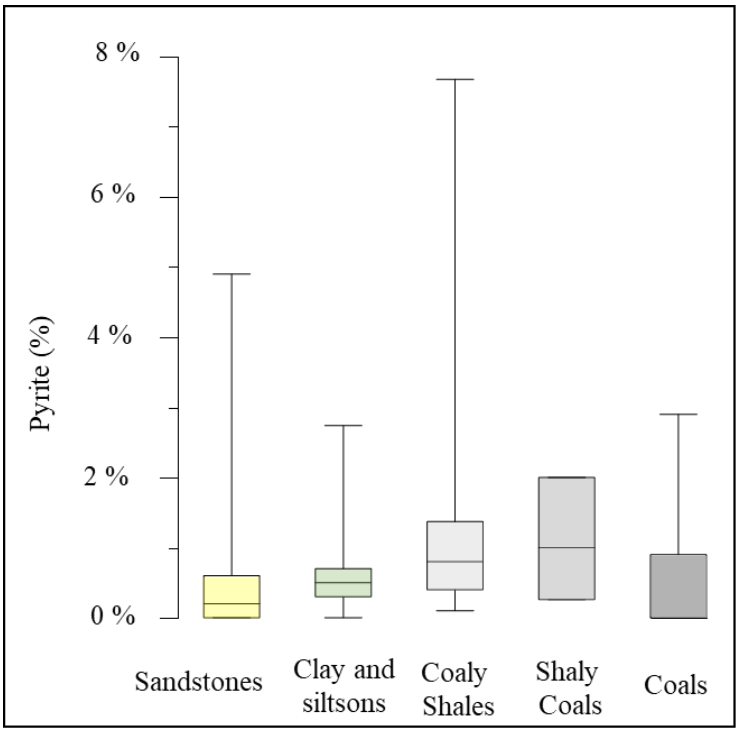
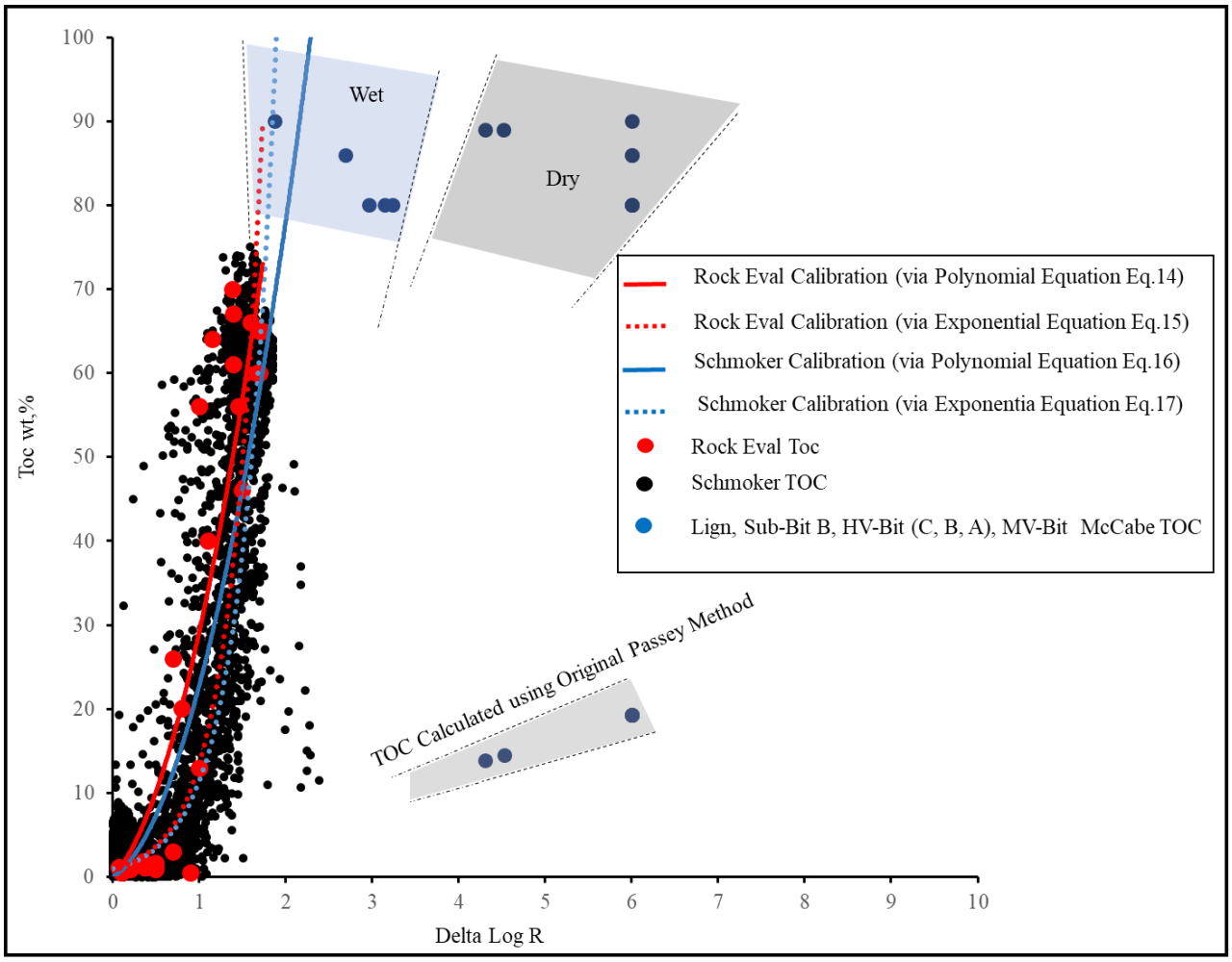


822

823 **Fig. 13:** Percentage of pyrite in different lithologies of Fols 1A and Dbl S1 wells. Data obtained

824 from XRD and petrographic analyses.



825

826 **Fig. 14:** Measured Rock Eval and calculated Schmoker TOC (wt%) values plotted against

827 Delta log R for the Fols 1A well.

828 **Tables**

829

Table 1. Vitrinite reflectance (%Ro) and Level of Organic Maturity determined after Hood *et al.* (1975) for samples from Fols 1A and DBLS 1 wells.

Well Name	Depth MD (m)	Vitrinite reflectance (%Ro)	Level of organic maturity (LOM)
Dbl S1	1300	0.96	10.65
Fols 1A	1094	0.84	10.12
Fols 1A	1100	0.85	10.17
Fols 1A	1150	0.89	10.36
Fols 1A	1160	0.84	10.12
Fols 1A	1162	0.89	10.36
Fols 1A	1267	0.84	10.12
Fols 1A	1286	0.93	10.53

Table 2. Delta log R Baseline values used for TOC calculations.

Well Name	Baseline Values	
	Resistivity (Ohm.m)	Sonic slowness (µs/ft)
Fols 1A	150	65
Dbl S1	100	80

838 **Table 3.** Table of resistivity data as a function of coal rank and TOC values for different coal types:
839 Resistivity data as a function of coal rank and TOC values for different coal types. The resistivity
840 values for bituminous coal (Max and Min) (Telford *et al.*, 1990), while the resistivity values for
841 sub-bituminous coal B and medium- and high-volatile bituminous coal (C, B and A) were derived
842 from the reference data study of McCabe and Tholey. (1945) .TOC values for each coal type were
843 based on the Passey equation and Rock Eval TOC values as reported by Mastalerz *et al*. (2011) (
844 [1]The wet coal samples were impregnated in water for 24 hours before being subjected to resistivity
845 measurement after McCabe and Tholey. (1945)).
846

Rank	Resistivity (ohm.m)		Delta log R		Passey TOC (wt%)		Expected TOC (wt%)
	Dry	Wet [1]	Dry	Wet [1]	Dry	Wet [1]	-
Sub-bituminous B Coal	3.10^6	5100	6	3.23	19.32	10.40	80
High volatile C bituminous Coal (1)	3.10^6	2740	6	2.96	19.32	9.53	80
High volatile C bituminous Coal (2)	3.10^6	4150	6	3.14	19.32	10.11	80
High volatile B bituminous Coal	3.10^6	ND	6	ND	19.32	ND	86
High volatile A bituminous Coal	3.10^6	1480	6	2.69	19.32	8.67	86
Medium volatile bituminous Coal	3.10^6	220	6	1.87	19.32	6	90
Bituminous Coal (Max)	10^5	ND	4.52	ND	14.56	ND	89
Bituminous Coal (Min)	6.10^4	ND	4.30	ND	13.85	ND	89

847

Table 4. Equations used in the calculation of TOC for the Fols 1A well. R^2: determination coefficient for each method. RMSE: Root Mean Squared Error for each method compared to TOC values obtained using the method by Schmoker (1979, 1981).

Methods Calibration		Eq	Modified TOC Equations	R^2	RMSE (wt. %)
TOC Schmoker/Passey Ratio		11	$TOC = \Delta Log\ R * 10^{(2.297-0.1688*LOM)} * (19.15 * ln(\Delta T) - 83.48)$	**0.82**	**8.52**
(Delta log R separation) **Vs** (TOC Calibration)	With Rock Eval TOC	13	$TOC = 22.117 * \Delta Log\ R^2 + 6.997 * \Delta Log\ R$	0.79	9.12
		14	$TOC = e^{2.6136*\Delta Log\ R}$	0.58	14
	With Schmoker TOC	15	$TOC = 16.262 * \Delta Log\ R^2 + 6.5631 * \Delta Log\ R$	0.79	7.04
		16	$TOC = e^{2.4374*\Delta Log\ R}$	0.62	5.23
Multivariate regression		19	$TOC = 0.73 * \Delta t - 0.065 * GammaRay + 0.02 * R - 46.29$	**0.82**	**6.6**

Table 5. Equations used in the calculation of TOC for the Dbl S1. R^2: determination coefficient for each method. RMSE, Root Mean Squared Error for each method compared to TOC values obtained using the method by Schmoker (1979, 1981).

Methods Calibration		Eq	Modified TOC Equations	R^2	RMSE (wt. %)
TOC Schmoker/Passey Ratio		12	$TOC = \Delta Log\ R * 10^{(2.297-0.1688*LOM)} * (23.298 * ln(\Delta T) - 103.48)$	**0.76**	**12**
(Delta log R separation) **Vs** (TOC Calibration)	With Rock Eval TOC	17	$TOC = -8.5903 * \Delta Log\ R^2 + 64.702 * \Delta Log\ R - 12.655$	0.62	17
	With Schmoker TOC	18	$TOC = -3.2901 * \Delta Log\ R^2 + 45.123 * \Delta Log\ R - 2.4875$	0.64	12
Multivariate regression		20	$TOC = 0.82 * \Delta t - 0.066 * GammaRay + 0.02 * R - 64.15$	**0.73**	**9.7**