GSA Data Repository 2020018

Bojanowski, M.J., et al., 2020, Pedogenic siderites fossilizing Ediacaran soil microorganisms on the Baltica paleocontinent: Geology, v. 48, https://doi.org/10.1130/G46746.1

Description of the material

Material for this study was selected from over six hundred samples representing the Ediacaran (Volyn, Redkino and Kotlin series) and Cambrian siliciclastic rocks, mostly mudstones. They were collected from 44 wells and 18 outcrops, located in the western area of the East European Craton (Arkhangelsk region, St. Petersburg region, Estonia, Lithuania, Belarus, Poland, Ukraine and Moldova). All samples were inspected by the quantitative XRD. Many of them are red-colored rocks that contain hematite and are siderite-free. Siderite was identified only in reduced greenish to gray rocks, where hematite is usually absent or insignificant. Some samples were concretions chiefly composed of siderite. Samples with >1% siderite were further inspected: stable C and O isotope analysis, organic geochemical investigations and optical microscopy and SEM on thin sections, were performed (Tab. A1). Evident pedogenic siderite was detected in three areas: St. Petersburg, Lithuania and eastern Belarus (Fig. 1B), representing northern and central parts of the Ediacaran sedimentary basin (Rozanov and Łydka, 1987). Siderite is rare in Lithuania, while in several profiles of the St. Petersburg area and eastern Belarus it is present in most of the Ediacaran samples above the Volyn series (Tab. A1). Average mineral contents were calculated for the St. Petersburg and eastern Belarus sections, where statistically significant number (102) of reduced gray-green samples with and without siderite was available. The sideritic samples are clearly enriched in kaolinite and fluoroapatite, whereas depleted in hematite, plagioclases and berthierine relative to the siderite-free samples. Significant differences were not observed for other minerals.

The most complete section with pedogenic siderites is from Bogushevsk-1 well (Makhnach et al., 2001), where they begin to occur in the uppermost part of the Volyn series

(Fig. S1). The greatest abundance is, however, in the Kotlin series. Pedogenic siderites were detected in eight horizons (out of twenty six sampled) within the top 200 m of the Ediacaran in this well (Fig. S1).

Biomarker indices based on *n*-alkanes, hopanes, and steranes

Location area & well name	Sample No.	*n*-alkanes		Hopanes	Steranes	S/H
		CPI	TAR	C31 S/(S+R)	C27/C29	
St. Petersburg, Russia						
Tajcy 2	Tajcy2/18	1.00	0.29	0.22	0.38	0.12
	Tajcy2/17	0.81	0.47	0.26	0.49	0.11
Vasilevskij Ostrov	5360/8	1.24	1.18	0.18	0.66	0.13
Bolshoya Izhora	BI-8B	0.93	0.38	0.19	0.45	0.09
Lakhta 77-1-270	L-46	1.52	0.94	0.19	0.52	0.14
Avloga	GDD200-25	1.25	2.40	0.21	0.35	0.13
Belarus						
Bogushevsk 2	BOG2-3	1.05	0.50	0.21	0.36	0.14
	BOG-52B	possibly contaminated		0.24	0.41	0.09
Lyozno 1	Lyozno-7	1.11	0.77	0.34	0.53	0.13

$CPI = \frac{C17+2(C19+C21+C23+\cdots+C31)}{2(C18+C20+C22+\cdots+C30)}$, in *m/z* 71 chromatogram

$TAR = \frac{(C27+C29+C31)}{(C15+C17+C19)}$, in *m/z* 71 chromatogram

$S/H = \frac{(C27\ \alpha\alpha\alpha\ S+\ C27\ \alpha\alpha\alpha\ R+\ C28\ \alpha\alpha\alpha\ S+C29\ \alpha\alpha\alpha\ S+\ C29\ \alpha\alpha\alpha\ R)}{(C29\alpha\beta+C29\beta\alpha+C30\alpha\beta+C30\beta\alpha+C31\alpha\beta\ S+C31\alpha\beta\ R+C30\beta\beta+C31\beta\alpha+C31\beta\beta)}$, in *m/z* 191 for hopanes and *m/z* 217 for steranes chromatograms.

Carbon Preference Index (CPI), refers to odd-over-even predominance (OEP) of numbers of C atoms in *n*-alkanes. Terrigenous OM is characterized by high values (>>1.0) of this parameter (Peters et al., 2005).

A predominance of long-chained odd-numbered *n*-alkanes (C_{27}, C_{29}, and C_{31}) characterize higher plants, while short-chained odd-numbered *n*-alkanes (C_{15}, C_{17}, and C_{19}) indicate

aquatic sources of OM. High values of **the Terrestrial (Terrigenous)/Aquatic Ratio (TAR)** shows the predominance of terrestrial-type OM (Bourbonniere and Meyers, 1996).

Hopanes have origins in bacteriohopanepolyols (BHPs), compounds contained in the lipid cell membranes of bacteria, while steranes are sterols derivatives and originated from eucariotic organisms (Peters et al., 2005). Low **Sterane/Hopane Ratio (S/H)** shows predominant input of prokaryotic organisms in OM.

Homohopanes are molecules which include carbon atoms from C_{31} to C_{35} with extended side chains, which isomerise at C-22 into two epimers, 22S and 22R. Biologically produced BHPs are characterised by the 22R configuration, which is converted gradually to 22S diastereomers during diagenesis. Equilibrium of the 22S/(22S+22R) ratio is achieved at ~0.5–0.6 (Peters et al., 2005). The lower values of **C_{31} S/(S+R)** ratio characterize the immature sample, below the oil window stage of OM maturation.

For the Precambrian and Palaeozoic source-rocks predominance of C_{27} steranes (cholestanes) is characteristic for red algae while C_{29} steranes (stigmastanes) for green algae (Schwark and Empt, 2006). Hence, low **C_{27}/C_{29}** ratio indicates predominance of green, photosynthetic algae.

References:

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Supplementary Figure Captions

Figure DR1. Litholog of the Ediacaran strata in Bogushevsk-1 well with locations of samples containing pedogenic siderite. Lithology compiled from own investigations on the available core, the description of Bogushevsk-1 well supplied by Oksana Kuzmenkova (Research and Production Center for Geology, Minsk, Belarus) and the nearby (Fig. 1B) Bogushevsk-2 well (Makhnach et al., 2001). Dev. - Devonian, Mesop. - Mesoproterozoic.

Figure DR2. Elemental composition of siderite cement. A: Results of EDS analyses (in mol%) for S1 and S2 siderite generations in sphaerosiderites and microcrystalline cements. B: WDS mapping illustrating major differences between S1 and S2 siderite generations in microcrystalline cement (sample Bog-8A). S1 contains P and is Mg-poor, whereas S2 is P-free and Mg-rich, which is observed in all samples. Mn content is slightly higher in S1 in this case, but it may differ in other samples. Ap- fluorapatite.

Figure DR3. Partial mass chromatogram (*m/z* 117) of L-46 sample showing the distribution of high molecular weight *n*-carboxylic acids with even-over-odd homologues preponderance. Numbers above peaks represent the number of C atoms in the molecule.

Figure DR4. Partial chromatograms (*m/z* 71) showing preponderance of long chain odd-carbon-number *n*-alkanes from siderite-bearing and surrounding siderite-free samples from Avloga well. Numbers above peaks denote number of carbon atoms in the molecule. Pr – pristine; Ph – phytane.

TABLE A1. LOCATION, MINERALOGICAL, PETROGRAPHIC AND GEOCHEMICAL DATA OF THE SIDERITE-BEARING SAMPLES STUDIED

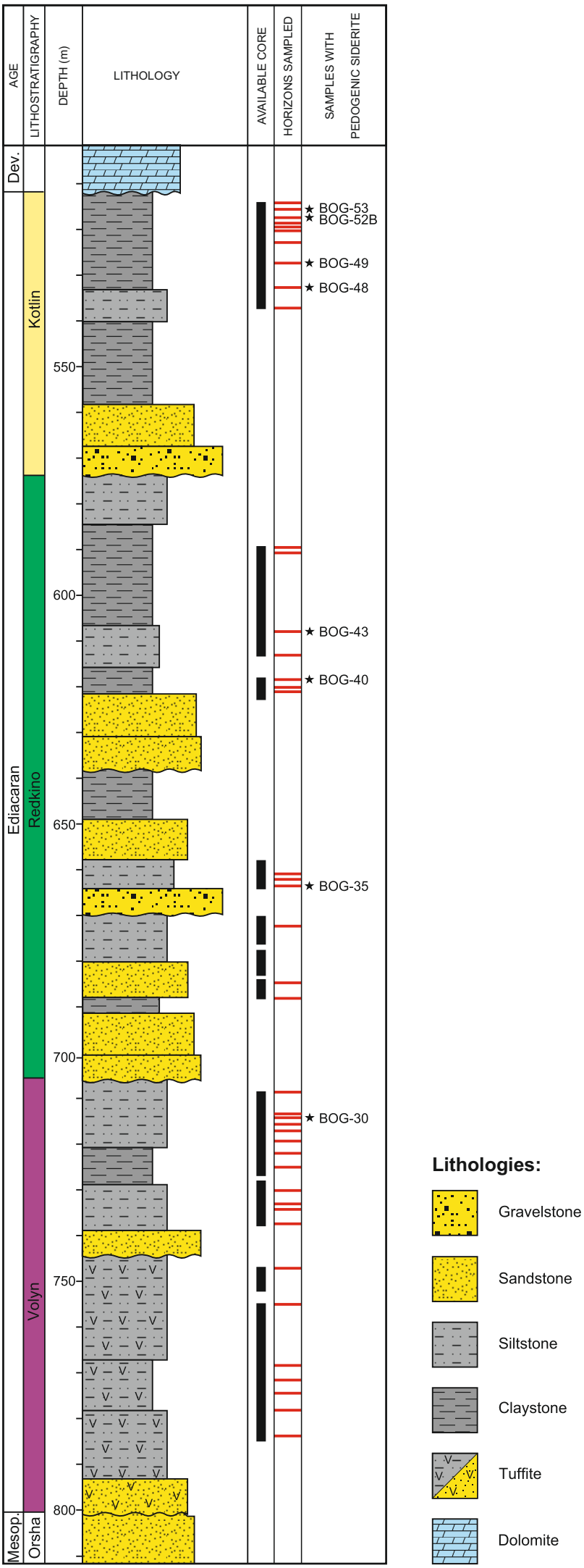
Location area & well/outcrop name	GPS coordinates	Core storage location	Sample No.	Sample depth (m)	Lithology	System & Lithostratigraphic unit	Siderite micromorphology	Mineral composition (wt%) Siderite	Calcite	Dolomite	Quartz	Feldspars	Micas	Chlorites	Hematite	Goethite	Pyrite	Apatite	Berthierine	Illite+IS	Anatase	Jarosite	Kaolinite	TOC (%)	Isotopic composition $\delta^{13}C$ (‰)	$\delta^{18}O$ (‰)
St. Petersburg, Russia																										
			Tajcy2/18	293.9	green mudstone	Ediacaran, Kotlin series	microcrystalline, encrusting	6.9	N.D.#	N.D.#	34.5	5.3	4.6	2.8	N.D.#	N.D.#	trace	N.D.#	4.2	30.7	0.3		10.7	no data	7.1	-6.9
Tajcy 2	N59.6611 E30.1386	liquidated hydrogeological drill core	Tajcy2/17	305.2	green mudstone	Ediacaran, Kotlin series		4.6	N.D.#	N.D.#	43.8	10.4	3.0	1.0	N.D.#	N.D.#	N.D.#	N.D.#	2.5	21.7	0.3		12.7	no data	7.2	-8.2
			Tajcy2/16	307.1	green mudstone	Ediacaran, Kotlin series		3.0	N.D.#	N.D.#	49.1	10.0	3.1	N.D.#	N.D.#	N.D.#	N.D.#	N.D.#	2.1	19.2	0.5		12.9	no data	-2.2	-8.6
Sosnovyj Bor	N59.8533 E29.0889	liquidated drill core	SB-2	43.2	mudstone	Ediacaran, Kotlin series	microcrystalline	2.2	N.D.#	N.D.#	24.1	8.4	24.3	8.7	N.D.#	N.D.#	trace	N.D.#	N.D.#	19.4	0.7	0.8	11.4	0.6	14.2	-6.4
Vasilevskij Ostrov	N59.9544 E30.2378	liquidated drill core	5360/11	40.2	green mudstone	Cambrian	sphaerosiderite, microcrystalline	20.1	N.D.#	trace	33.0	7.6	12.5	3.5	N.D.#	N.D.#	0.7	trace	N.D.#	15.1	N.D.#	N.D.#	7.4	0.0	7.6	-6.6
			5360/8	59.2	brecciated green sandy mudstone	Ediacaran, Kotlin series	sphaerosiderite	1.3	N.D.#	N.D.#	35.5	7.7	17.6	6.9	N.D.#	N.D.#	trace	N.D.#	N.D.#	20.3	N.D.#	N.D.#	10.9	no data	9.6	-7.2
			BI-6	surface	concretionary siderite in mudstone	Ediacaran, Kotlin series	microcrystalline	39.6	N.D.#	N.D.#	8.9	3.3	9.5	1.5	N.D.#	N.D.#	trace	17.0	N.D.#	10.0	N.D.#	N.D.#	10.3	0.7	9.7	-6.9
Bolshoya Izhora	N59.9378 E29.5703	outcrop	BI-8A	surface	concretionary siderite in mudstone	Ediacaran, Kotlin series	microcrystalline, encrusting	28.2	N.D.#	N.D.#	8.4	1.7	19.0	2.6	N.D.#	4.3*	trace	19.9	N.D.#	9.7	N.D.#	N.D.#	6.1	no data	13.9	-6.5
			BI-8B	surface	concretionary siderite in mudstone	Ediacaran, Kotlin series	microcrystalline	43.4	N.D.#	N.D.#	5.6	1.4	25.2	N.D.#	N.D.#	8.7*	trace	trace	N.D.#	11.5	N.D.#	N.D.#	4.2	no data	10.2	-7.7
			L-39	39.0	concretionary siderite and dolomite in mudstone	Ediacaran, Kotlin series	sphaerosiderite, microcrystalline	28.1	N.D.#	14.4	20.5	12.9	11.1	N.D.#	N.D.#	N.D.#	trace	N.D.#	N.D.#	10.4	N.D.#	N.D.#	2.4	no data	2.1	-7.0
Lakhta 77-1-270	N59.9869 E30.1764	liquidated technical drill core	L-41	41.0	mudstone	Ediacaran, Kotlin series	microcrystalline, encrusting(?)	4.9	N.D.#	N.D.#	35.4	7.1	22.7	1.4	N.D.#	N.D.#	N.D.#	N.D.#	5.9	13.2	0.2	N.D.#	8.9	0.2	5.9	-7.0
			L-46	46.0	mudstone	Ediacaran, Kotlin series		1.6	N.D.#	N.D.#	30.2	6.5	25.0	1.7	N.D.#	N.D.#	N.D.#	N.D.#	6.9	15.7	N.D.#	0.6	12.0		11.1	-7.9
			L-107	107.0	siltstone	Ediacaran, Kotlin series	microcrystalline	2.2	N.D.#	N.D.#	59.8	13.2	4.0	1.7	N.D.#	N.D.#	trace	N.D.#	N.D.#	7.6	N.D.#	N.D.#	11.5	0.1	-3.0	-8.5
		Core repository of Institute of Precambrian	GDD200-25	123.5	grey mudstone	Ediacaran, Kotlin series	encrusting, microcrystalline	5.8	0.2	N.D.#	35.0	4.6	6.5	5.6	N.D.#	N.D.#	0.4	N.D.#	N.D.#	31.3	0.5	N.D.#	10.3	0.4	9.8	-7.8
Avloga	N60.2653 E30.4642	Geology and Geochronology RAS in St. Petersburg	GDD200-21	148.8	grey mudstone	Ediacaran, Kotlin series		2.4	0.4	N.D.#	65.3	23.9	1.2	N.D.#	N.D.#	N.D.#	N.D.#	N.D.#	N.D.#	2.6	0.2	N.D.#	4.3	0.2	1.3	-7.6
			GDD200-20	152.5	grey mudstone	Ediacaran, Kotlin series		1.5	N.D.#	N.D.#	39.1	14.9	8.7	N.D.#	N.D.#	N.D.#	0.4	N.D.#	3.5	14.1	0.3	N.D.#	17.5	0.2	-5.2	-8.1
Lithuania																										
			VIL-20	345.4	grey mudstone	Cambrian	microcrystalline	4.9	N.D.#	1.7	26.2	18.8	10.9	N.D.#	0.5	N.D.#	0.3	N.D.#	N.D.#	20.5	0.3	N.D.#	15.7	1.0	-5.3	-4.9
Vilkiskiai 68	N54.4665 E25.4147	Core repository of Lithuanian Geological Survey in Vievis	VIL-18A	376.0	silt-/sandstone	Ediacaran, Kotlin series	sphaerosiderite	7.2	N.D.#	3.1	38.8	N.D.#	9.0	N.D.#	1.0	N.D.#	trace	N.D.#	N.D.#	6.0	1.4	N.D.#	33.4	0.5	-5.4	-5.1
			VIL-18B	376.0	violet siltstone	Ediacaran, Kotlin series	sphaerosiderite	5.5	N.D.#	N.D.#	32.2	0.6	8.0	N.D.#	2.3	N.D.#	N.D.#	N.D.#	N.D.#	13.7	1.1	N.D.#	36.3	no data	-5.1	-5.5
Belarus																										
Bogushevsk 2	N54.84 E30.21**	Belarussian Geological Survey in Minsk	BOG2-3	554.0	concretionary siderite in siltstone	Ediacaran, Kotlin series	microcrystalline, encrusting	27.0	N.D.#	N.D.#	15.8	8.1	2.7	N.D.#	N.D.#	N.D.#	0.5	12.2	N.D.#	22.3	N.D.#	N.D.#	11.4	no data	0.9	-8.1
			BOG-53	516.0	siltstone	Ediacaran, Kotlin series	encrusting, microcrystalline	7.9	2.6	N.D.#	28.0	21.6	7.0	N.D.#	N.D.#	N.D.#	0.8	trace	3.8	7.4	0.2	N.D.#	20.9	0.6	-2.9	-5.8
			BOG-52B	517.7	concretionary siderite in siltstone	Ediacaran, Kotlin series	microcrystalline	62.7	N.D.#	N.D.#	12.7	6.6	5.4	N.D.#	N.D.#	N.D.#	trace	N.D.#	N.D.#	1.5	N.D.#	N.D.#	11.0	no data	-2.0	-5.5
			BOG-49	527.0	grey mudstone	Ediacaran, Kotlin series		2.0	1.0	N.D.#	43.1	14.3	7.8	N.D.#	N.D.#	0.3	N.D.#	N.D.#	6.1	10.0	0.3	N.D.#	15.1	0.3	-4.2	-6.7
Bogushevsk 1	N54.84 E30.21**	Core repository of Belarussian Geological Survey in Sluck	BOG-48	533.0	grey mudstone	Ediacaran, Kotlin series		2.1	N.D.#	N.D.#	47.9	12.9	6.4	N.D.#	N.D.#	0.8	N.D.#	N.D.#	3.3	12.8	0.5	N.D.#	13.1	0.1	-7.1	-6.1
			BOG-43	608.0	grey mudstone	Ediacaran, Redklino series	sphaerosiderite	3.3	N.D.#	N.D.#	24.7	23.3	9.7	0.8	N.D.#	1.3	0.3	N.D.#	5.9	14.8	0.5	N.D.#	15.3	0.4	-11.1	-8.7
			BOG-40	618.0	grey mudstone	Ediacaran, Redklino series	microcrystalline	1.1	N.D.#	N.D.#	21.7	25.5	7.2	N.D.#	N.D.#	1.3	1.7	N.D.#	14.1	12.9	0.3	N.D.#	14.2	0.3	-11.3	-8.2
			BOG-35	663.0	concretionary siderite in mudstone	Ediacaran, Redklino series	encrusting, microcrystalline	18.8	9.0	N.D.#	15.4	12.1	5.6	4.8	N.D.#	1.0	trace	N.D.#	13.1	N.D.#	0.7	N.D.#	19.7	no data	-17.6	-7.7
			BOG-30	715.3	concretionary siderite in mudstone with volcanoclastic component	Ediacaran, Volyn series	encrusting, microcrystalline	40.8	N.D.#	N.D.#	18.9	8.5	1.9	N.D.#	N.D.#	1.5	0.5	N.D.#	3.9	4.0	0.5	N.D.#	19.3	0.5	-19.5	-6.6
Lyozno 1	N55.03 E30.80**	Core repository of Belarussian Geological Survey in Sluck	Lyozno-7	615.0	grey mudstone	Ediacaran, Kotlin series		1.0	N.D.#	N.D.#	22.2	18.5	10.1	N.D.#	N.D.#	1.3	1.8	N.D.#	7.9	17.5	0.2	N.D.#	19.4	0.3	-12.4	-5.4
			Lyozno-2	657.0	grey mudstone	Ediacaran, Kotlin series		1.4	N.D.#	N.D.#	26.6	22.2	3.5	N.D.#	1.2	1.0	N.D.#	N.D.#	7.9	13.4	0.4	N.D.#	22.3	0.3	-8.2	-7.5

*Goethite associated with modern weathering and oxidation of siderite

#N.D. = not detected

**Precise location information is classified. Location of the nearest town is given.

Fig. DR1


AGE
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DEPTH (m)
LITHOLOGY
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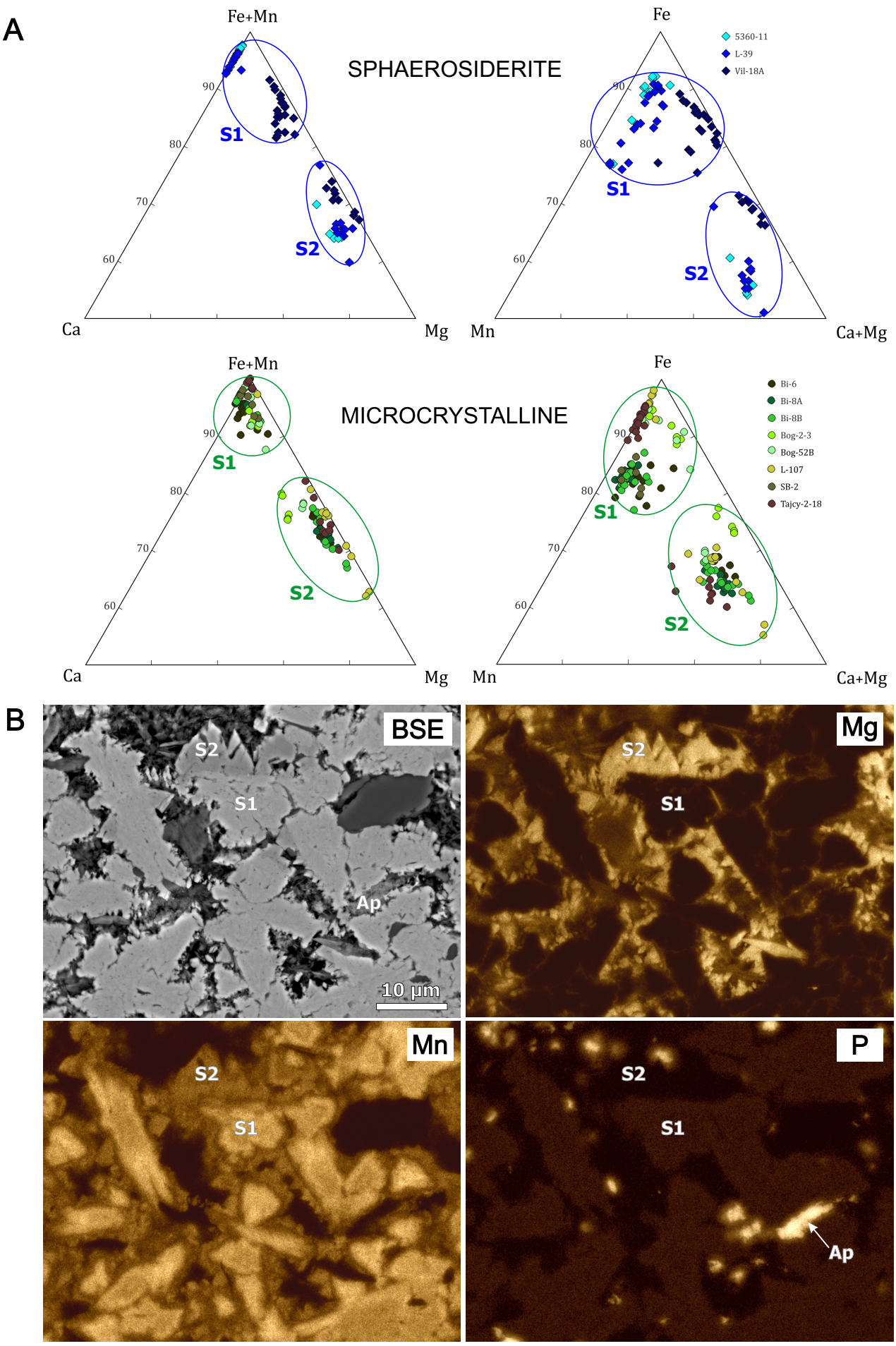
SAMPLES WITH PEDOGENIC SIDERITE
Dev.
Ediacaran
Kotlin
Redkino
Volyn
Mesop.
Orsha
550
600
650
700
750
800
BOG-53
BOG-52B
BOG-49
BOG-48
BOG-43
BOG-40
BOG-35
BOG-30
Lithologies:
Gravelstone
Sandstone
Siltstone
Claystone
Tuffite
Dolomite

Fig. DR2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SPHAEROSIDERITE
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Mg
Fe
Mn
Ca+Mg
S1
S2
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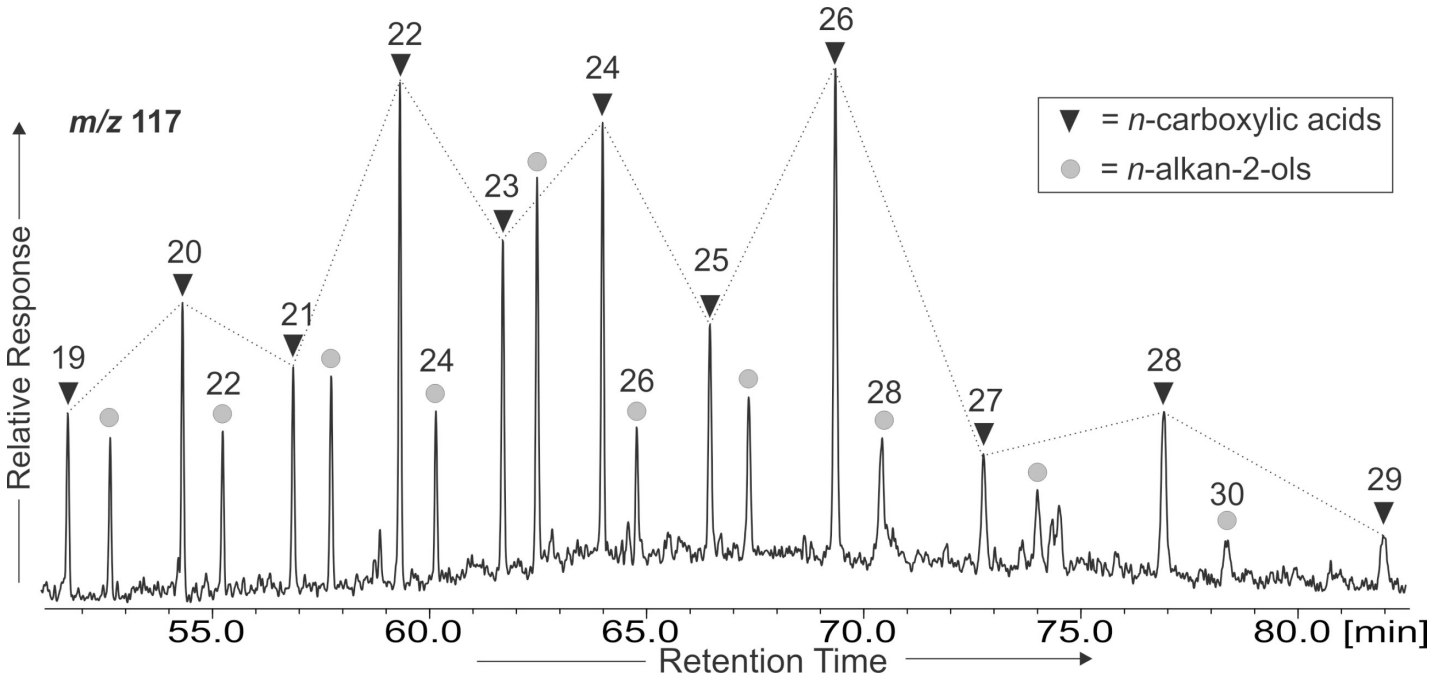
80
70
60
5360-11
L-39
Vil-18A
MICROCRYSTALLINE
Bi-6
Bi-8A
Bi-8B
Bog-2-3
Bog-52B
L-107
SB-2
Tajcy-2-18
B
BSE
Mg
Mn
P
Ap
10 µm

Fig. DR3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Relative Response
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= n-alkan-2-ols
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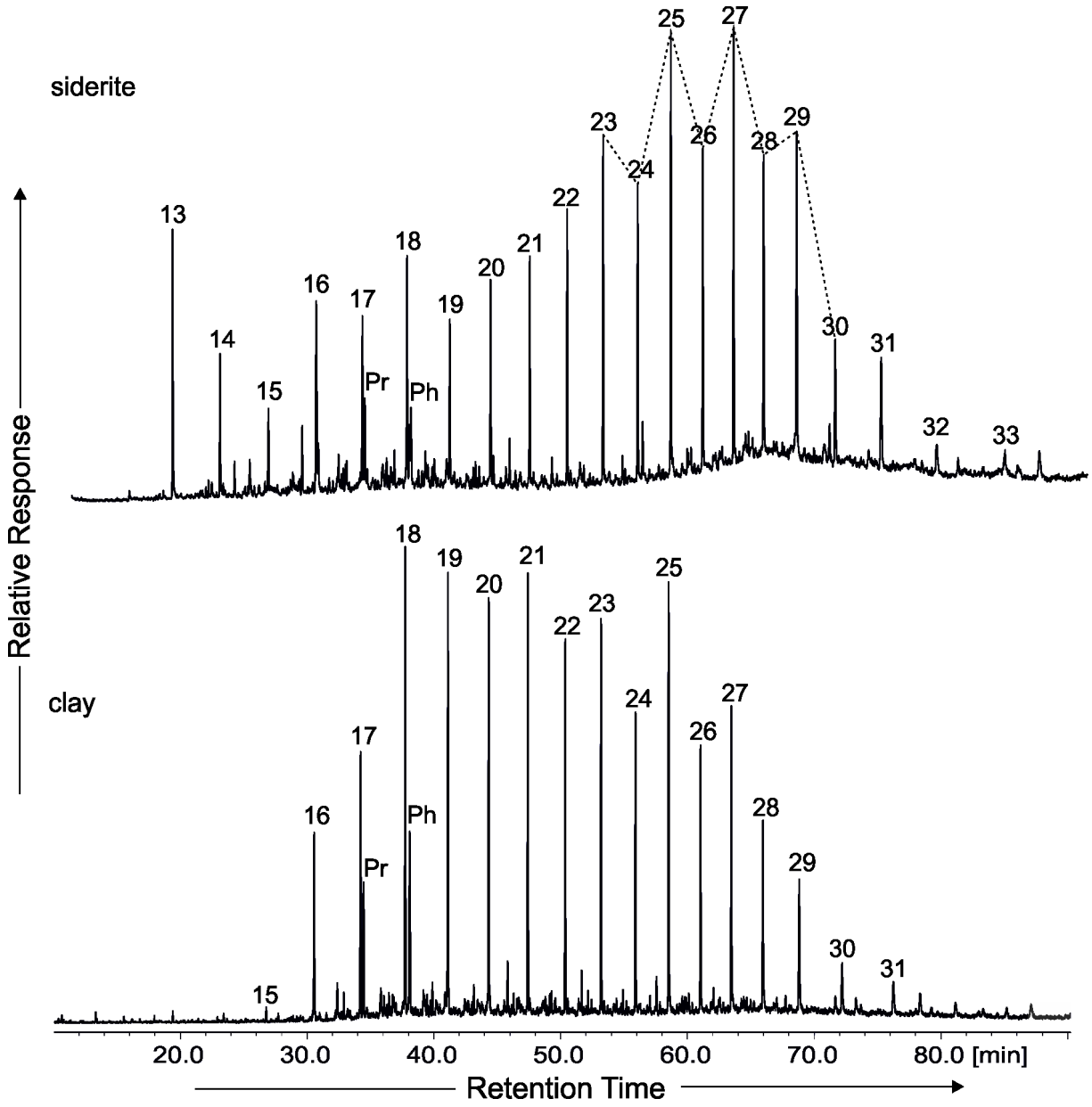
21
22
24
23
24
26
25
26
28
27
28
30
29
55.0
60.0
65.0
70.0
75.0
80.0 [min]
Retention Time

Fig. DR4


siderite
clay
Relative Response
Retention Time
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15
16
17
Pr
18
Ph
19
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27
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