Supplementary Information

Influence of minor hydrocarbon seepage on sulfur cycling in marine subsurface sediments and its significance for hydrocarbon reservoir detection

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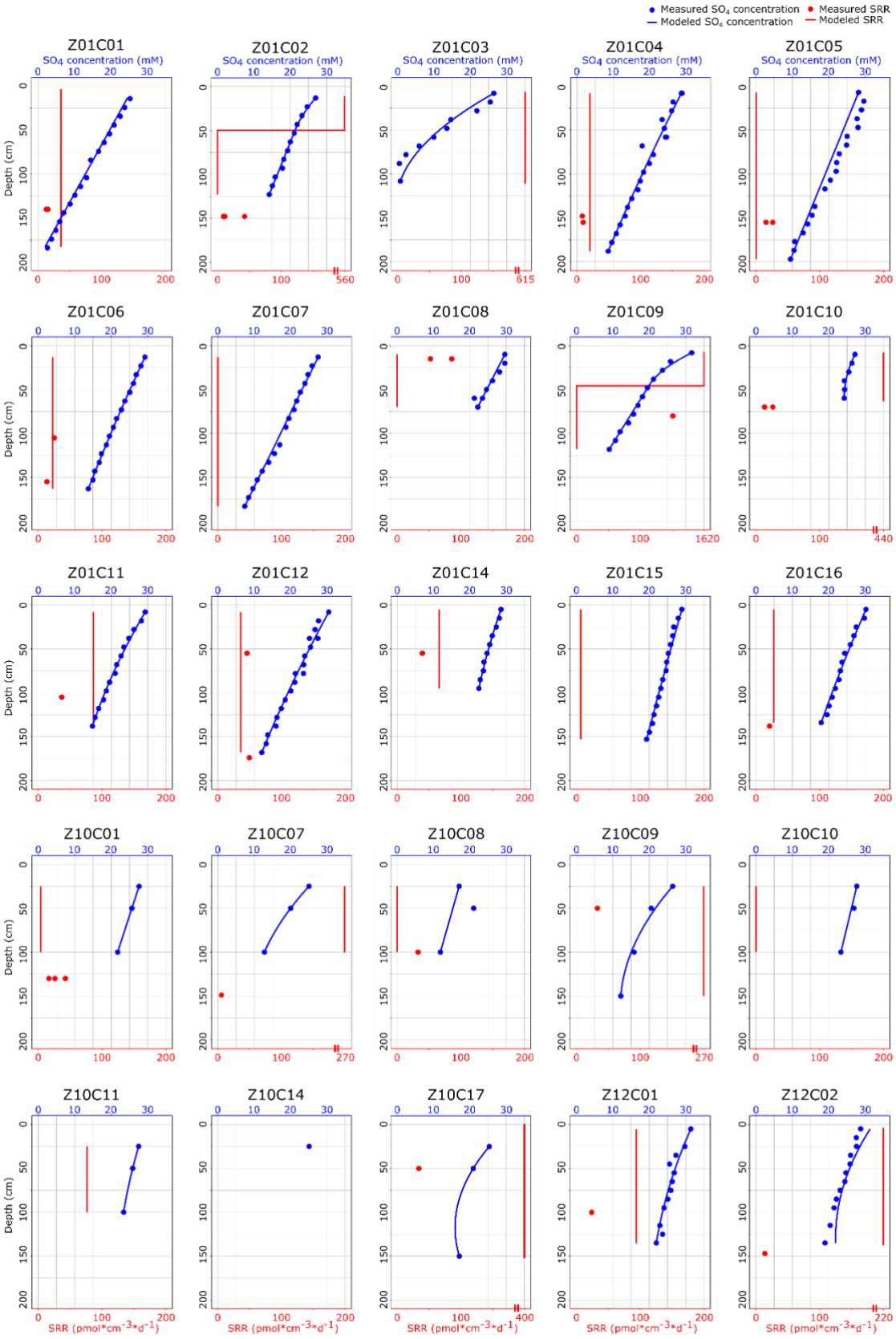
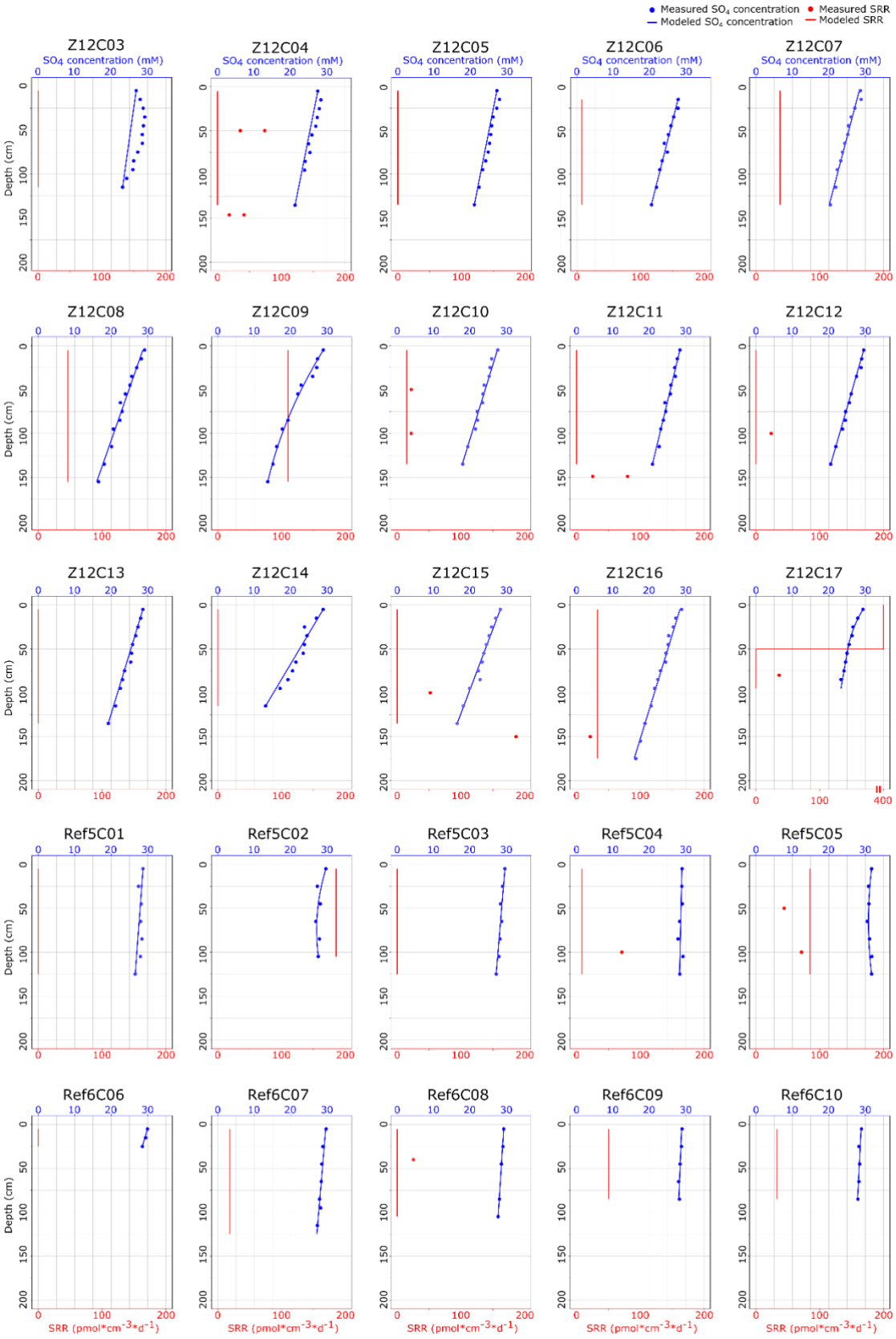

Measured SO_4 concentration
Modeled SO_4 concentration
Measured SRR
Modeled SRR
Z01C01
Z01C02
Z01C03
Z01C04
Z01C05
Z01C06
Z01C07
Z01C08
Z01C09
Z01C10
Z01C11
Z01C12
Z01C14
Z01C15
Z01C16
Z10C01
Z10C07
Z10C08
Z10C09
Z10C10
Z10C11
Z10C14
Z10C17
Z12C01
Z12C02
SO_4 concentration (mM)
Depth (cm)
SRR (pmol*cm^{-3}*d^{-1})


Measured SO4 concentration
Modeled SO4 concentration
Measured SRR
Modeled SRR
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Z12C05
Z12C06
Z12C07
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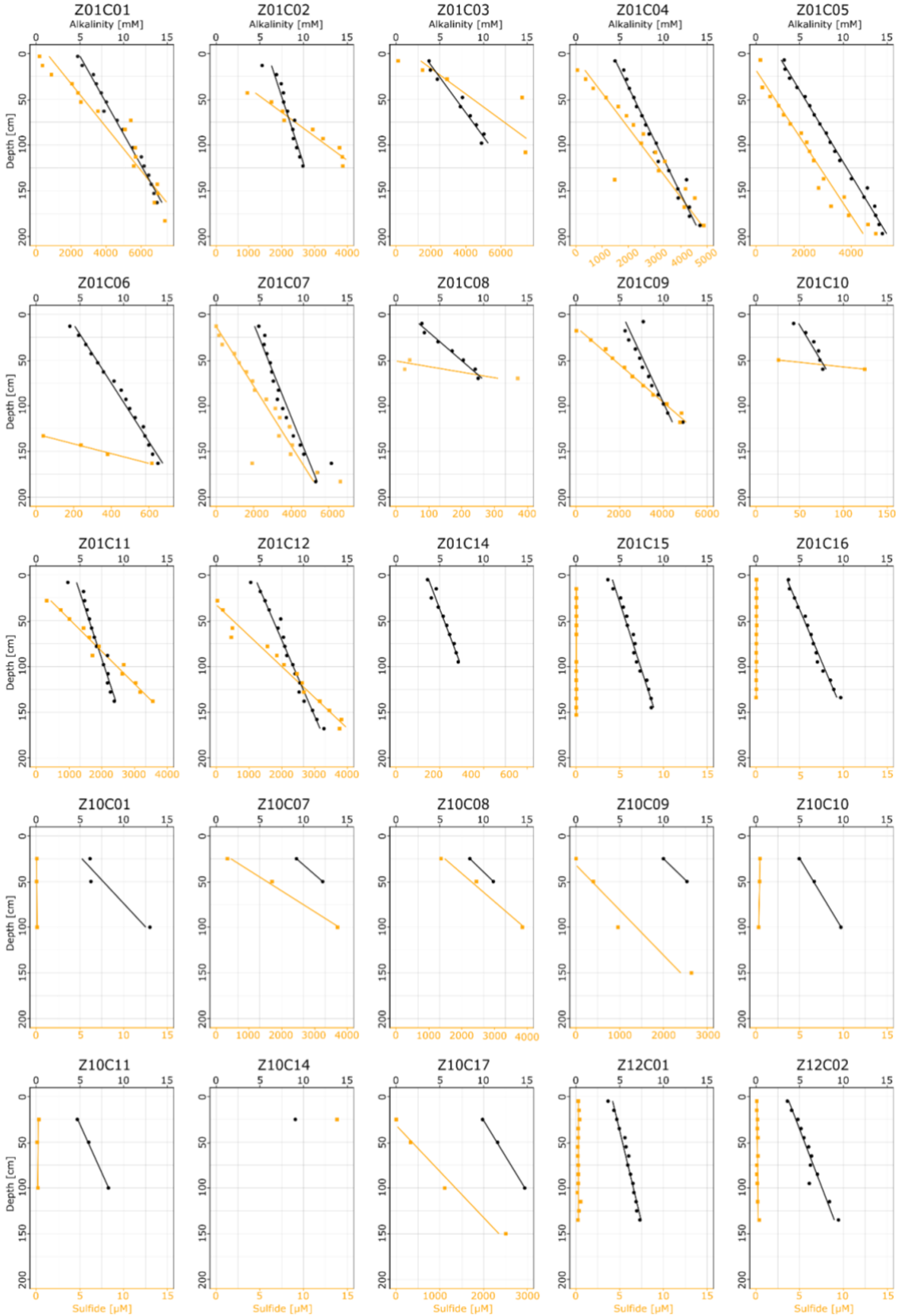
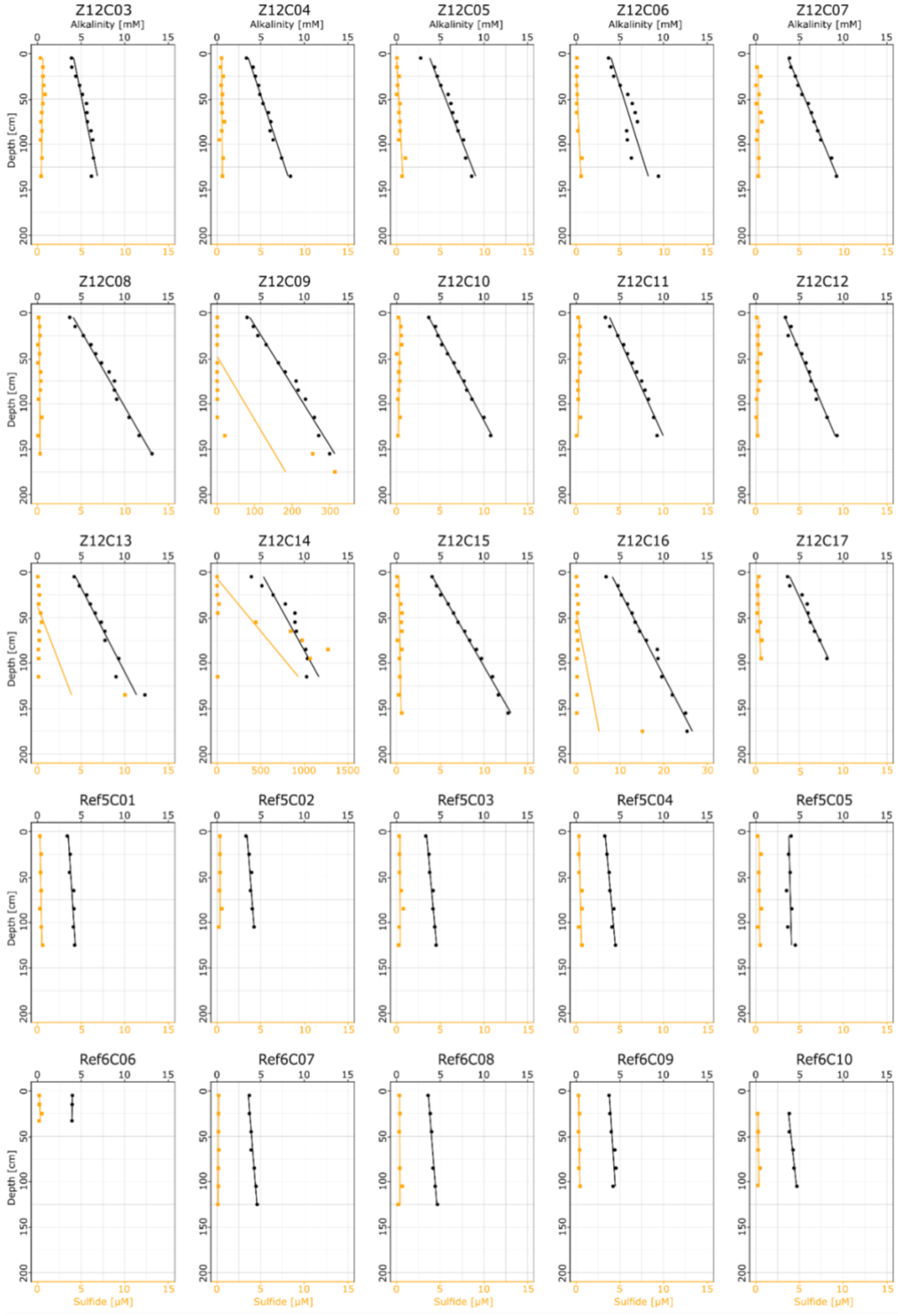
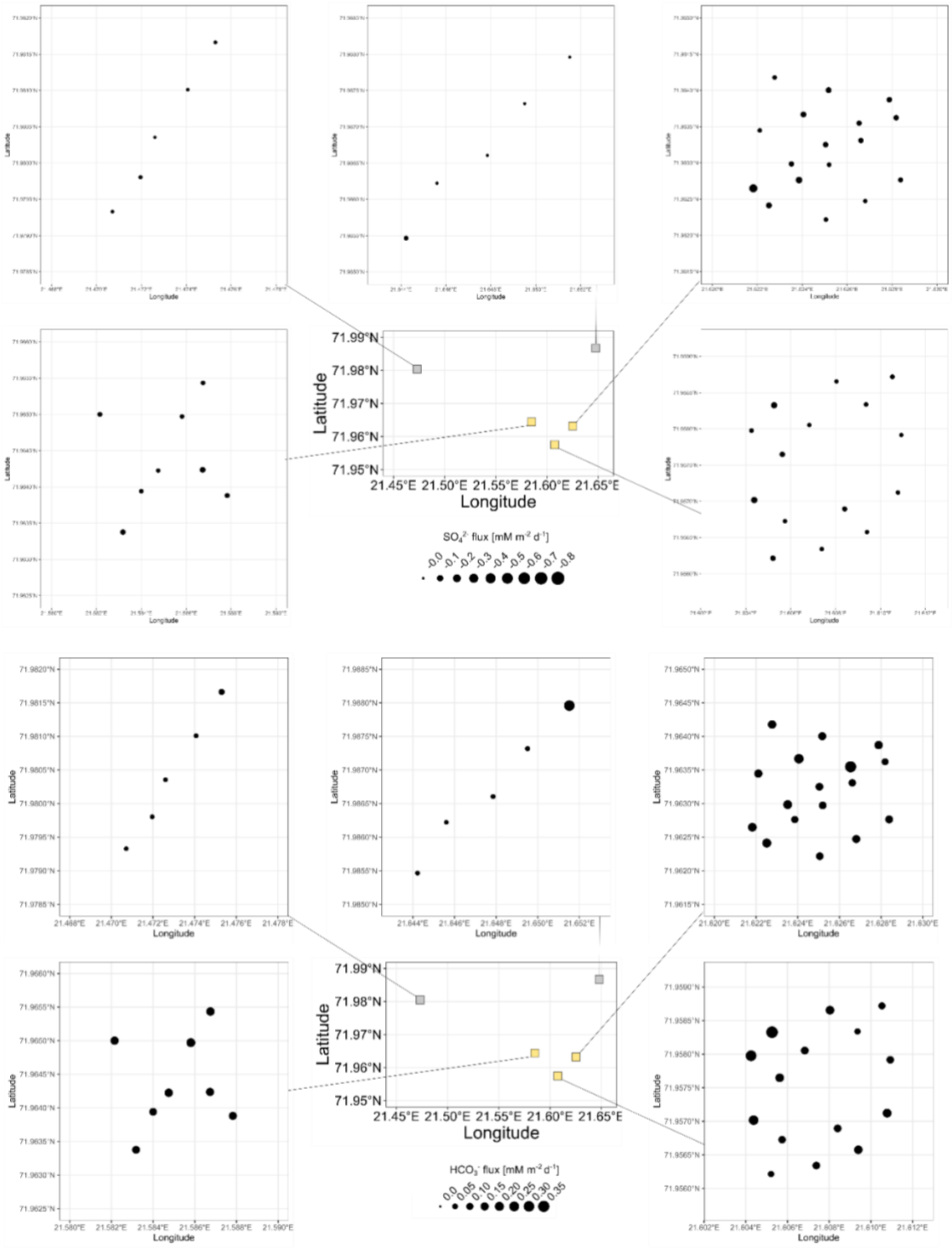
Z12C09
Z12C10
Z12C11
Z12C12
Z12C13
Z12C14
Z12C15
Z12C16
Z12C17
Ref5C01
Ref5C02
Ref5C03
Ref5C04
Ref5C05
Ref6C06
Ref6C07
Ref6C08
Ref6C09
Ref6C10
SO4 concentration (mM)
Depth (cm)
SRR (pmol*cm-3*d-1)

Supplementary Figure S1. Measured pore water sulfate concentrations (blue dots) and modelled sulfate reduction rates (red lines) and sulfate concentrations (blue lines).

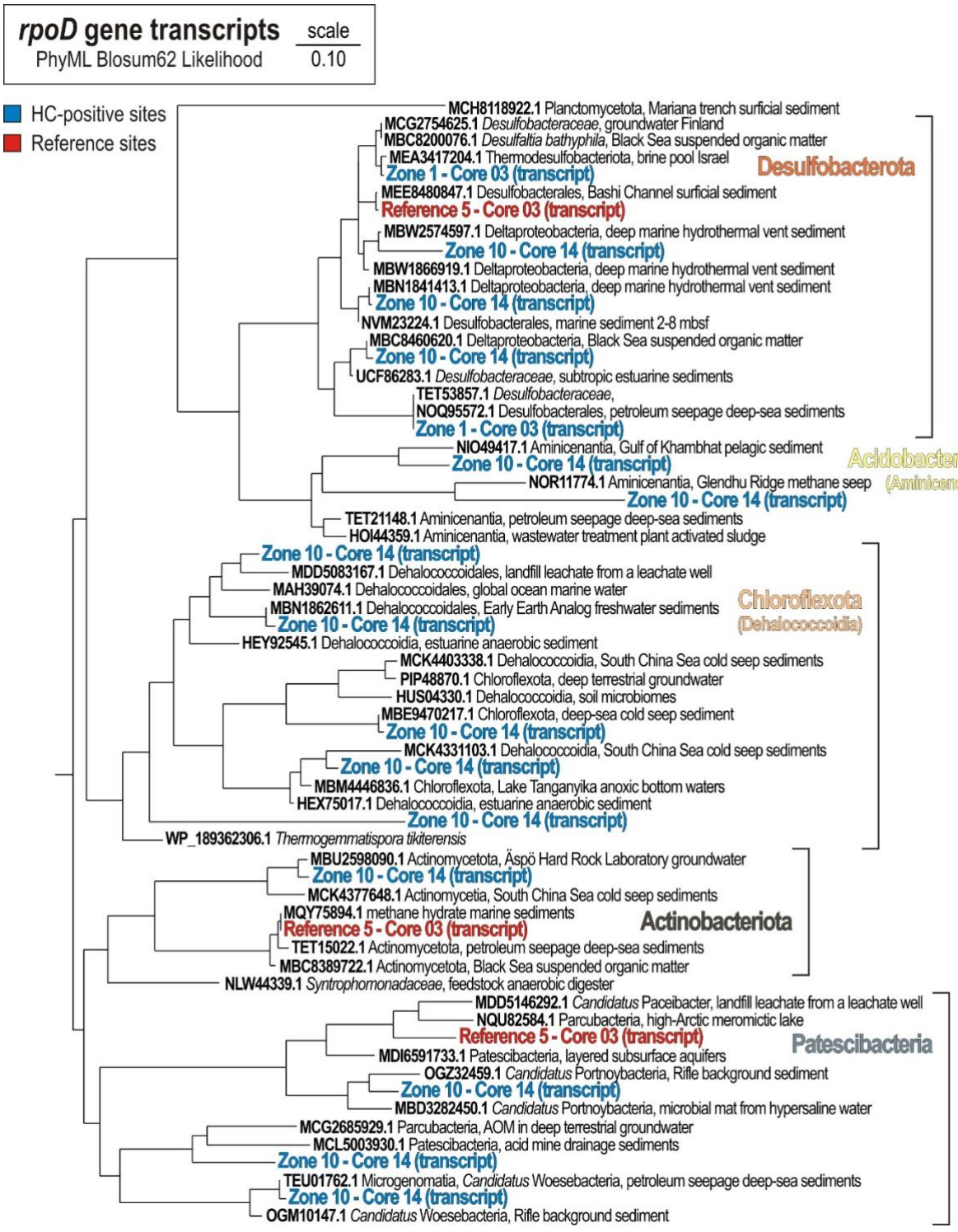

Z01C01
Z01C02
Z01C03
Z01C04
Z01C05
Z01C06
Z01C07
Z01C08
Z01C09
Z01C10
Z01C11
Z01C12
Z01C14
Z01C15
Z01C16
Z10C01
Z10C07
Z10C08
Z10C09
Z10C10
Z10C11
Z10C14
Z10C17
Z12C01
Z12C02
Alkalinity [mM]
Depth [cm]
Sulfide [µM]


Z12C03
Z12C04
Z12C05
Z12C06
Z12C07
Z12C08
Z12C09
Z12C10
Z12C11
Z12C12
Z12C13
Z12C14
Z12C15
Z12C16
Z12C17
Ref5C01
Ref5C02
Ref5C03
Ref5C04
Ref5C05
Ref6C06
Ref6C07
Ref6C08
Ref6C09
Ref6C10
Alkalinity [mM]
Depth [cm]
Sulfide [µM]

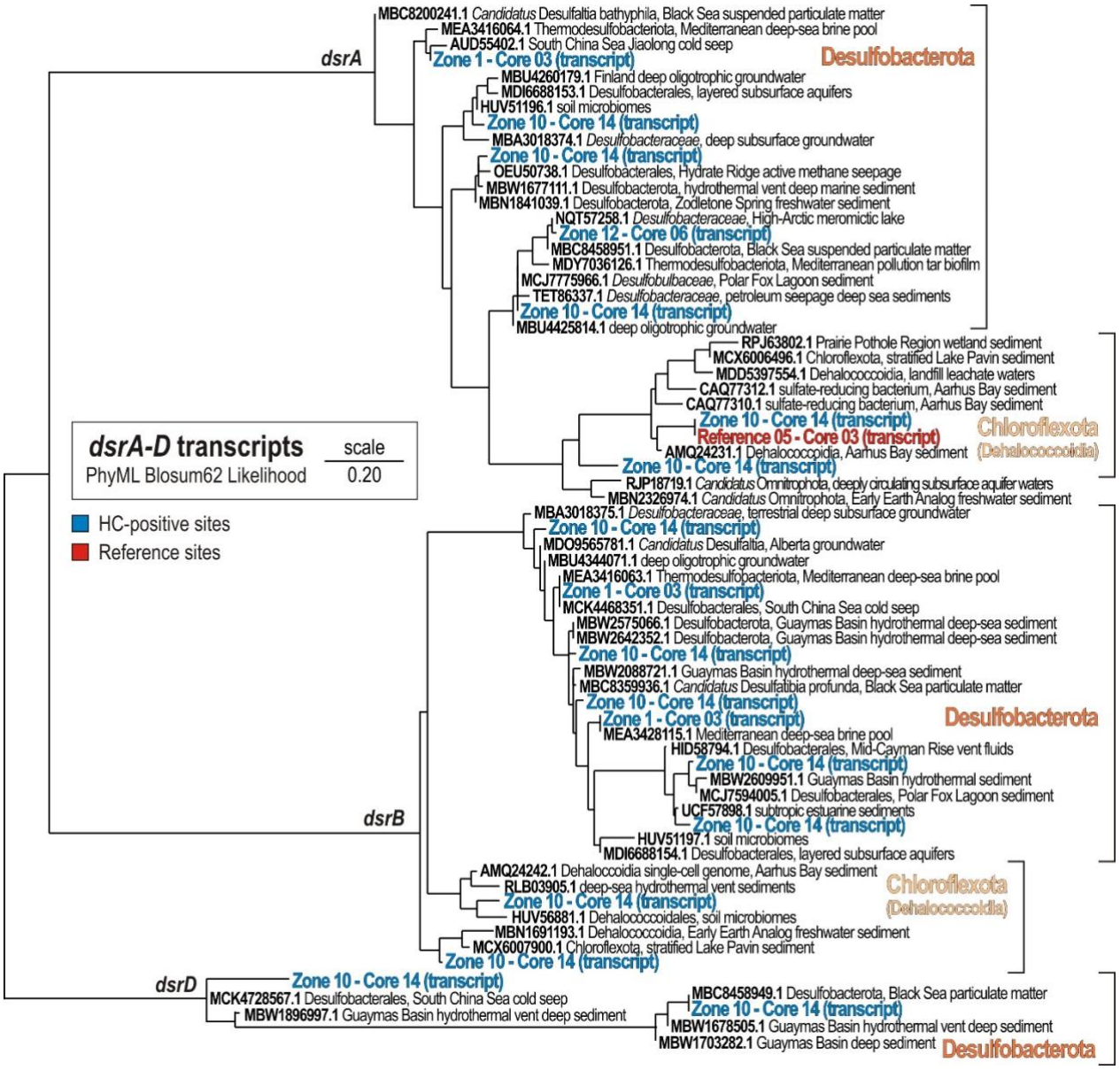
Supplementary Figure S2. Measured pore water alkalinity (black dots) and sulfide profiles (yellow dots) and their respective linear regressions


71.99°N
71.98°N
71.97°N
71.96°N
71.95°N
Latitude
21.45°E 21.50°E 21.55°E 21.60°E 21.65°E
Longitude
SO_4^{2-} flux [mM m^{-2} d^{-1}]
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
HCO_3^- flux [mM m^{-2} d^{-1}]
0.0 0.05 0.10 0.15 0.20 0.25 0.30 0.35

Supplementary Figure S3. Fluxes of SO_4^{2-} (top) and HCO_3^- (bottom) at each sampling site.

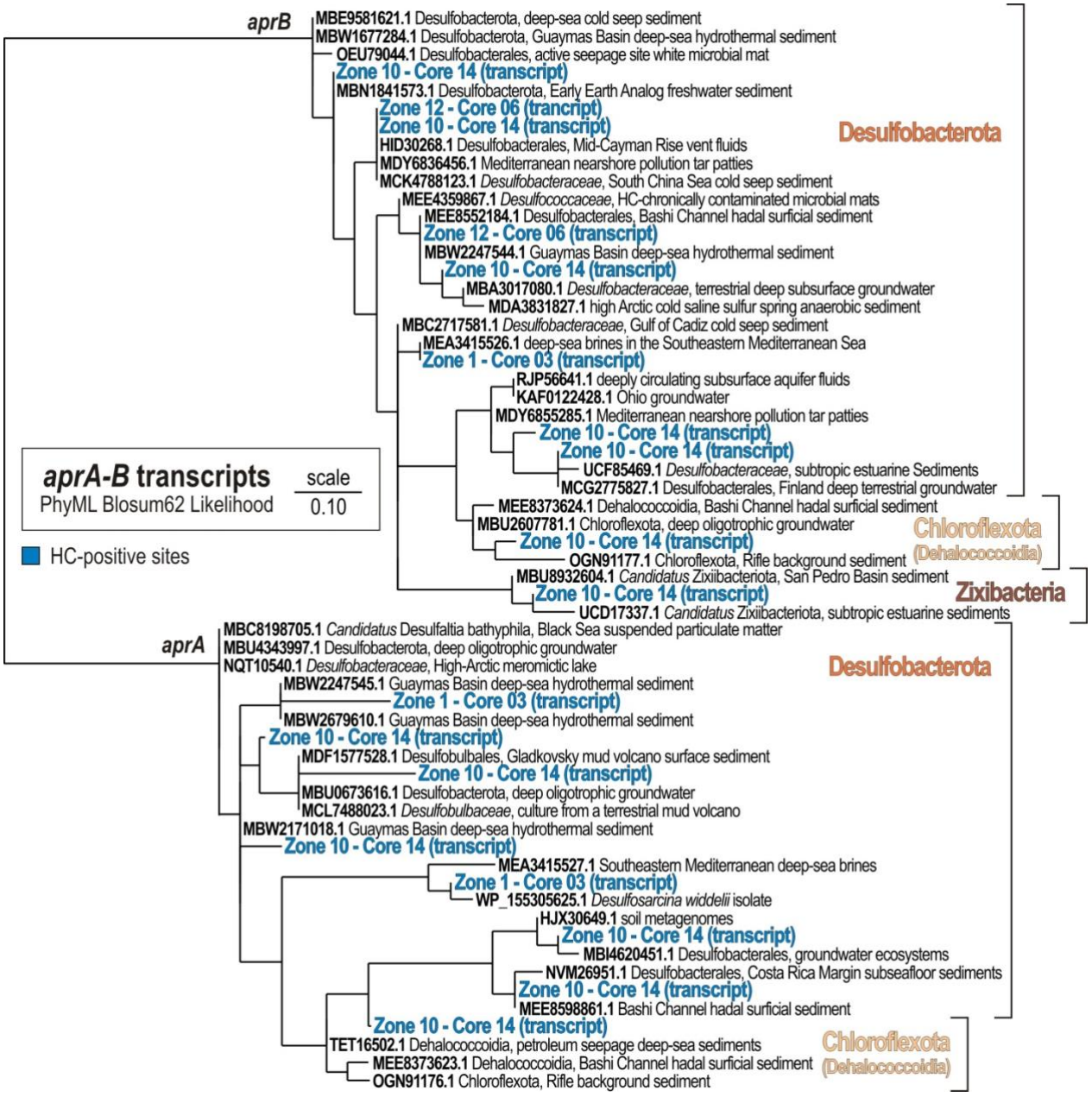

rpoD gene transcripts
PhyML Blosum62 Likelihood
scale
0.10
HC-positive sites
Reference sites
MCH8118922.1 Planctomycetota, Mariana trench surficial sediment
MCG2754625.1 Desulfobacteraceae, groundwater Finland
MBC8200076.1 Desulfaltia bathyphila, Black Sea suspended organic matter
MEA3417204.1 Thermodesulfobacteriota, brine pool Israel
Zone 1 - Core 03 (transcript)
Desulfobacterota
MEE8480847.1 Desulfobacterales, Bashi Channel surficial sediment
Reference 5 - Core 03 (transcript)
MBW2574597.1 Deltaproteobacteria, deep marine hydrothermal vent sediment
Zone 10 - Core 14 (transcript)
MBW1866919.1 Deltaproteobacteria, deep marine hydrothermal vent sediment
MBN1841413.1 Deltaproteobacteria, deep marine hydrothermal vent sediment
Zone 10 - Core 14 (transcript)
NVM23224.1 Desulfobacterales, marine sediment 2-8 mbsf
MBC8460620.1 Deltaproteobacteria, Black Sea suspended organic matter
Zone 10 - Core 14 (transcript)
UCF86283.1 Desulfobacteraceae, subtropic estuarine sediments
TET53857.1 Desulfobacteraceae,
NOQ95572.1 Desulfobacterales, petroleum seepage deep-sea sediments
Zone 1 - Core 03 (transcript)
NIO49417.1 Aminicenantia, Gulf of Khambhat pelagic sediment
Zone 10 - Core 14 (transcript)
Acidobacteriota
(Aminicenantia)
NOR11774.1 Aminicenantia, Glendhu Ridge methane seep
Zone 10 - Core 14 (transcript)
TET21148.1 Aminicenantia, petroleum seepage deep-sea sediments
HOI44359.1 Aminicenantia, wastewater treatment plant activated sludge
Zone 10 - Core 14 (transcript)
MDD5083167.1 Dehalococcoidales, landfill leachate from a leachate well
MAH39074.1 Dehalococcoidales, global ocean marine water
MBN1862611.1 Dehalococcoidales, Early Earth Analog freshwater sediments
Zone 10 - Core 14 (transcript)
Chloroflexota
(Dehalococcoidia)
HEY92545.1 Dehalococcoidia, estuarine anaerobic sediment
MCK4403338.1 Dehalococcoidia, South China Sea cold seep sediments
PIP48870.1 Chloroflexota, deep terrestrial groundwater
HUS04330.1 Dehalococcoidia, soil microbiomes
MBE9470217.1 Chloroflexota, deep-sea cold seep sediment
Zone 10 - Core 14 (transcript)
MCK4331103.1 Dehalococcoidia, South China Sea cold seep sediments
Zone 10 - Core 14 (transcript)
MBM4446836.1 Chloroflexota, Lake Tanganyika anoxic bottom waters
HEX75017.1 Dehalococcoidia, estuarine anaerobic sediment
Zone 10 - Core 14 (transcript)
WP_189362306.1 Thermogemmatispora tikiterensis
MBU2598090.1 Actinomycetota, Äspö Hard Rock Laboratory groundwater
Zone 10 - Core 14 (transcript)
MCK4377648.1 Actinomycetia, South China Sea cold seep sediments
MQY75894.1 methane hydrate marine sediments
Reference 5 - Core 03 (transcript)
Actinobacteriota
TET15022.1 Actinomycetota, petroleum seepage deep-sea sediments
MBC8389722.1 Actinomycetota, Black Sea suspended organic matter
NLW44339.1 Syntrophomonadaceae, feedstock anaerobic digester
MDD5146292.1 Candidatus Paceibacter, landfill leachate from a leachate well
NQU82584.1 Parcubacteria, high-Arctic meromictic lake
Reference 5 - Core 03 (transcript)
Patescibacteria
MDI6591733.1 Patescibacteria, layered subsurface aquifers
OGZ32459.1 Candidatus Portnoybacteria, Rifle background sediment
Zone 10 - Core 14 (transcript)
MBD3282450.1 Candidatus Portnoybacteria, microbial mat from hypersaline water
MCG2685929.1 Parcubacteria, AOM in deep terrestrial groundwater
MCL5003930.1 Patescibacteria, acid mine drainage sediments
Zone 10 - Core 14 (transcript)
TEU01762.1 Microgenomatia, Candidatus Woesebacteria, petroleum seepage deep-sea sediments
Zone 10 - Core 14 (transcript)
OGM10147.1 Candidatus Woesebacteria, Rifle background sediment

Supplementary Figure S4. Phylogenetic tree of *rpoD* protein-encoding genes. PhyML maximum likelihood tree of transcript ORFs (708 aligned amino acids) encoding the RNA polymerase sigma-70 factor (*RpoD*), based on 100 bootstrap replicates with BLOSUM62 as evolutive model. Boldface types signify sequence accession numbers to the NCBI database.



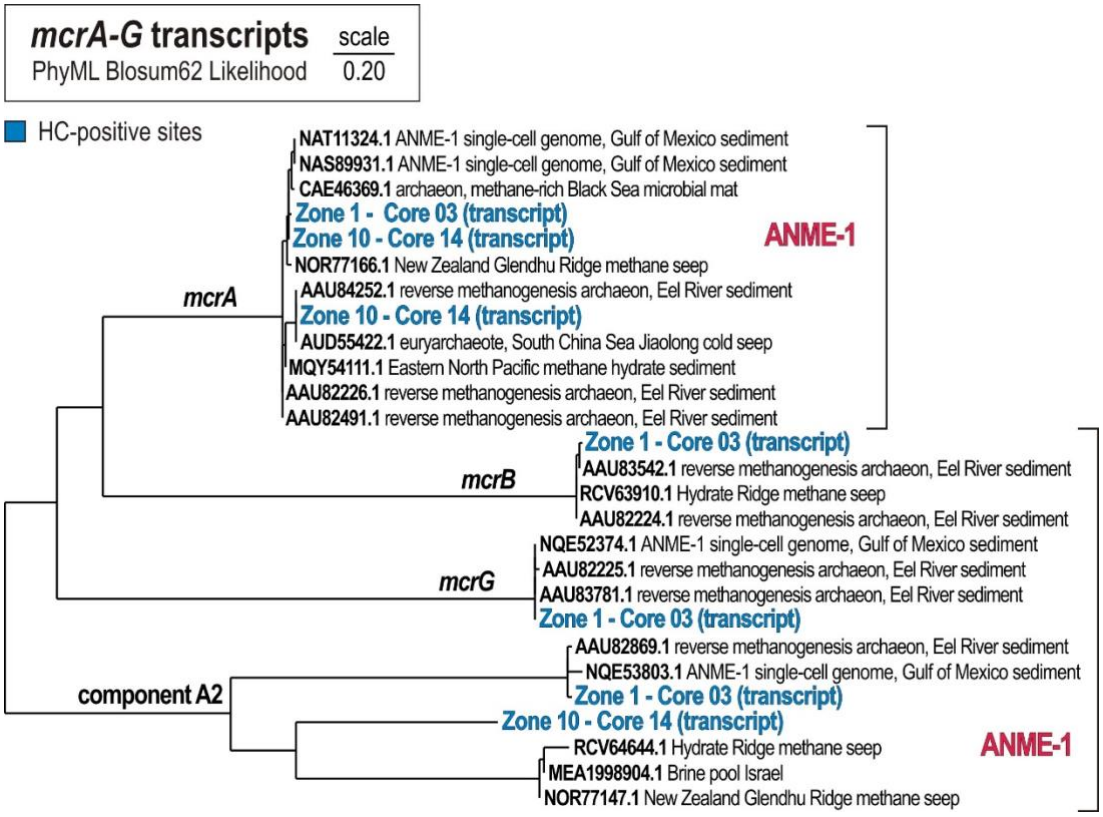
Supplementary Figure S5. Phylogenetic tree of *dsrA-D* protein-encoding genes. PhyML maximum likelihood tree of transcript ORFs (493 aligned amino acids) encoding the dissimilatory sulfite reductase subunit alpha (*dsrA*), beta (*dsrB*) and

delta (*dsrD*), based on 100 bootstrap replicates with BLOSUM62 as evolutive model. Boldface types signify sequence accession numbers to the NCBI database.



Supplementary Figure S6. Phylogenetic tree of *aprA-B* protein-encoding genes. PhyML maximum likelihood tree of transcript ORFs (714 aligned amino acids) encoding the adenylylsulfate reductase subunit alpha (*aprA*) and beta (*aprB*), based

on 100 bootstrap replicates with BLOSUM62 as evolutive model. Boldface types signify sequence accession numbers to the NCBI database.



Supplementary Figure S7. Phylogenetic tree of *mcrA-G* protein-encoding genes. PhyML maximum likelihood tree of transcript ORFs (698 aligned amino acids) encoding the methyl-coenzyme M reductase reductase subunit alpha (*mcrA*), beta (*mcrB*), gamma (*mcrG*) and component A2, based on 100 bootstrap replicates with BLOSUM62 as evolutive model. Boldface types signify sequence accession numbers to the NCBI database.

Supplementary Table S1. Assembly statistics for all samples.

		Sampling area				
		Zone 1	**Zone 10**	**Zone 12**	**Reference 5**	**Reference 6**
MetaG	**Replicates**	4	2	2	3	1
	Reads	25119029	13313285	12378731	21674342	7,700,785
	Scaffolds	228,637	153,150	144,433	285,446	116,305
	Average length	2,780	2,876	2,361	2,443	2,344
	Predicted genes*	353,429	233,499	234,922	404,878	144,642
	ORFs	153,976	111,101	108,403	140,145	85,781
	High-Q MAGs	61	51	45	98	23
MetaT	**Replicates**	1	1	1	1	1
	Sequencing depth	93.9 Gps (pooled)			1.2 Gps (pooled)	
	Mapped reads	86.30%	94.60%	47.90%	95.20%	94.70%
	ribosomal RNA	72.5%	80.3%	20.5%	78.8%	78.2%
	Assigned CDS	8.9%	2.9%	15.7%	7.0%	5.6%
	Predicted genes	4,072	35,288	1,151	6,169	636
	ORFs	3,743	24,098	1,137	5,461	614

Supplementary Table S2. Pearson correlations

Zone	Core	SO_4^{2-}/Alkalinity	SO_4^{2-}/Sulfide	Alkalinity/Sulfide
Ref5	1	-0.51	N.A.	N.A.
Ref5	2	-0.60	N.A.	N.A.
Ref5	3	-0.90	N.A.	N.A.
Ref5	4	-0.57	N.A.	N.A.
Ref5	5	0.53	N.A.	N.A.
Ref6	6	1.00	N.A.	N.A.
Ref6	7	-0.84	N.A.	N.A.
Ref6	8	-0.98	N.A.	N.A.
Ref6	9	-0.91	N.A.	N.A.
Ref6	10	-0.76	N.A.	N.A.
Z01	1	-0.99	-0.86	0.87
Z01	2	-0.97	-0.98	0.92
Z01	3	-0.99	-0.93	0.99
Z01	4	-0.98	-0.92	0.88
Z01	5	-0.99	-0.98	0.97
Z01	6	-1.00	-0.65	0.60
Z01	7	-0.96	-0.89	0.75
Z01	8	-0.99	-0.68	0.61
Z01	9	-0.82	-0.97	0.91
Z01	10	-0.97	-0.52	0.55
Z01	11	-0.97	-0.99	0.93
Z01	12	-0.98	-0.97	0.94
Z01	14	-0.97	N.A.	N.A.
Z01	15	-0.99	N.A.	N.A.
Z01	16	-0.99	N.A.	N.A.
Z10	1	-0.95	N.A.	N.A.
Z10	7	-1.00	-1.00	1.00
Z10	8	-0.76	-0.62	0.98
Z10	9	-0.99	-0.90	0.94

Z10	10	-0.98	N.A.	N.A.
Z10	11	-1.00	N.A.	N.A.
Z10	17	-0.94	-0.90	0.98
Z12	1	-0.97	N.A.	N.A.
Z12	2	-0.95	N.A.	N.A.
Z12	3	-0.58	N.A.	N.A.
Z12	4	-0.90	N.A.	N.A.
Z12	5	-0.92	N.A.	N.A.
Z12	6	-0.82	N.A.	N.A.
Z12	7	-0.98	N.A.	N.A.
Z12	8	-0.99	N.A.	N.A.
Z12	9	-0.99	N.A.	N.A.
Z12	10	-0.99	N.A.	N.A.
Z12	11	-0.97	N.A.	N.A.
Z12	12	-0.99	N.A.	N.A.
Z12	13	-0.97	N.A.	N.A.
Z12	14	-0.86	-0.87	0.63
Z12	15	-0.98	N.A.	N.A.
Z12	16	-0.99	N.A.	N.A.
Z12	17	-0.98	N.A.	N.A.