TABLE DR1.

Sol. no.	Conditions	Input concentrations (mmol L^{-1}) SO_4^{2-}	HS^-	TA	DIC	Ca^{2+}	Mg^{2+}	Na^+	Cl^-	T°C	Calculated pH	Saturation indices Aragonite	Calcite	Dolomite
1	Seawater	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
2	Seawater	27.9	0.1	2.3	2.2	10	50	469	530	10	7.842	0.03	0.19	1.03
3	Seawater	27.8	0.2	2.5	2.4	10	50	469	530	10	7.539	-0.24	-0.08	0.49
4	Seawater	27.5	0.5	3.1	3	10	50	469	530	10	7.187	-0.51	-0.36	-0.05
5	Seawater	27	1	4.1	4	10	50	469	530	10	7.007	-0.58	-0.43	-0.20
6	Seawater	26.5	1.5	5.1	5	10	50	469	530	10	6.931	-0.57	-0.42	-0.17
7	Seawater	26	2	6.1	6	10	50	469	530	10	6.888	-0.54	-0.38	-0.11
8	Seawater	24.5	3.5	9.1	9	10	50	469	530	10	6.827	-0.43	-0.28	0.10
9	Seawater	23	5	12.1	12	10	50	469	530	10	6.800	-0.34	-0.19	0.29
10	Seawater	20.5	7.5	17.1	17	10	50	469	530	10	6.778	-0.21	-0.06	0.54
11	Seawater	18	10	22.1	22	10	50	469	530	10	6.766	-0.11	0.04	0.74
12	Seawater	13	15	32.1	32	10	50	469	530	10	6.754	0.04	0.19	1.04
13	Seawater	8	20	42.1	42	10	50	469	530	10	6.748	0.15	0.30	1.26
14	Seawater	0	28	58.1	58	10	50	469	530	10	6.743	0.29	0.44	1.53
15	Seawater, 10% CH_4	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
16	Seawater, 10% CH_4	27.9	0.1	2.3	2.19	10	50	469	530	10	7.884	0.07	0.23	1.11
17	Seawater, 10% CH_4	27.8	0.2	2.5	2.38	10	50	469	530	10	7.599	-0.18	-0.03	0.61
18	Seawater, 10% CH_4	27.5	0.5	3.1	2.95	10	50	469	530	10	7.246	-0.45	-0.30	0.06
19	Seawater, 10% CH_4	27	1	4.1	3.9	10	50	469	530	10	7.066	-0.53	-0.37	-0.09
20	Seawater, 10% CH_4	26.5	1.5	5.1	4.85	10	50	469	530	10	6.991	-0.52	-0.36	-0.06
21	Seawater, 10% CH_4	26	2	6.1	5.8	10	50	469	530	10	6.949	-0.49	-0.33	0.00
22	Seawater, 10% CH_4	24.5	3.5	9.1	8.65	10	50	469	530	10	6.888	-0.38	-0.23	0.21
23	Seawater, 10% CH_4	23	5	12.1	11.5	10	50	469	530	10	6.862	-0.29	-0.13	0.39
24	Seawater, 10% CH_4	20.5	7.5	17.1	16.25	10	50	469	530	10	6.840	-0.16	-0.01	0.65
25	Seawater, 10% CH_4	18	10	22.1	21	10	50	469	530	10	6.829	-0.06	0.09	0.84
26	Seawater, 10% CH_4	13	15	32.1	30.5	10	50	469	530	10	6.817	0.09	0.24	1.14
27	Seawater, 10% CH_4	8	20	42.1	40	10	50	469	530	10	6.811	0.20	0.36	1.37
28	Seawater, 10% CH_4	0	28	58.1	55.2	10	50	469	530	10	6.806	0.34	0.50	1.64
29	Seawater, 50% CH_4	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
30	Seawater, 50% CH_4	27.9	0.1	2.3	2.15	10	50	469	530	10	8.050	0.23	0.38	1.42
31	Seawater, 50% CH_4	27.8	0.2	2.5	2.3	10	50	469	530	10	7.878	0.09	0.24	1.14

32	Seawater, 50% CH_4	27.5	0.5	3.1	2.75	10	50	469	530	10	7.570	-0.15	0.01	0.68
33	Seawater, 50% CH_4	27	1	4.1	3.5	10	50	469	530	10	7.388	-0.23	-0.07	0.51
34	Seawater, 50% CH_4	26.5	1.5	5.1	4.25	10	50	469	530	10	7.314	-0.22	-0.07	0.52
35	Seawater, 50% CH_4	26	2	6.1	5	10	50	469	530	10	7.273	-0.20	-0.04	0.58
36	Seawater, 50% CH_4	24.5	3.5	9.1	7.25	10	50	469	530	10	7.216	-0.09	0.06	0.78
37	Seawater, 50% CH_4	23	5	12.1	9.5	10	50	469	530	10	7.192	0.00	0.15	0.96
38	Seawater, 50% CH_4	20.5	7.5	17.1	13.25	10	50	469	530	10	7.172	0.12	0.28	1.21
39	Seawater, 50% CH_4	18	10	22.1	17	10	50	469	530	10	7.162	0.22	0.38	1.41
40	Seawater, 50% CH_4	13	15	32.1	24.5	10	50	469	530	10	7.151	0.37	0.53	1.71
41	Seawater, 50% CH_4	8	20	42.1	32	10	50	469	530	10	7.146	0.48	0.64	1.93
42	Seawater, 50% CH_4	0	28	58.1	44	10	50	469	530	10	7.142	0.62	0.78	2.21
43	Seawater, 80% CH_4	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
44	Seawater, 80% CH_4	27.9	0.1	2.3	2.12	10	50	469	530	10	8.164	0.33	0.49	1.63
45	Seawater, 80% CH_4	27.8	0.2	2.5	2.24	10	50	469	530	10	8.100	0.29	0.45	1.55
46	Seawater, 80% CH_4	27.5	0.5	3.1	2.6	10	50	469	530	10	7.951	0.21	0.37	1.39
47	Seawater, 80% CH_4	27	1	4.1	3.2	10	50	469	530	10	7.818	0.17	0.32	1.31
48	Seawater, 80% CH_4	26.5	1.5	5.1	3.8	10	50	469	530	10	7.751	0.18	0.33	1.33
49	Seawater, 80% CH_4	26	2	6.1	4.4	10	50	469	530	10	7.713	0.20	0.36	1.38
50	Seawater, 80% CH_4	24.5	3.5	9.1	6.2	10	50	469	530	10	7.658	0.30	0.45	1.56
51	Seawater, 80% CH_4	23	5	12.1	8	10	50	469	530	10	7.634	0.39	0.54	1.74
52	Seawater, 80% CH_4	20.5	7.5	17.1	11	10	50	469	530	10	7.615	0.51	0.66	1.98
53	Seawater, 80% CH_4	18	10	22.1	14	10	50	469	530	10	7.605	0.60	0.76	2.17
54	Seawater, 80% CH_4	13	15	32.1	20	10	50	469	530	10	7.595	0.75	0.90	2.47
55	Seawater, 80% CH_4	8	20	42.1	26	10	50	469	530	10	7.590	0.86	1.02	2.69
56	Seawater, 80% CH_4	0	28	58.1	35.6	10	50	469	530	10	7.585	1.00	1.15	2.96
57	Seawater, 100% CH_4	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
58	Seawater, 100% CH_4	27.9	0.1	2.3	2.1	10	50	469	530	10	8.234	0.39	0.55	1.75
59	Seawater, 100% CH_4	27.8	0.2	2.5	2.2	10	50	469	530	10	8.233	0.41	0.57	1.79
60	Seawater, 100% CH_4	27.5	0.5	3.1	2.5	10	50	469	530	10	8.230	0.46	0.62	1.90
61	Seawater, 100% CH_4	27	1	4.1	3	10	50	469	530	10	8.227	0.54	0.70	2.05
62	Seawater, 100% CH_4	26.5	1.5	5.1	3.5	10	50	469	530	10	8.225	0.61	0.76	2.18
63	Seawater, 100% CH_4	26	2	6.1	4	10	50	469	530	10	8.223	0.66	0.82	2.30
64	Seawater, 100% CH_4	24.5	3.5	9.1	5.5	10	50	469	530	10	8.221	0.80	0.96	2.57
65	Seawater, 100% CH_4	23	5	12.1	7	10	50	469	530	10	8.219	0.90	1.06	2.78
66	Seawater, 100% CH_4	20.5	7.5	17.1	9.5	10	50	469	530	10	8.218	1.04	1.19	3.04

67	Seawater, 100% CH_4	18	10	22.1	12	10	50	469	530	10	8.217	1.14	1.29	3.25
68	Seawater, 100% CH_4	13	15	32.1	17	10	50	469	530	10	8.216	1.29	1.45	3.55
69	Seawater, 100% CH_4	8	20	42.1	22	10	50	469	530	10	8.215	1.40	1.56	3.78
70	Seawater, 100% CH_4	0	28	58.1	30	10	50	469	530	10	8.213	1.54	1.70	4.05
71	N:C = 1:8	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
72	N:C = 1:8	27.9	0.1	2.325	2.2	10	50	469	530	10	7.946	0.13	0.29	1.24
73	N:C = 1:8	27.8	0.2	2.55	2.4	10	50	469	530	10	7.698	-0.08	0.08	0.82
74	N:C = 1:8	27.5	0.5	3.225	3	10	50	469	530	10	7.358	-0.33	-0.17	0.31
75	N:C = 1:8	27	1	4.35	4	10	50	469	530	10	7.184	-0.39	-0.23	0.19
76	N:C = 1:8	26.5	1.5	5.475	5	10	50	469	530	10	7.112	-0.37	-0.21	0.23
77	N:C = 1:8	26	2	6.6	6	10	50	469	530	10	7.073	-0.33	-0.18	0.30
78	N:C = 1:8	24.5	3.5	9.975	9	10	50	469	530	10	7.018	-0.22	-0.06	0.53
79	N:C = 1:8	23	5	13.35	12	10	50	469	530	10	6.994	-0.12	0.04	0.73
80	N:C = 1:8	20.5	7.5	18.975	17	10	50	469	530	10	6.974	-0.95	0.01	0.99
81	N:C = 1:8	18	10	24.6	22	10	50	469	530	10	6.964	0.11	0.27	1.19
82	N:C = 1:8	13	15	35.85	32	10	50	469	530	10	6.954	0.27	0.42	1.50
83	N:C = 1:8	8	20	47.1	42	10	50	469	530	10	6.949	0.38	0.53	1.72
84	N:C = 1:8	0	28	65.1	58	10	50	469	530	10	6.944	0.52	0.67	2.00
85	nC16 fatty acid	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
86	nC16 fatty acid	27.9	0.1	2.3	2.1563	10	50	469	530	10	8.025	0.20	0.36	1.37
87	nC16 fatty acid	27.8	0.2	2.5	2.3125	10	50	469	530	10	7.831	0.04	0.20	1.05
88	nC16 fatty acid	27.5	0.5	3.1	2.7813	10	50	469	530	10	7.507	-0.21	-0.05	0.56
89	nC16 fatty acid	27	1	4.1	3.5625	10	50	469	530	10	7.325	-0.29	-0.13	0.39
90	nC16 fatty acid	26.5	1.5	5.1	4.3438	10	50	469	530	10	7.251	-0.28	-0.12	0.41
91	nC16 fatty acid	26	2	6.1	5.125	10	50	469	530	10	7.210	-0.25	-0.10	0.47
92	nC16 fatty acid	24.5	3.5	9.1	7.4688	10	50	469	530	10	7.153	-0.15	0.01	0.67
93	nC16 fatty acid	23	5	12.1	9.8125	10	50	469	530	10	7.128	-0.06	0.10	0.85
94	nC16 fatty acid	20.5	7.5	17.1	13.719	10	50	469	530	10	7.108	0.07	0.22	1.10
95	nC16 fatty acid	18	10	22.1	17.625	10	50	469	530	10	7.098	0.17	0.32	1.30
96	nC16 fatty acid	13	15	32.1	25.438	10	50	469	530	10	7.087	0.32	0.47	1.60
97	nC16 fatty acid	8	20	42.1	33.25	10	50	469	530	10	7.082	0.43	0.59	1.83
98	nC16 fatty acid	0	28	58.1	45.75	10	50	469	530	10	7.077	0.57	0.72	2.10
99	Ca:C = 1:1	28	0	2.1	2	10	50	469	530	10	8.235	0.37	0.53	1.72
100	Ca:C = 1:1	27.9	0.1	2.3	2.2	10.2	50	469	530	10	7.841	0.04	0.19	1.04

101	Ca:C = 1:1	27.8	0.2	2.5	2.4	10.4	50	469	530	10	7.538	-0.22	-0.07	0.51
102	Ca:C = 1:1	27.5	0.5	3.1	3	11	50	469	530	10	7.186	-0.47	-0.32	-0.01
103	Ca:C = 1:1	27	1	4.1	4	12	50	469	530	10	7.005	-0.51	-0.35	-0.12
104	Ca:C = 1:1	26.5	1.5	5.1	5	13	50	469	530	10	6.929	-0.46	-0.31	-0.07
105	Ca:C = 1:1	26	2	6.1	6	14	50	469	530	10	6.885	-0.40	-0.24	0.02
106	Ca:C = 1:1	24.5	3.5	9.1	9	17	50	469	530	10	6.822	-0.21	-0.06	0.31
107	Ca:C = 1:1	23	5	12.1	12	20	50	469	530	10	6.792	-0.05	0.10	0.56
108	Ca:C = 1:1	20.5	7.5	17.1	17	25	50	469	530	10	6.767	0.16	0.32	0.89
109	Ca:C = 1:1	18	10	22.1	22	30	50	469	530	10	6.751	0.33	0.49	1.16
110	Ca:C = 1:1	13	15	32.1	32	40	50	469	530	10	6.732	0.59	0.75	1.55
111	Ca:C = 1:1	8	20	42.1	42	50	50	469	530	10	6.719	0.79	0.94	1.85
112	Ca:C = 1:1	0	28	58.1	58	66	50	469	530	10	6.703	1.02	1.18	2.19
113	Lagoa Vermelha	67	0	5	3.1	24	140	1200	1300	10	9.394	1.64	1.80	4.37
114	Lagoa Vermelha	66.9	0.1	5.2	3.3	24	140	1200	1300	10	9.293	1.63	1.78	4.33
115	Lagoa Vermelha	66.8	0.2	5.4	3.5	24	140	1200	1300	10	9.202	1.60	1.76	4.29
116	Lagoa Vermelha	66.5	0.5	6	4.1	24	140	1200	1300	10	8.961	1.53	1.68	4.14
117	Lagoa Vermelha	66	1	7	5.1	24	140	1200	1300	10	8.598	1.35	1.51	3.78
118	Lagoa Vermelha	65.5	1.5	8	6.1	24	140	1200	1300	10	8.192	1.07	1.23	3.22
119	Lagoa Vermelha	65	2	9	7.1	24	140	1200	1300	10	7.724	0.69	0.84	2.45
120	Lagoa Vermelha	63.5	3.5	12	10.1	24	140	1200	1300	10	7.112	0.22	0.37	1.51
121	Lagoa Vermelha	62	5	15	13.1	24	140	1200	1300	10	6.929	0.13	0.29	1.35
122	Lagoa Vermelha	59.5	7.5	20	18.1	24	140	1200	1300	10	6.798	0.13	0.29	1.34
123	Lagoa Vermelha	57	10	25	23.1	24	140	1200	1300	10	6.735	0.16	0.32	1.41
124	Lagoa Vermelha	52	15	35	33.1	24	140	1200	1300	10	6.671	0.25	0.40	1.57
125	Lagoa Vermelha	47	20	45	43.1	24	140	1200	1300	10	6.640	0.32	0.48	1.73
126	Lagoa Vermelha	37	30	65	63.1	24	140	1200	1300	10	6.609	0.45	0.61	1.98
127	Lagoa Vermelha	0	67	139	137.1	24	140	1200	1300	10	6.576	0.74	0.90	2.56
128	Alkaline - low Ca	28.0	0.0	22	22	1	5	469	530	10	7.970	0.19	0.35	1.34
129	Alkaline - low Ca	27.9	0.1	22.2	22.2	1	5	469	530	10	7.916	0.14	0.30	1.24
130	Alkaline - low Ca	27.8	0.2	22.4	22.4	1	5	469	530	10	7.866	0.09	0.25	1.15
131	Alkaline - low Ca	27.5	0.5	23	23	1	5	469	530	10	7.733	-0.03	0.13	0.90
132	Alkaline - low Ca	27.0	1.0	24	24	1	5	469	530	10	7.572	-0.17	-0.02	0.61
133	Alkaline - low Ca	26.5	1.5	25	25	1	5	469	530	10	7.463	-0.27	-0.11	0.42
134	Alkaline - low Ca	26.0	2.0	26	26	1	5	469	530	10	7.383	-0.33	-0.18	0.29
135	Alkaline - low Ca	24.5	3.5	29	29	1	5	469	530	10	7.235	-0.44	-0.29	0.07

136	Alkaline - low Ca	23.0	5.0	32	32	1	5	469	530	10	7.150	-0.49	-0.34	-0.03
137	Alkaline - low Ca	20.5	7.5	37	37	1	5	469	530	10	7.064	-0.52	-0.37	-0.09
138	Alkaline - low Ca	18.0	10.0	42	42	1	5	469	530	10	7.012	-0.52	-0.37	-0.09
139	Alkaline - low Ca	13.0	15.0	52	52	1	5	469	530	10	6.950	-0.50	-0.34	-0.04
140	Alkaline - low Ca	8.0	20.0	62	62	1	5	469	530	10	6.915	-0.46	-0.30	0.04
141	Alkaline - low Ca	0.0	28.0	78	78	1	5	469	530	10	6.881	-0.39	-0.23	0.17

TABLE DR2.

Depth (cm)	T (°C)	pH	DIC (mmol L^{-1})	Ca^{2+} (mmol L^{-1})	Mg^{2+} (mmol L^{-1})	Na^{+} (mmol L^{-1})	K^{+} (mmol L^{-1})	Cl^{-} (mmol L^{-1})	SO_4^{2-} (mmol L^{-1})	HS^{-} (mmol L^{-1})	Calculated SI Aragonite	Calculated SI Calcite	Calculated SI Dolomite
0.0	25	8.03	3.70	14.40	78.93	694.70	15.16				0.74	0.88	2.70
3.0								798.73	44.28	0.00			
5.0	25	7.44	8.74	14.61	83.97	735.40	15.95	822.96	41.41	2.89	0.54	0.68	2.32
7.5		8.00	1.96										
10.0	25			13.00	79.78	687.07	15.01				0.42	0.56	2.11
12.0								783.81	43.55	0.00			
13.5		7.75	3.46										
15.0	25	7.46	10.24	13.10	89.76	760.73	16.30	731.67	39.33	1.61	0.58	0.72	2.47
16.5	25	7.74	9.67	14.66	83.04	765.87	15.54				0.88	1.03	3.00
18.0								777.67	38.37	3.50			
20.0	25	7.18	13.91	12.51	92.93	781.81	16.97				0.41	0.55	2.17
21.0								530.27	27.58	4.10			
22.5	25			11.91	94.82	832.67	17.17				0.52	0.66	2.42
24.0								755.06	34.18	4.99			
27.0								793.56	35.18	4.71			
28.5	25	7.62	14.01	11.74	75.77	708.72	14.55				0.84	0.98	2.97
30.0								801.58	35.22	5.11			
33.0								796.47	34.07	5.57			
34.5										3.40			
36.0								828.74	34.43	5.76			
37.5	25			12.08	87.25	785.20	16.57				0.77	0.91	2.88
39.0								878.40	35.14	4.88			
42.0								672.70	28.23	5.46			
45.0								948.13	36.07	5.06			
48.0								905.64	34.39	6.21			
49.5	25	7.63	16.35	11.34	92.32	827.52	17.82				0.89	1.03	3.17
51.0								941.37	34.03	5.46			
52.5										4.22			
54.0								894.16	32.14	5.79			
56.5		7.38	17.03										
57.0								768.34	28.97	4.92			
58.5	25			11.00	90.21	846.05	18.46				0.74	0.88	2.88
60.0								882.77	31.72	5.71			

61.5		7.61	17.65										
63.0								818.60	29.37	5.83			
66.0								978.80	33.06	4.60			
67.5	25			10.42	89.79	909.42	18.67				0.71	0.85	2.85
69.0								945.72	32.42	4.88			
70.5	25	7.39	17.28	10.53	91.88	923.99	18.88				0.64	0.78	2.71
71.5	25	7.15	17.72	10.11	87.09	843.21	18.49				0.39	0.53	2.21
72.0								944.94	31.18	6.00			
75.0										4.71			
78.0										5.55			
81.0										5.44			
84.0										5.51			

Table DR3.

Depth (cm)	delta$^{13}C_{TIC}$ ‰ (VPDB)	delta$^{13}C_{DIC}$ ‰ (VPDB)	‰ (VPDB)
0.0		-2.25	
5.0		-8.46	
7.5		-7.99	
8.5	-6.43		
10.0	-6.01		
12.5		-9.81	
15.0		-10.11	
18.0	-5.49		
20.0		-9.58	-9.46
22.5	-4.01	-10.98	
25.0		-10.87	
27.5		-9.26	-9.46
30.0	-7.62		
33.0	-4.45		
41.0	-5.14		
44.0	-5.63		
47.0	-10.84		
50.0	-10.40		
55.0	-8.49		
60.0	0.48		