Biogeosciences

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Supplement of

Spatial gradients in the characteristics of soil-carbon fractions are associated with abiotic features but not microbial communities

Aditi Sengupta et al.

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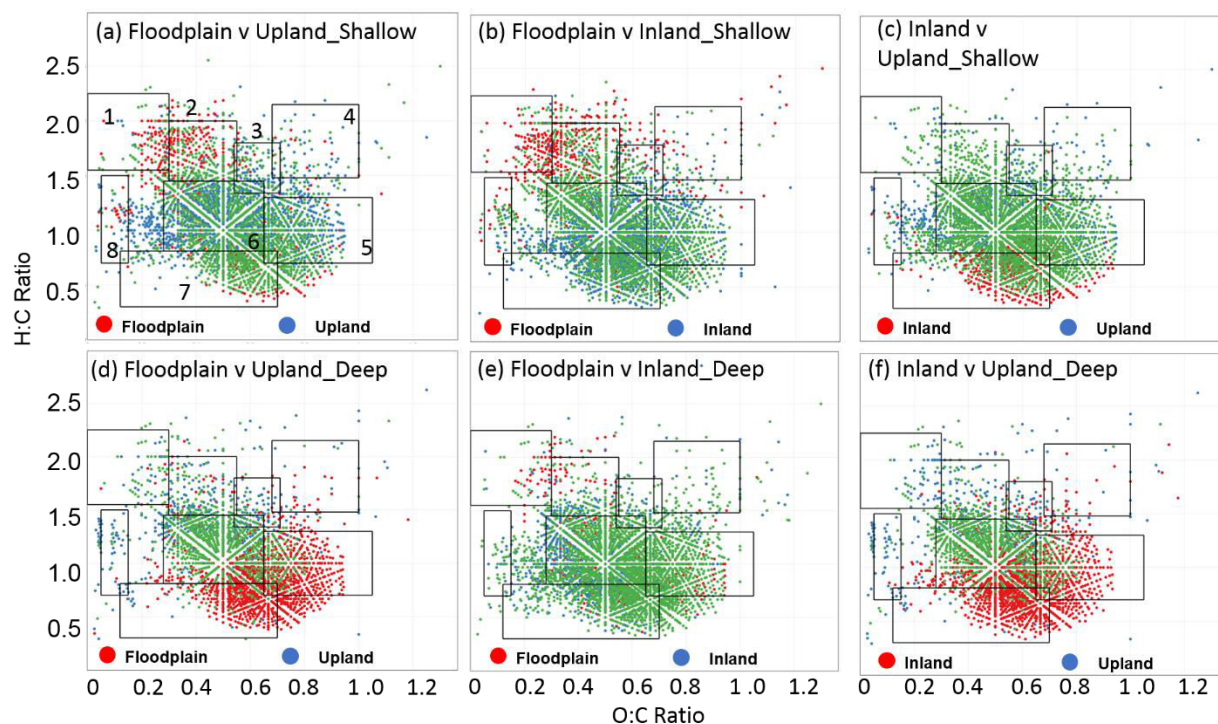
**Figure S1.** van Krevelen diagrams (O : C vs. H : C ratio plot) of unique versus shared peaks observed in water-fraction samples grouped according to their landscape position and depth. Floodplain locations include BC2, BC3, BC12, and BC13. Inland locations include BC4 and BC14. Terrestrial end-member indicates BC15 site. Red and blue dots indicate unique peaks while green indicates peaks observed in both sample groups. The compound classes are numbered as follows: 1) Lipid-like, 2) Protein-like, 3) Amino Sugar-like, 4) Carbohydrate-like, 5) Tannin-like, 6) Lignin-like, 7) Condensed Hydrocarbon-like, and 8) Unsaturated Hydrocarbon-like. Compound classes are reported on counts of C, H, and O for the following H:C and O:C ranges; lipids ($0 <$ O:C ≤ 0.3, $1.5 \leq$ H:C ≤ 2.5), unsaturated hydrocarbons ($0 \leq$ O:C ≤ 0.125, $0.8 \leq$ H:C < 2.5), proteins ($0.3 <$ O:C ≤ 0.55, $1.5 \leq$ H:C ≤ 2.3), amino sugars ($0.55 <$ O:C ≤ 0.7, $1.5 \leq$ H:C ≤ 2.2), carbohydrates ($0.7 <$ O:C ≤ 1.5, $1.5 \leq$ H:C ≤ 2.5), lignin ($0.125 <$ O:C ≤ 0.65, $0.8 \leq$ H:C < 1.5), tannins ($0.65 <$ O:C ≤ 1.1, $0.8 \leq$ H:C < 1.5), and condensed hydrocarbons ($0 \leq$ O:C ≤ 0.95, $0.2 \leq$ H:C < 0.8). Unnamed compounds are calculated as the proportion of identified C that does not fit within the above defined H:C and O:C ranges
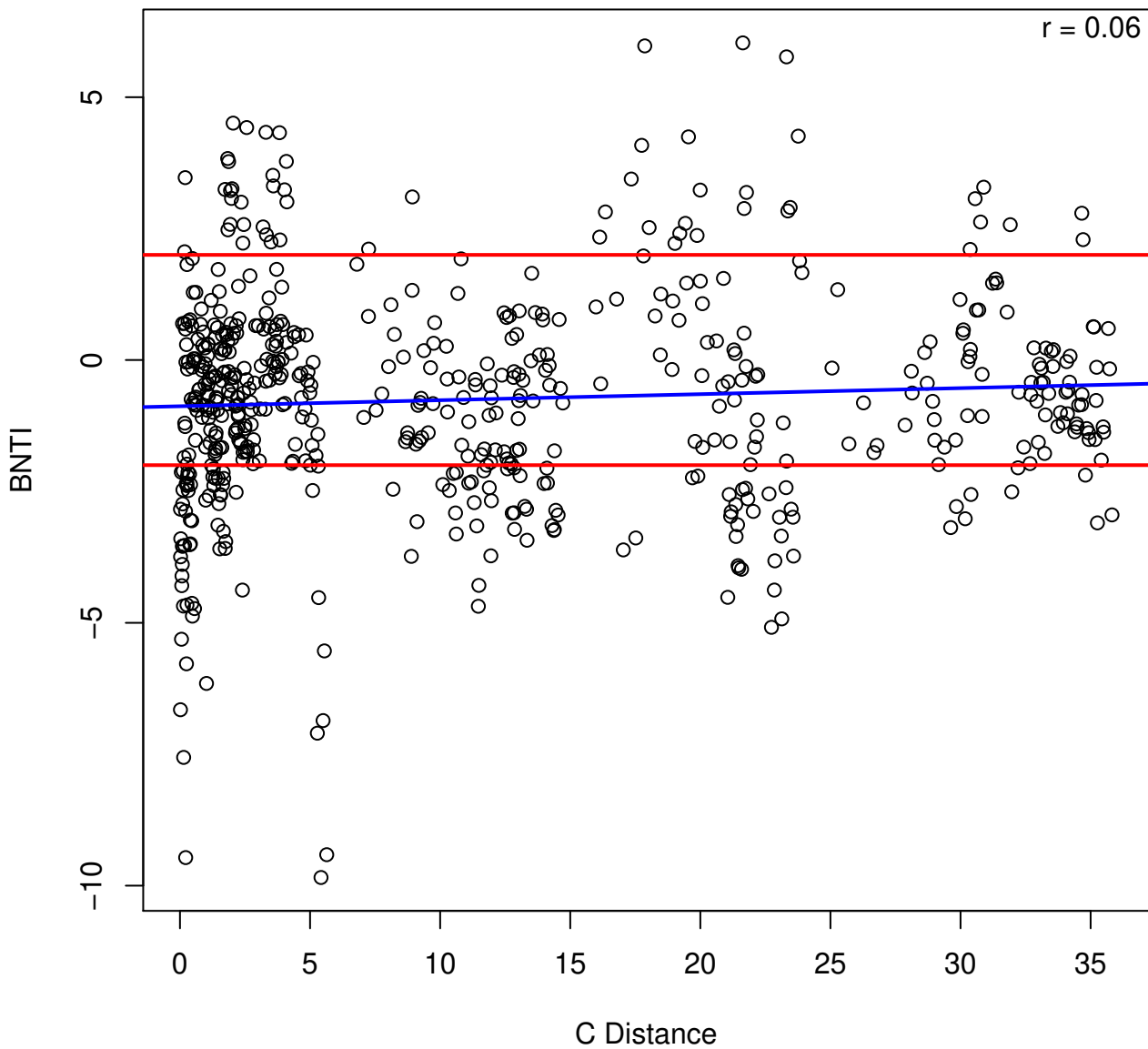
Figure S2 BetaNTI metric regressed against soil environmental variables
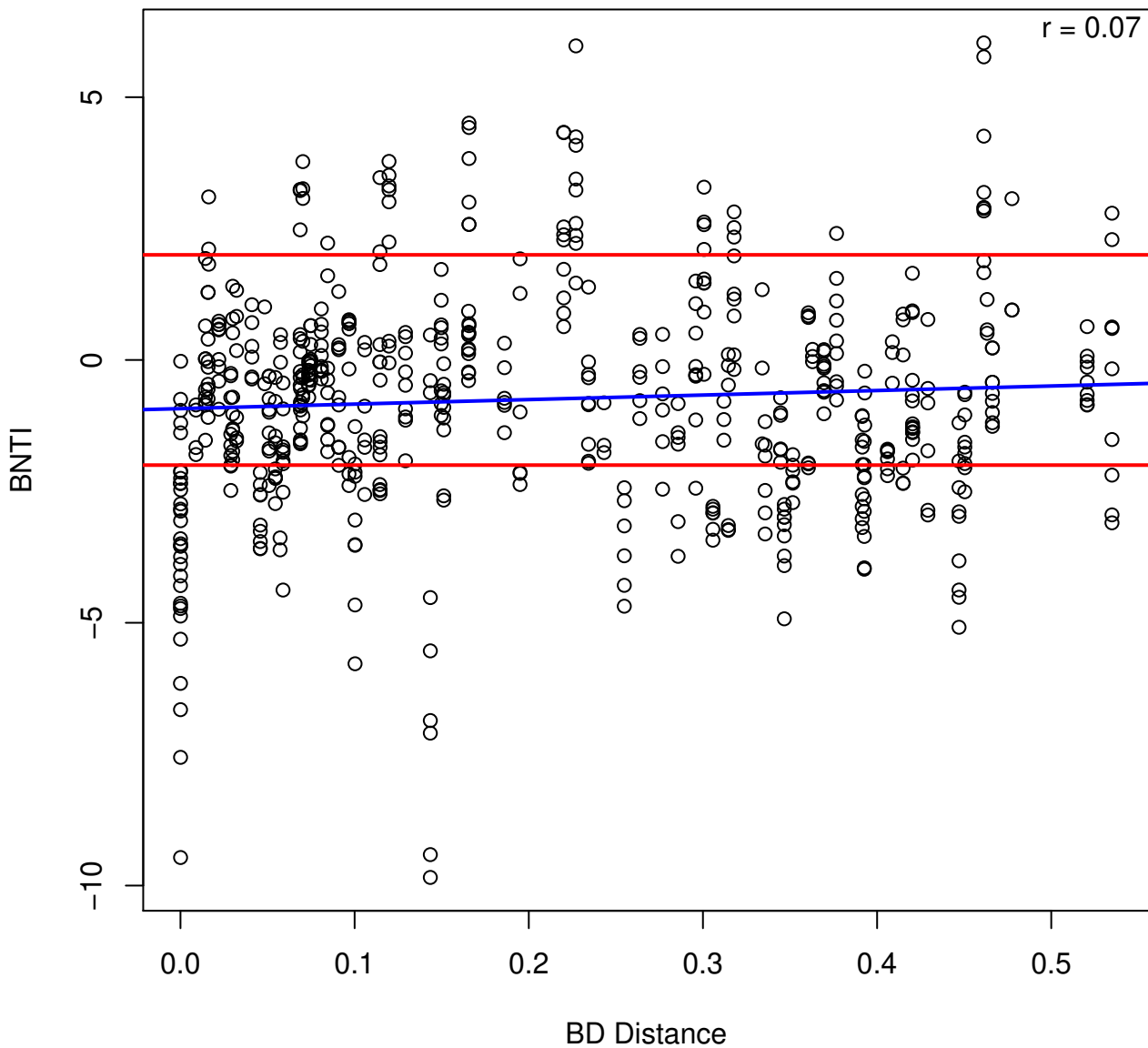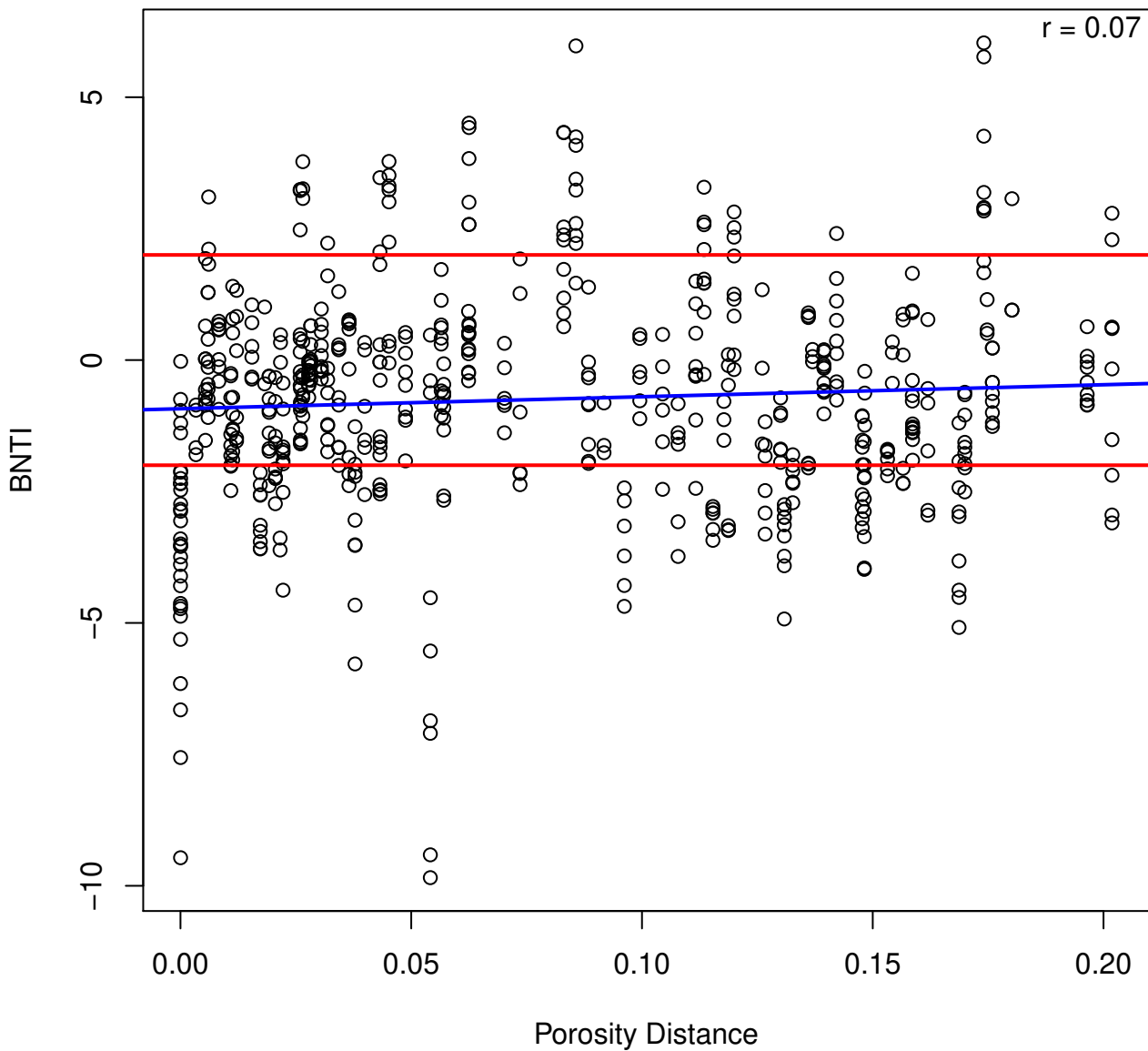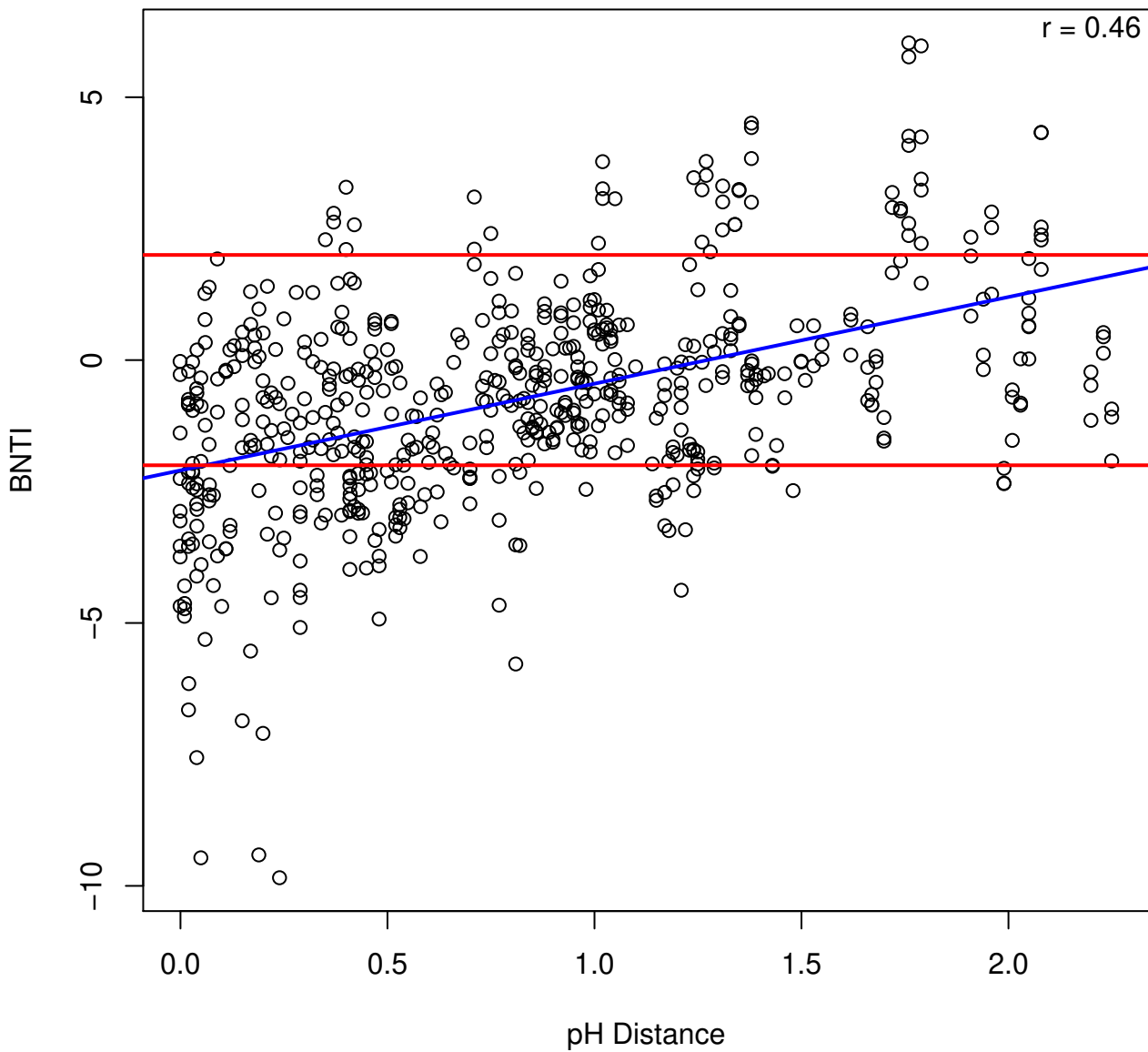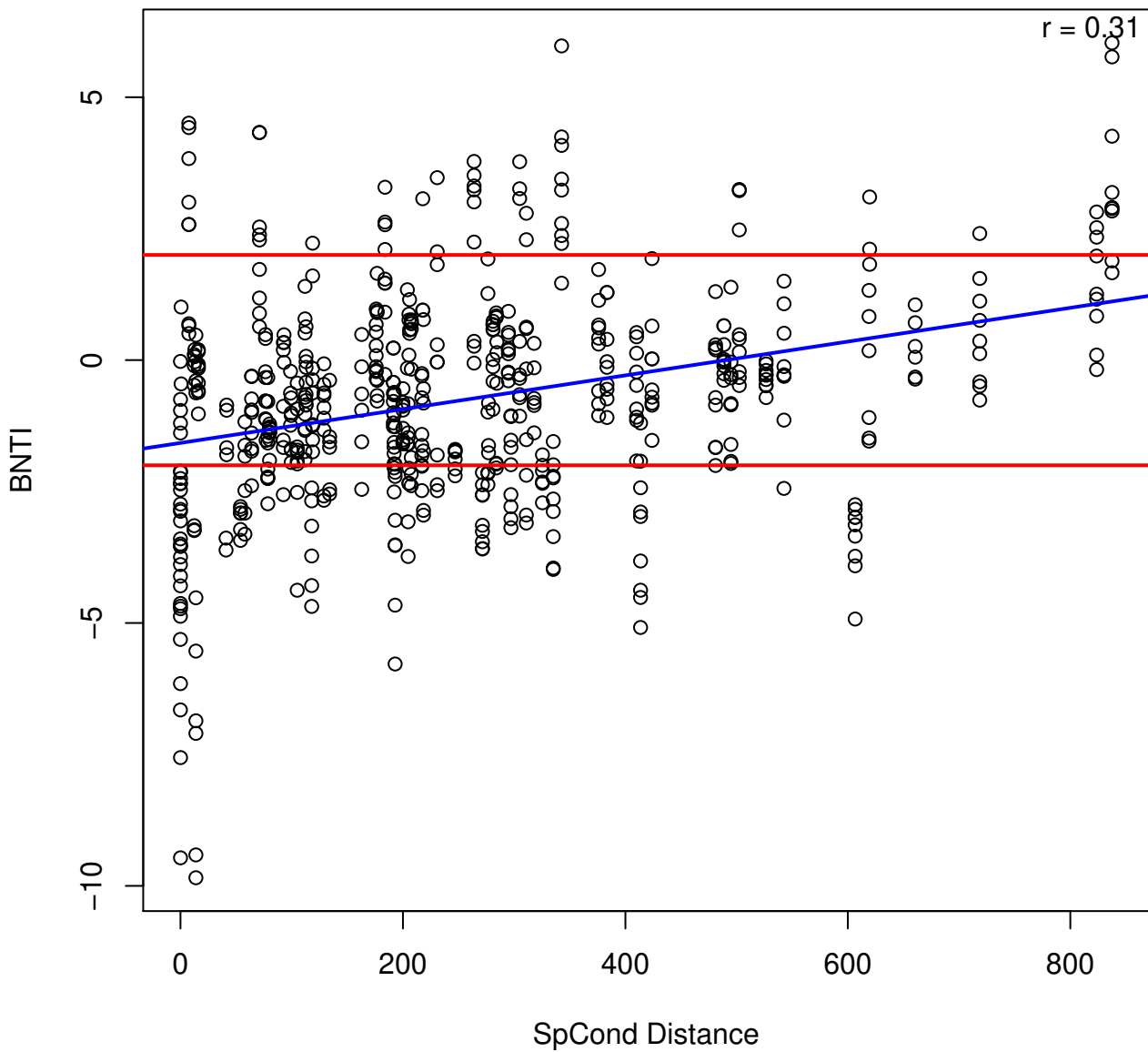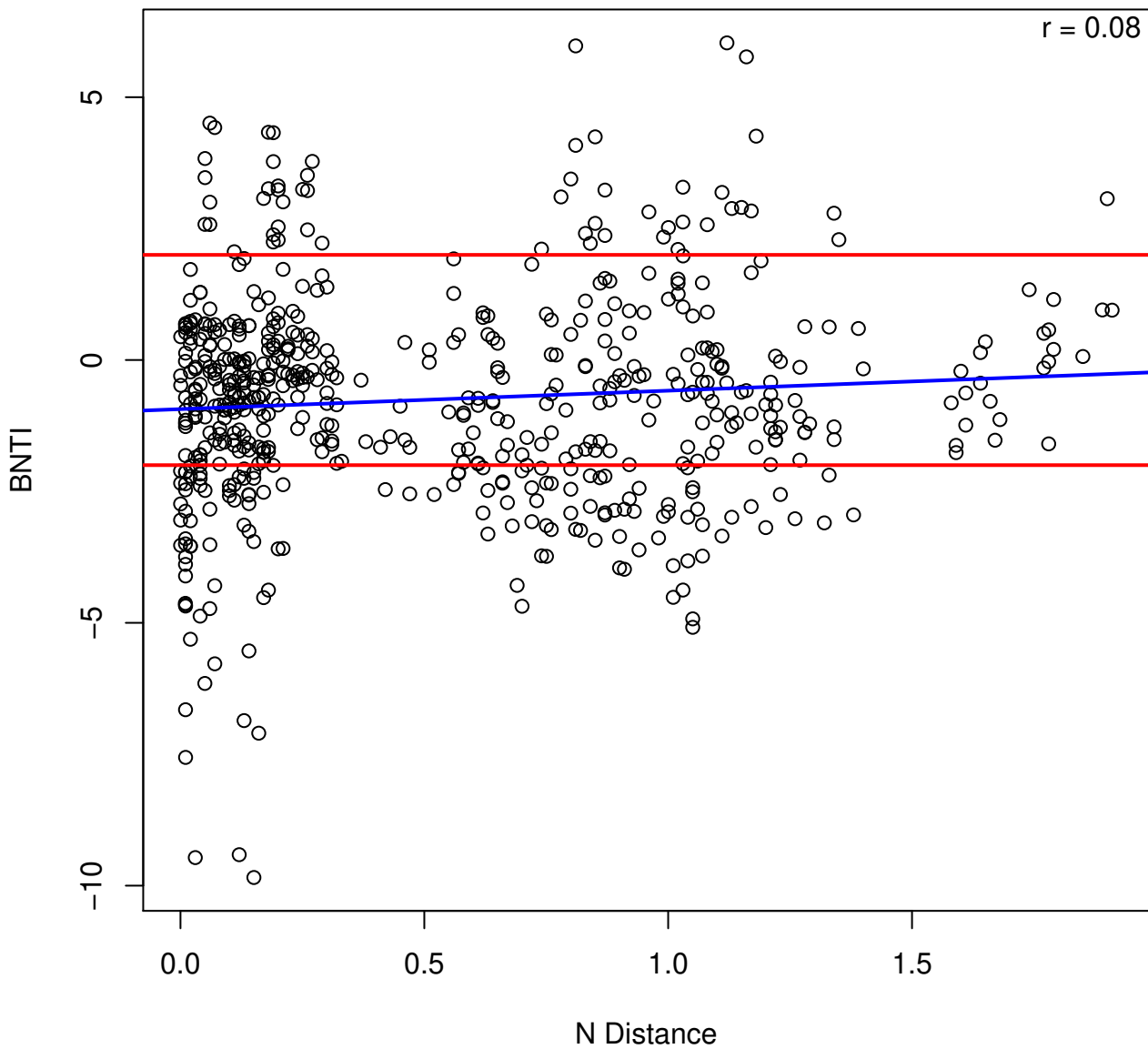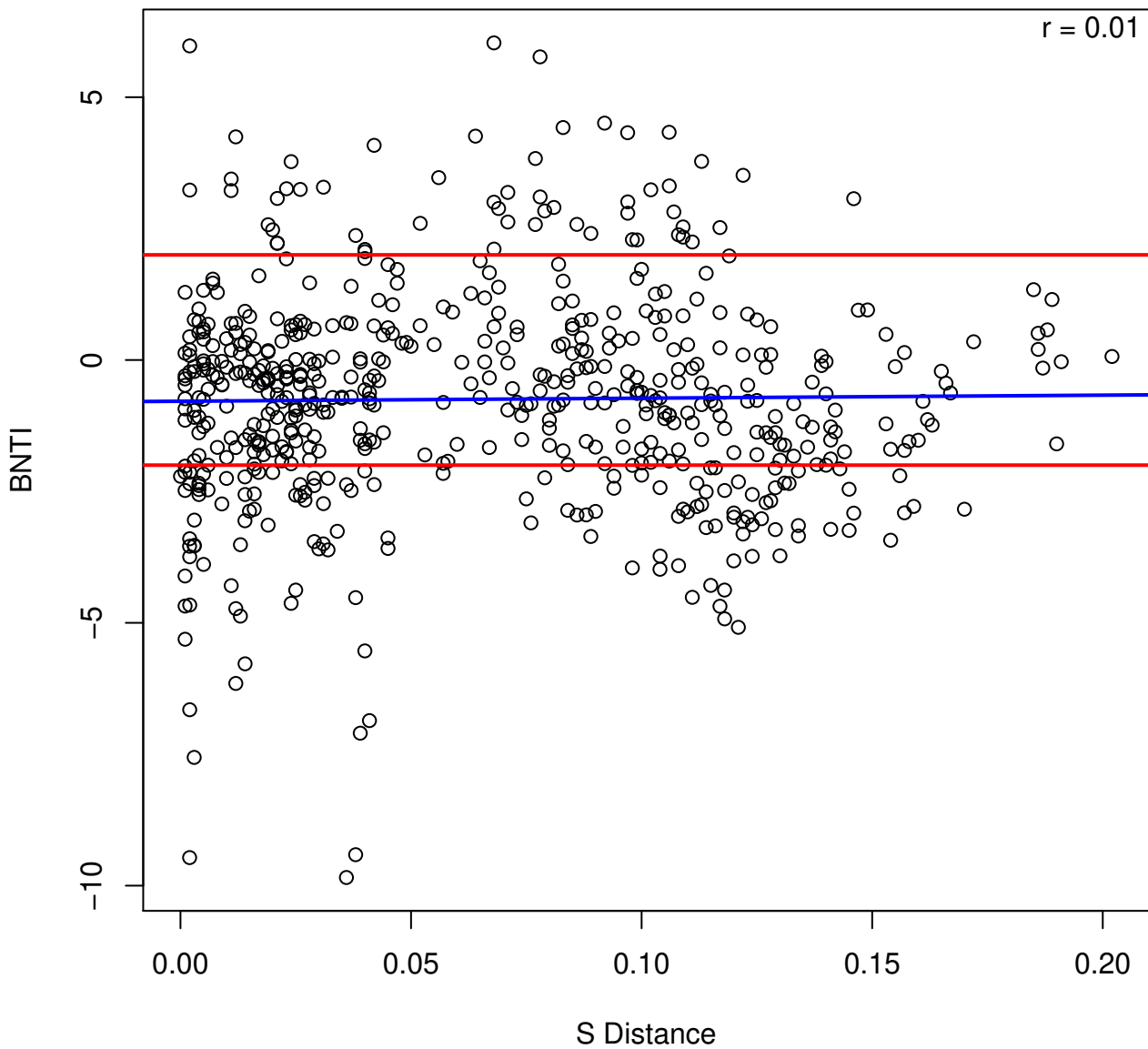
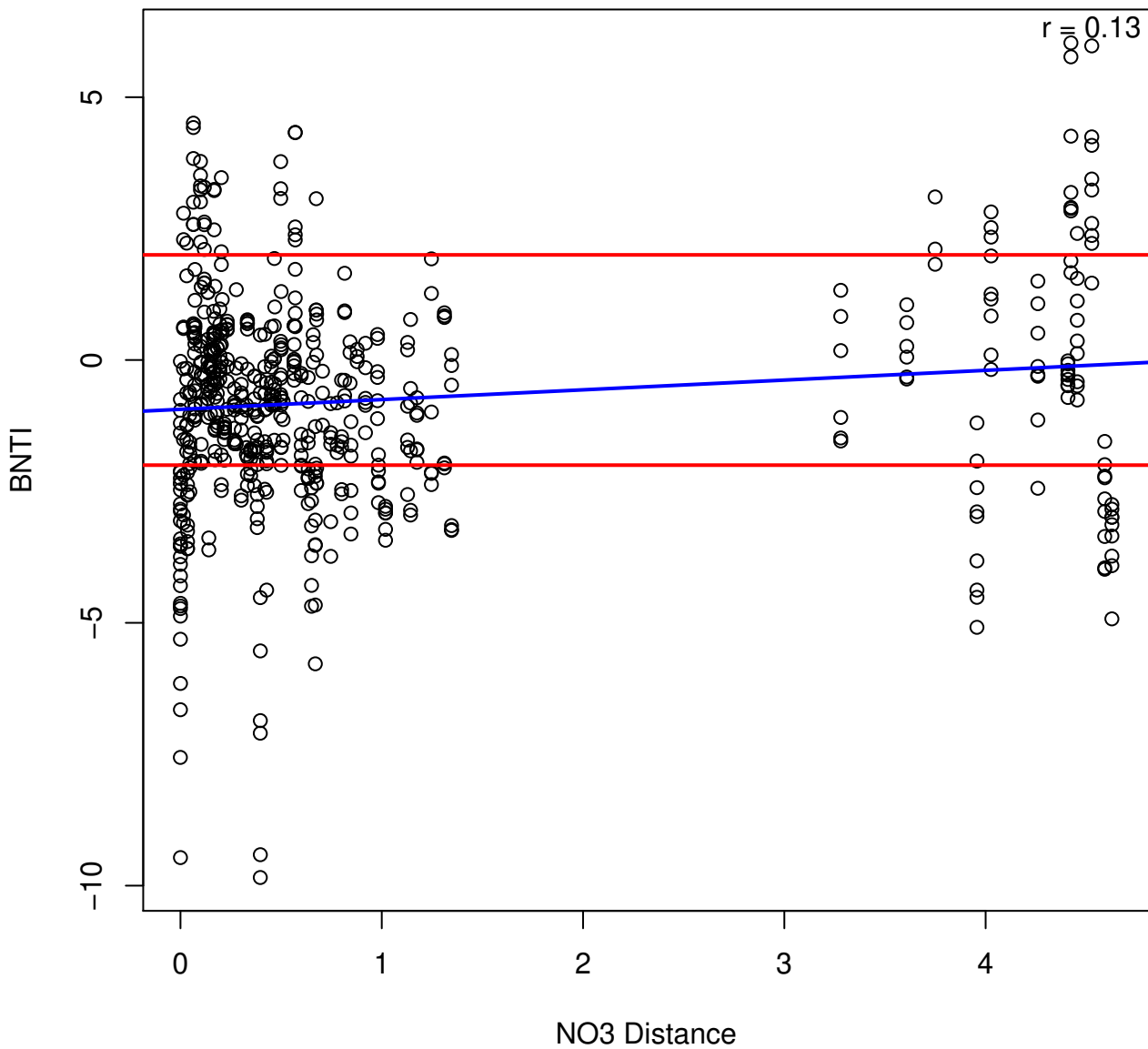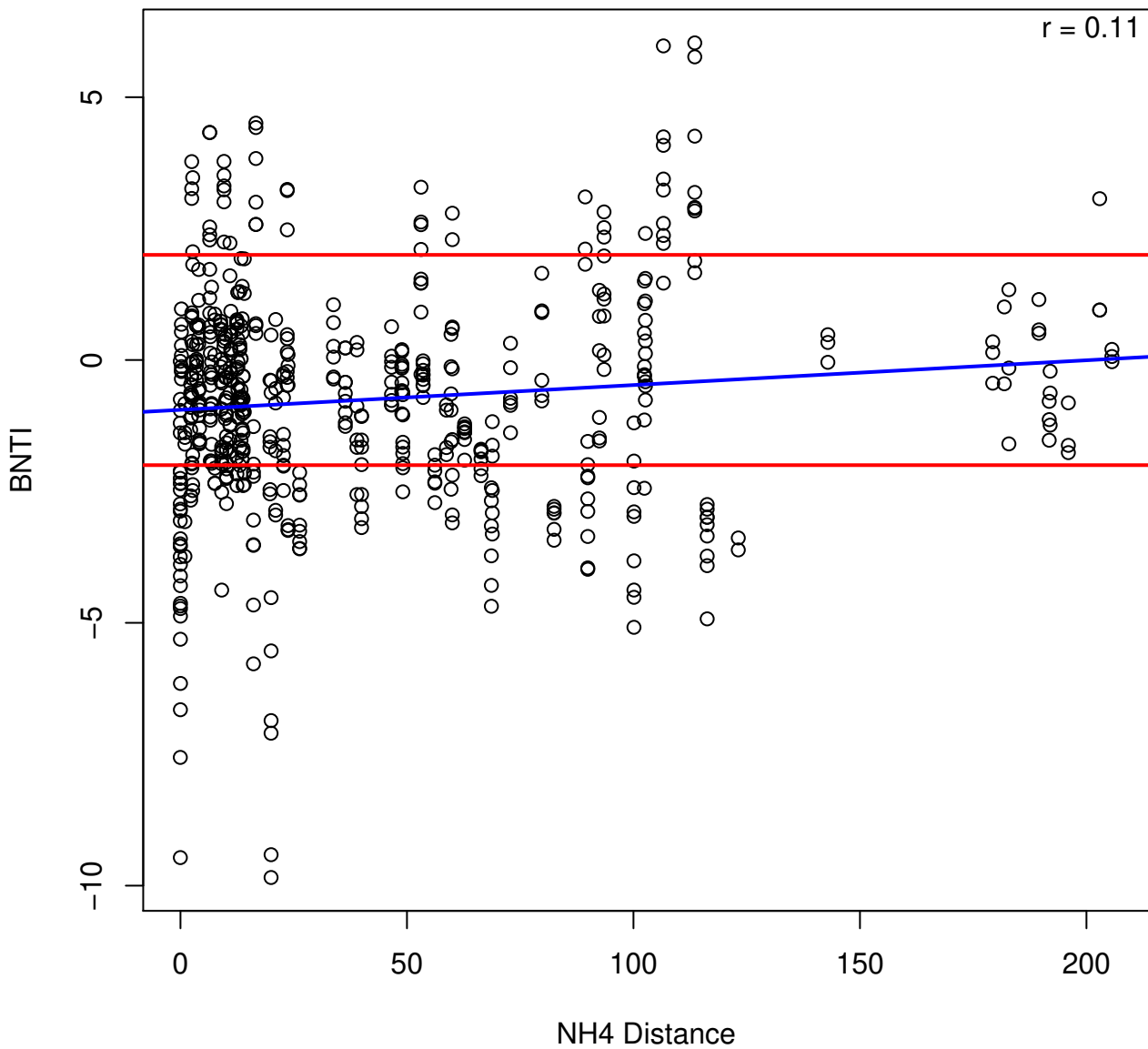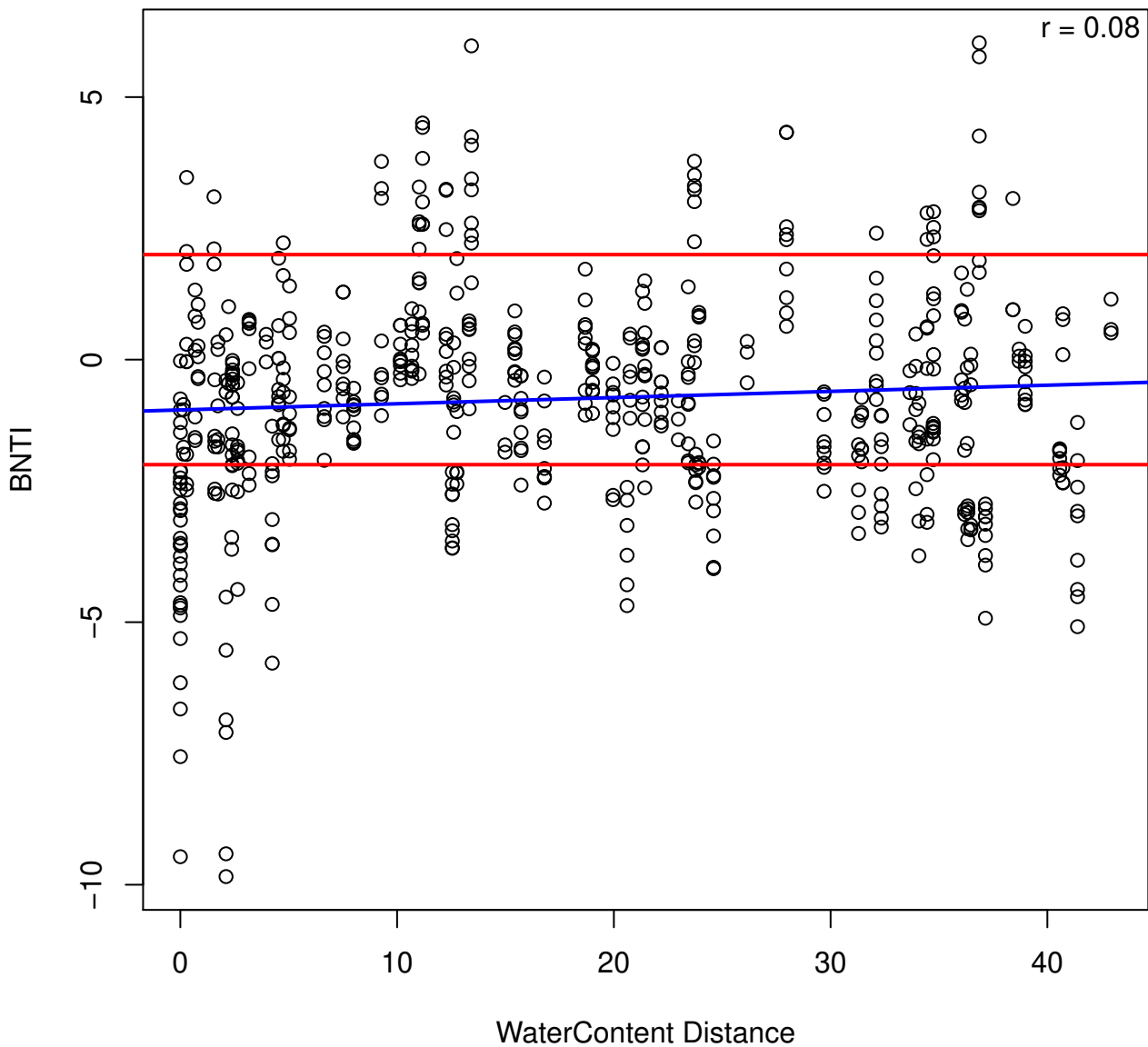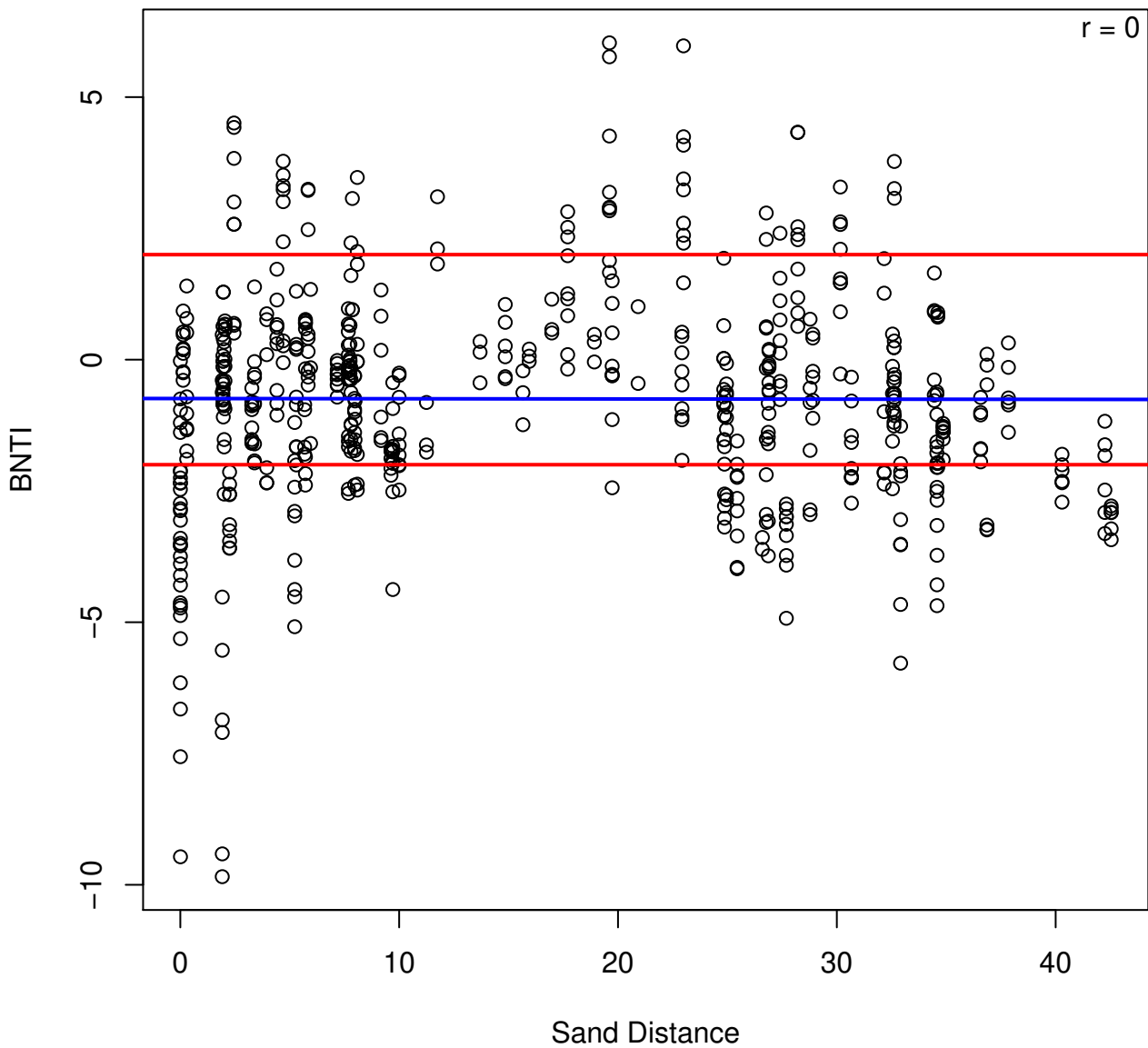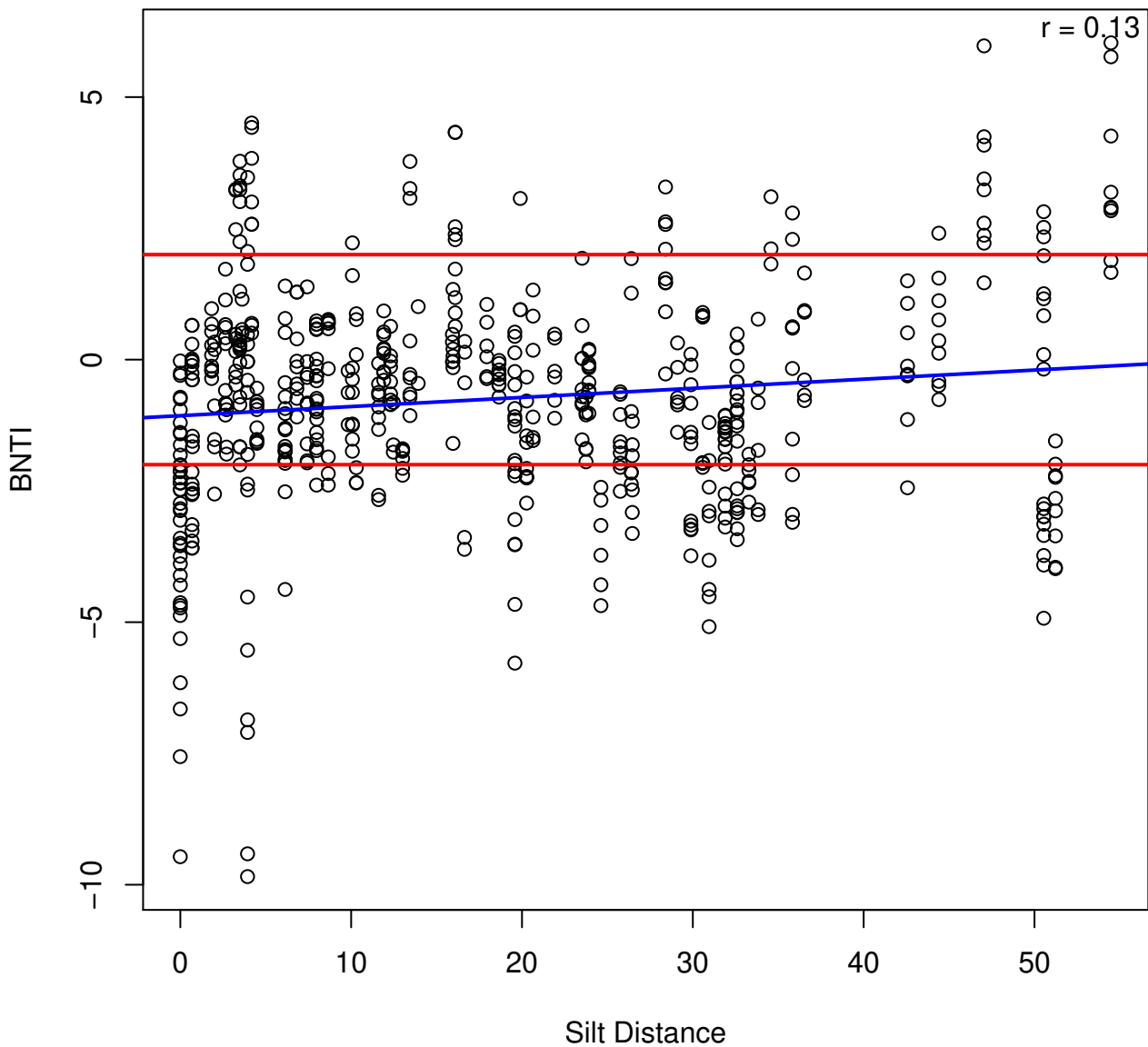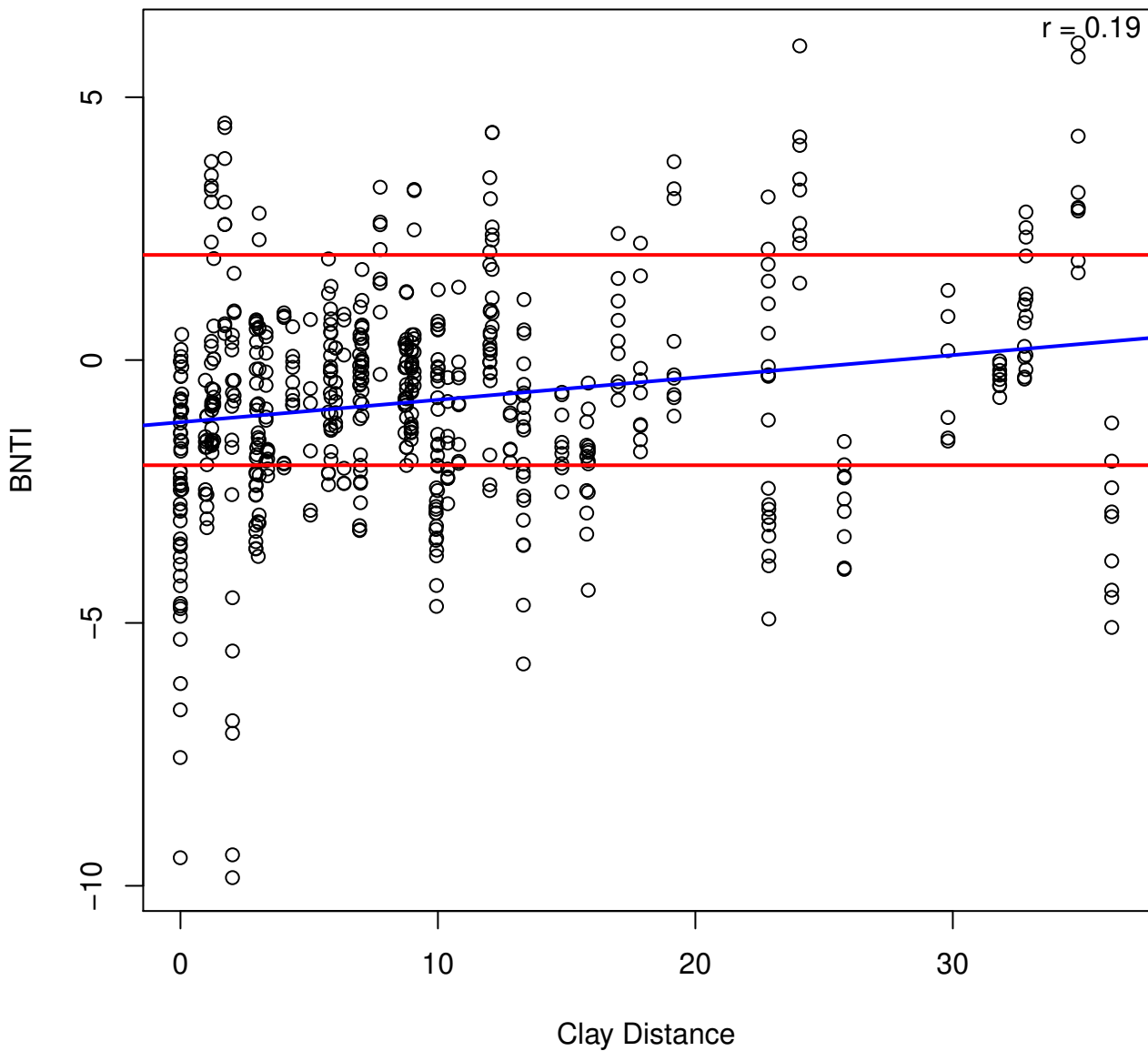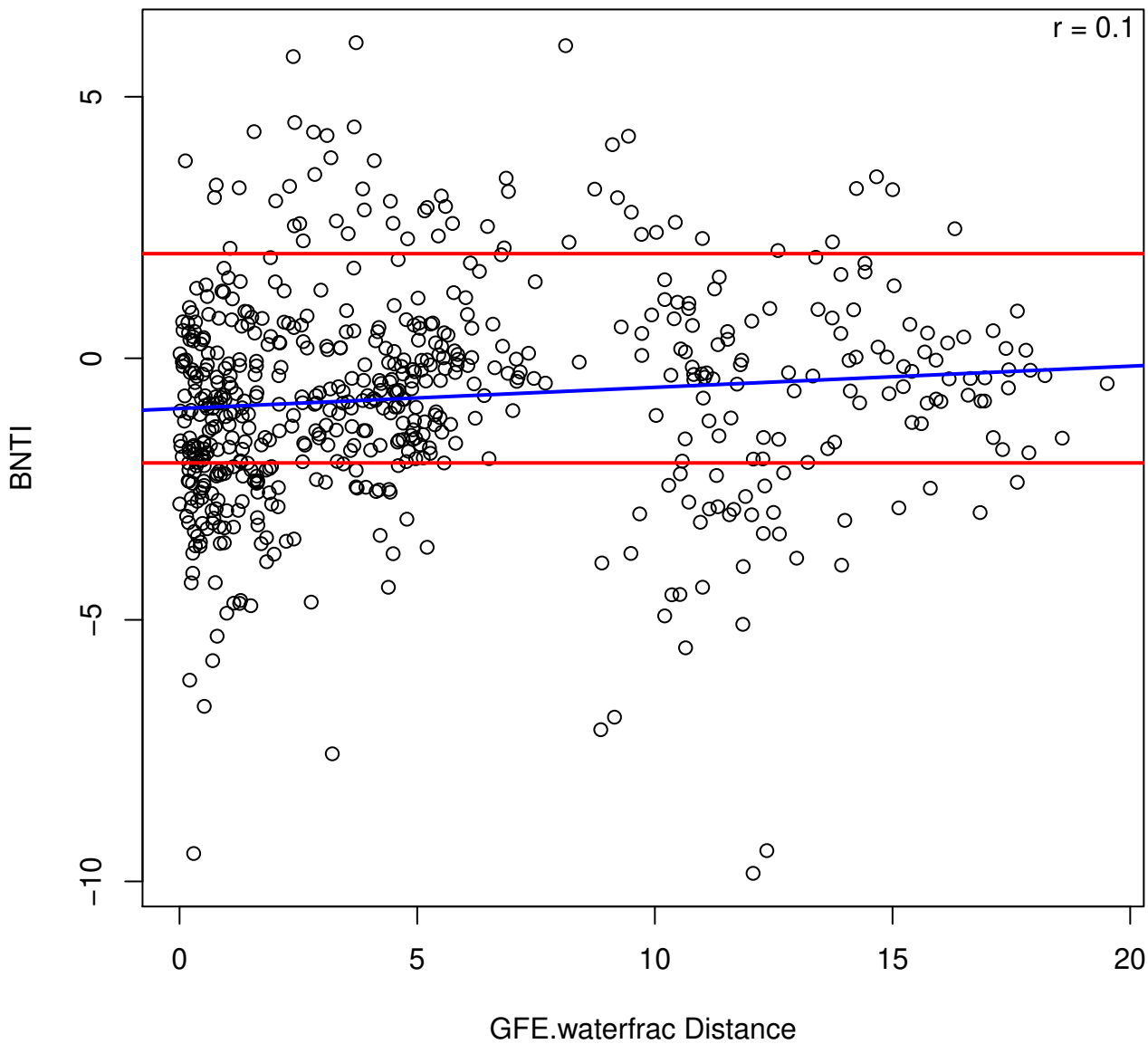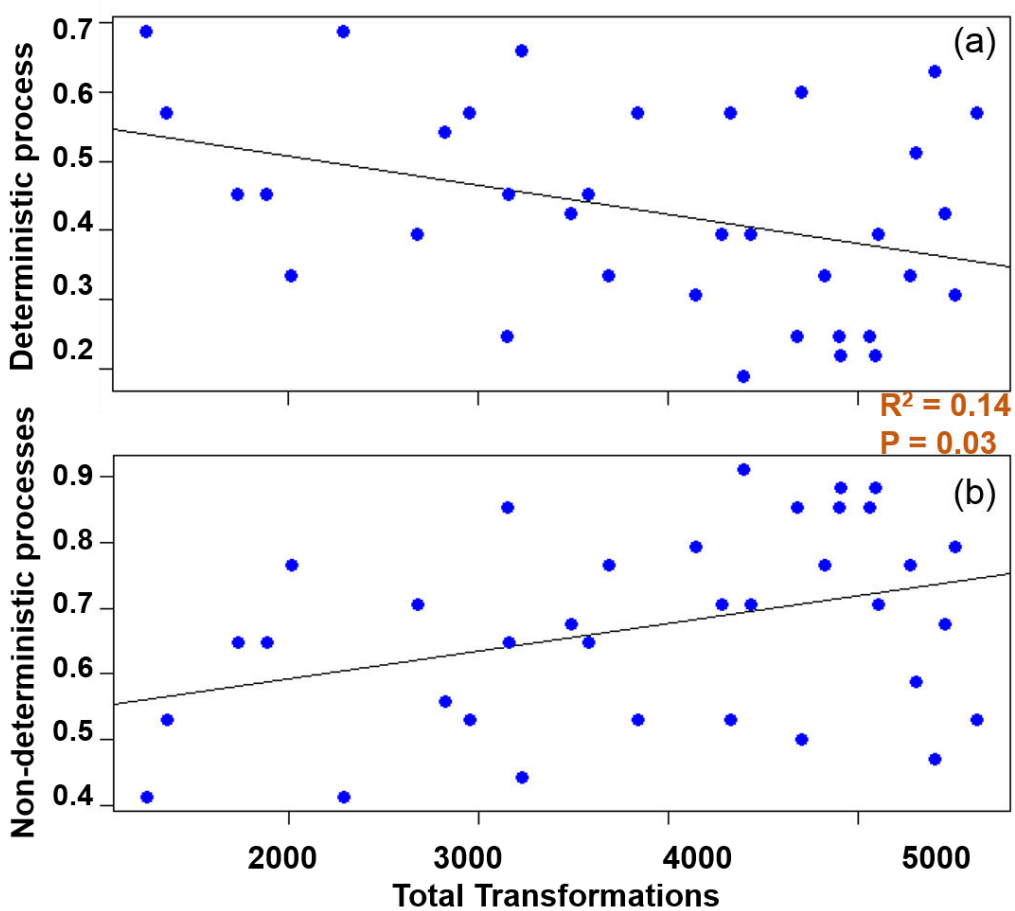**Supplementary Figure 3** Inferred biogeochemical transformations regressed against deterministic (a) and non-deterministic (b) microbial community assembly metric

Figure S4 Regression of Sorensen presence/absence of compound peaks against environmental and community assembly variables
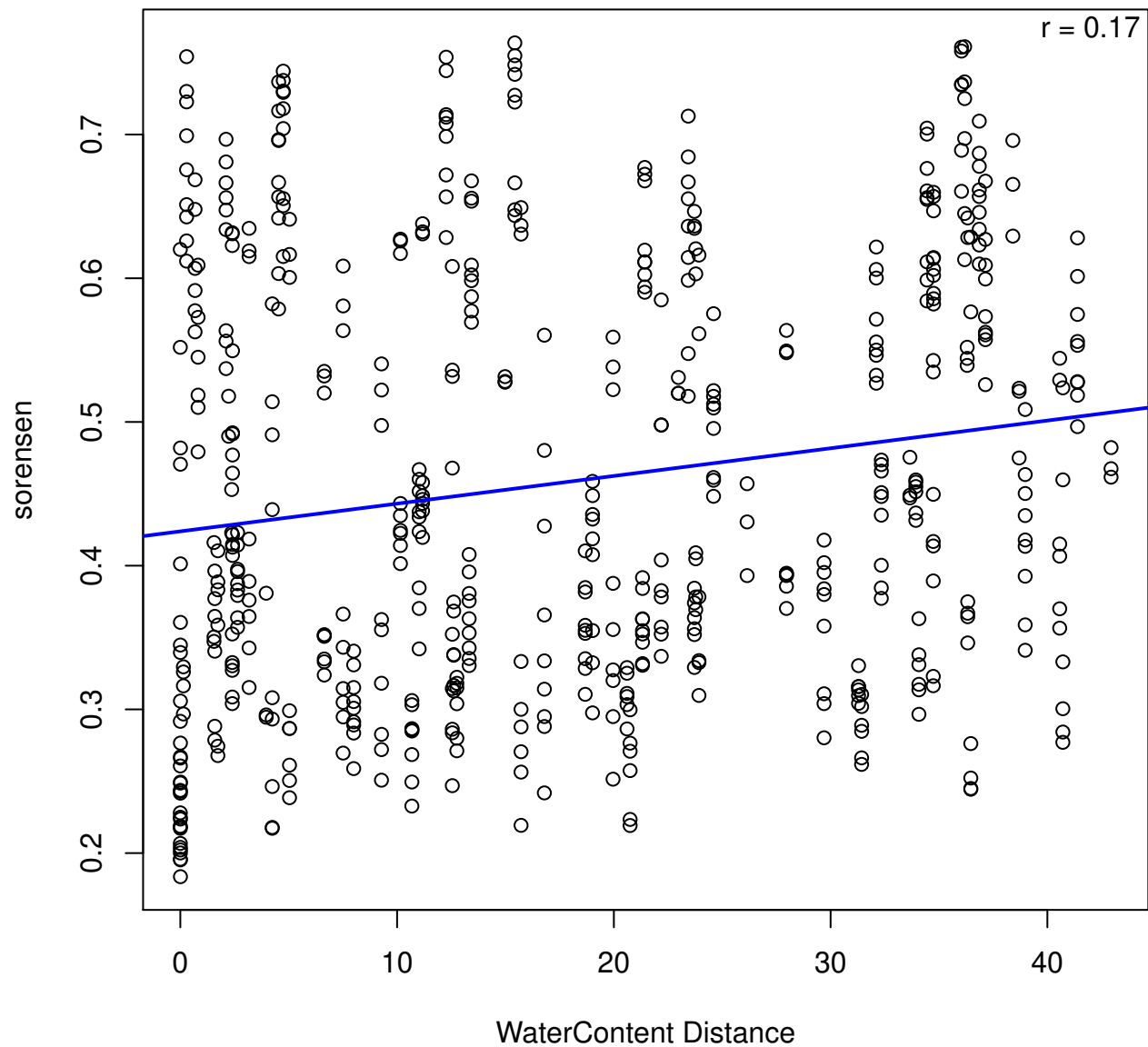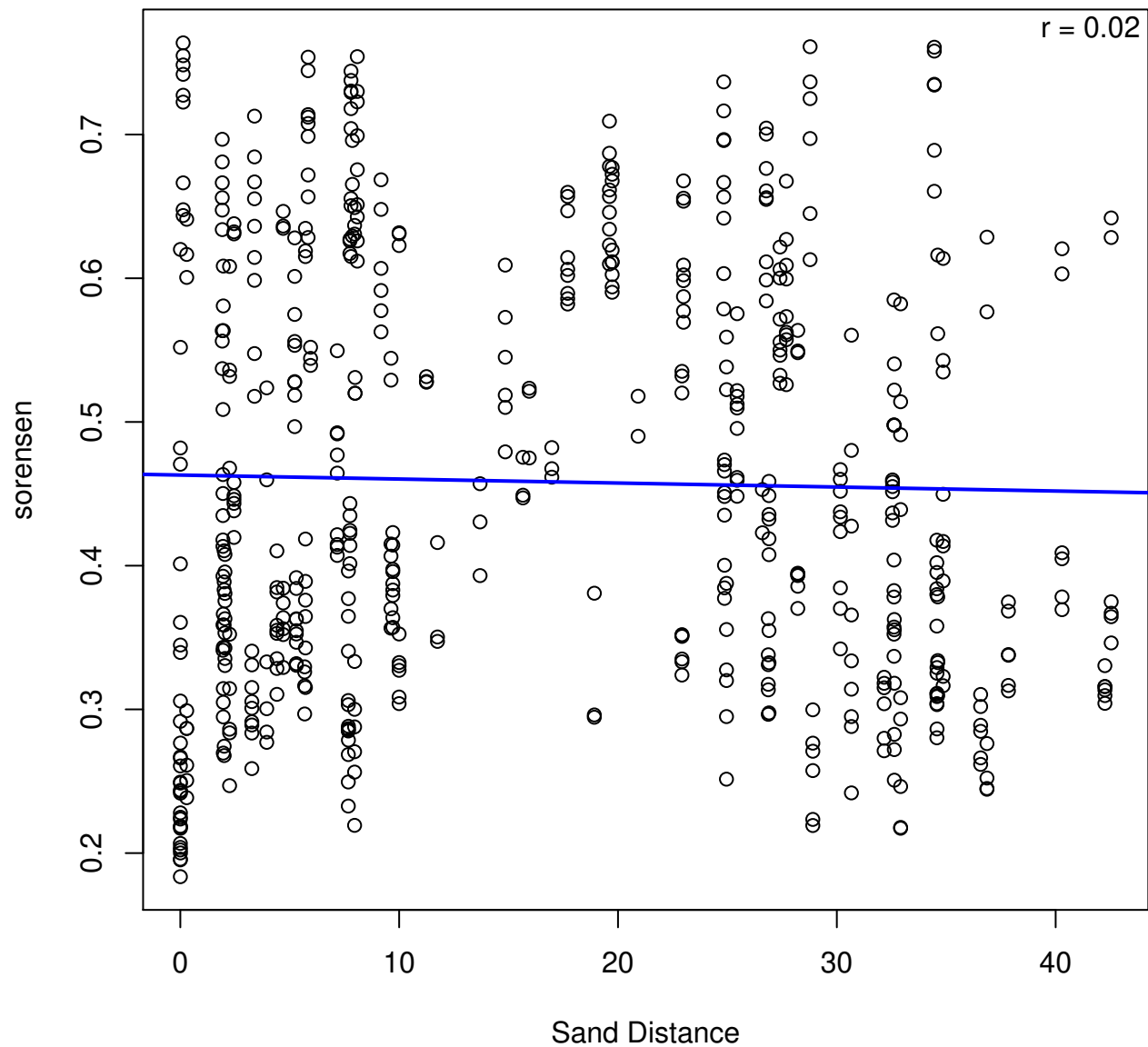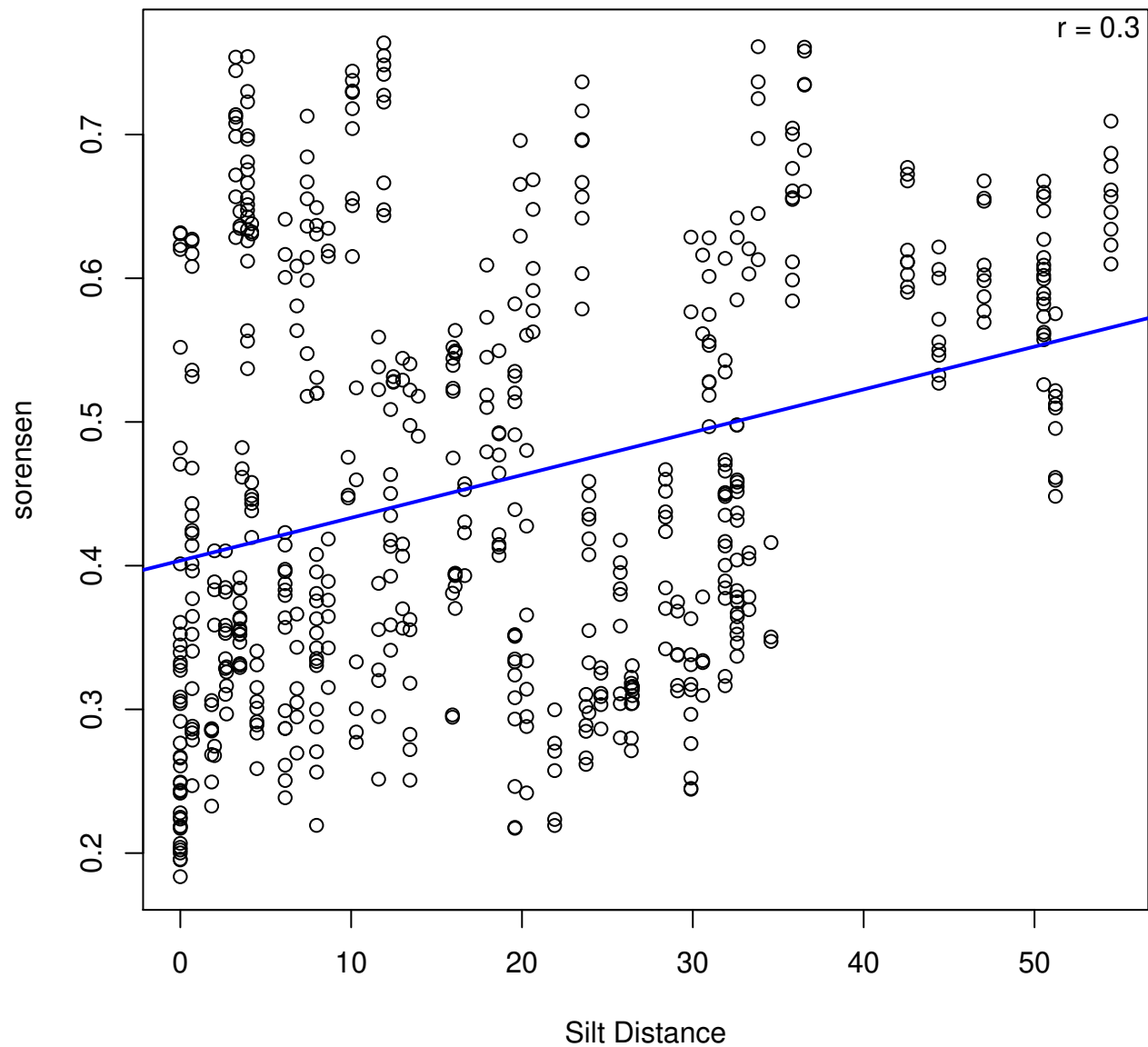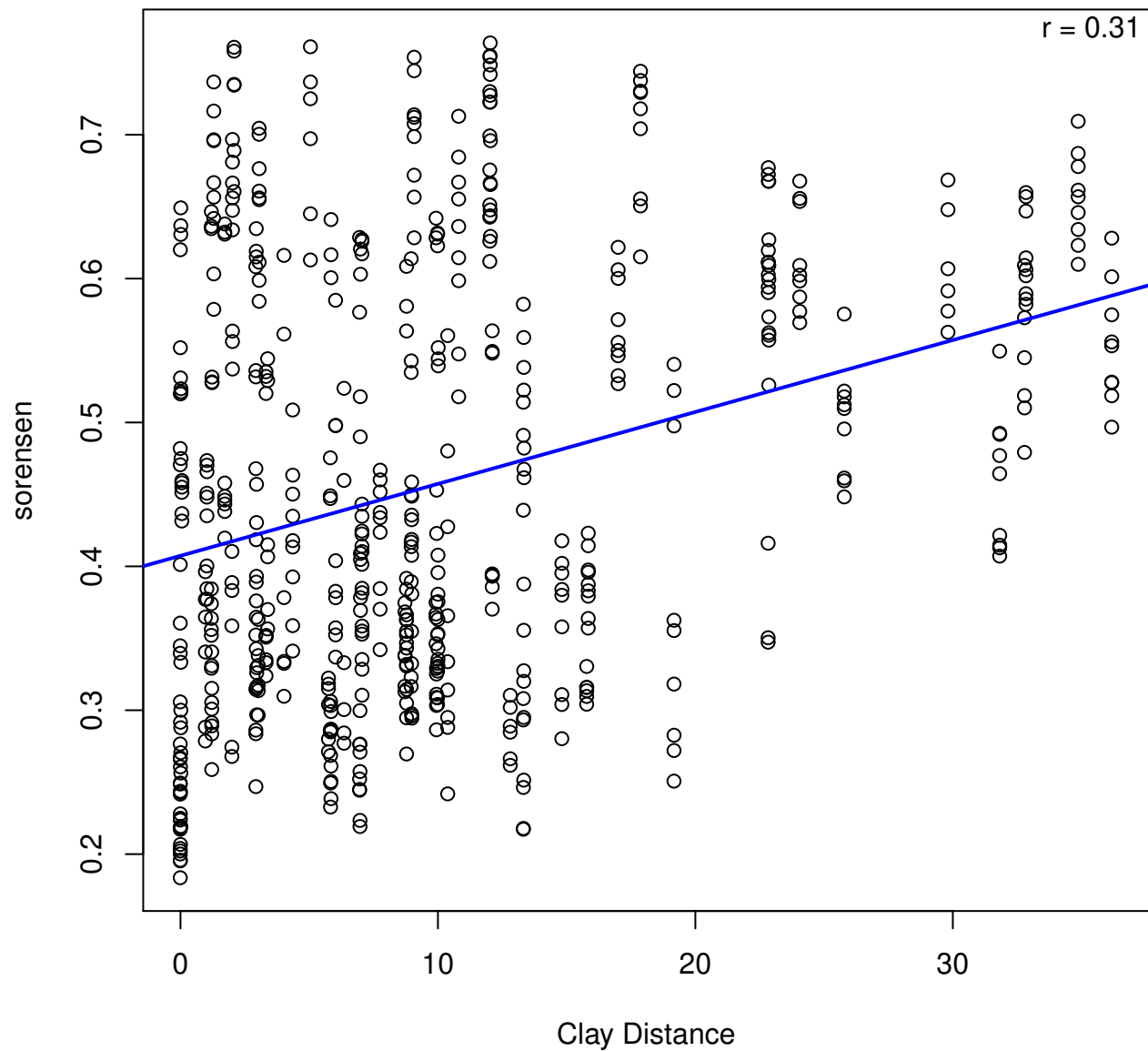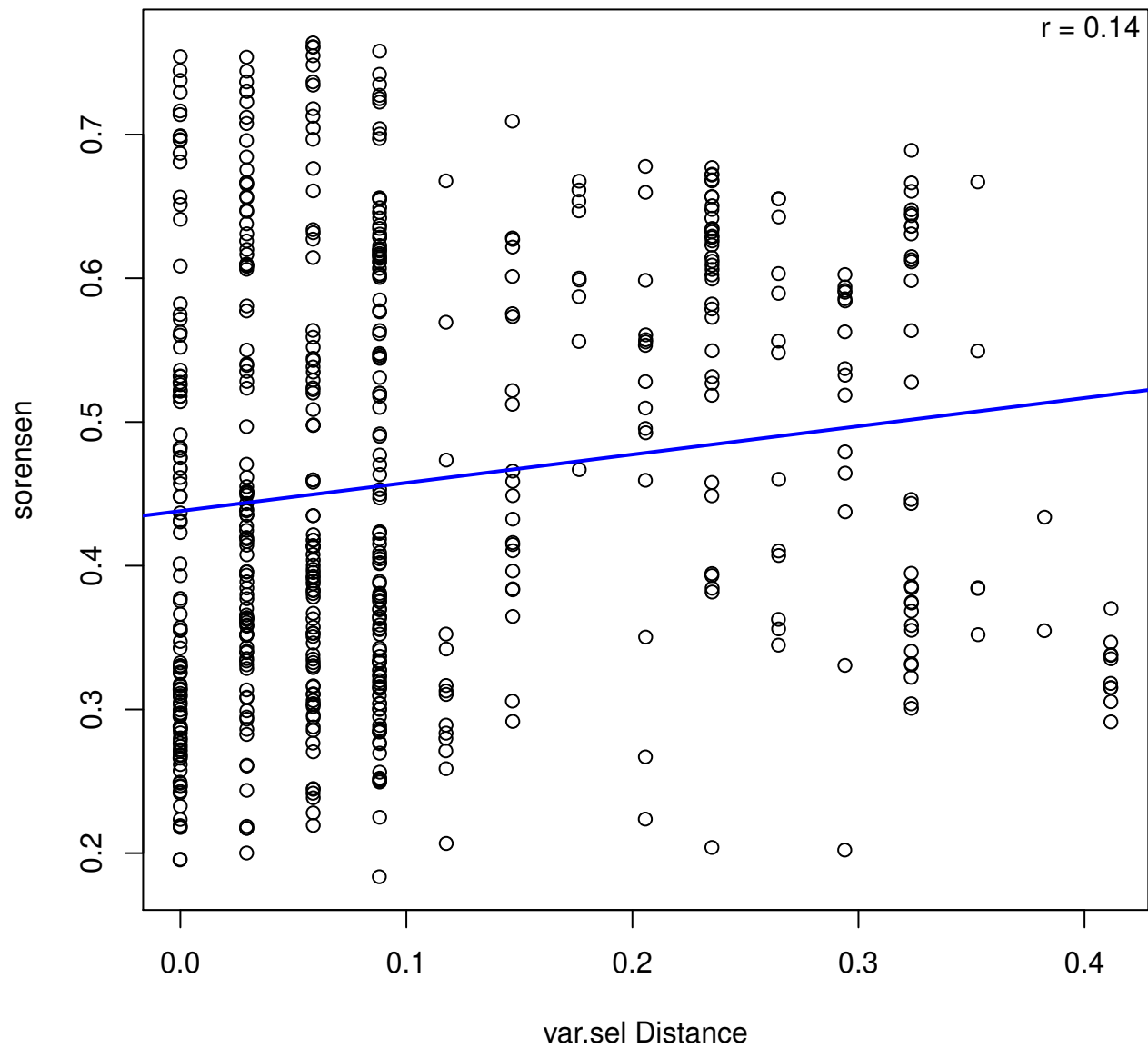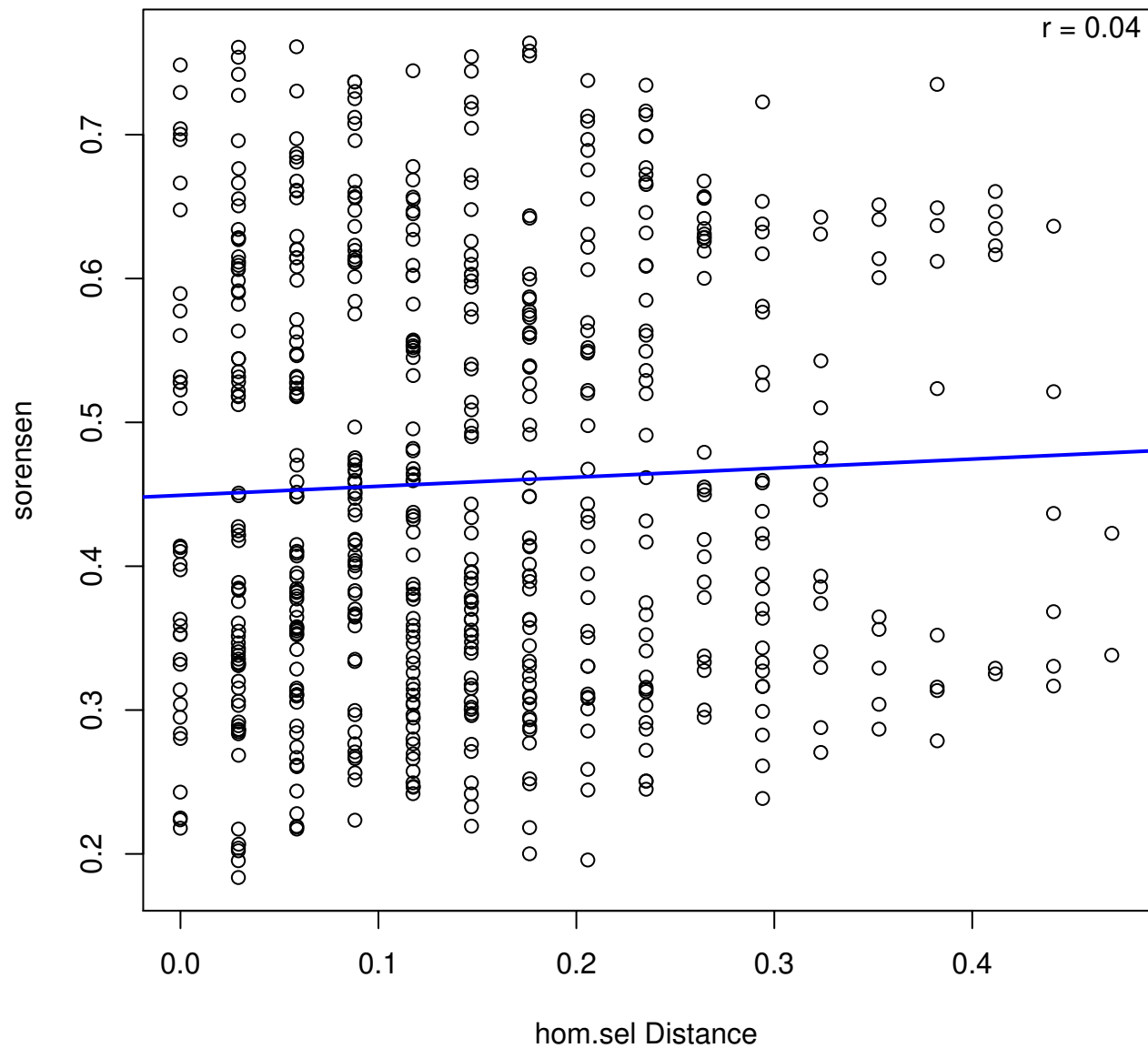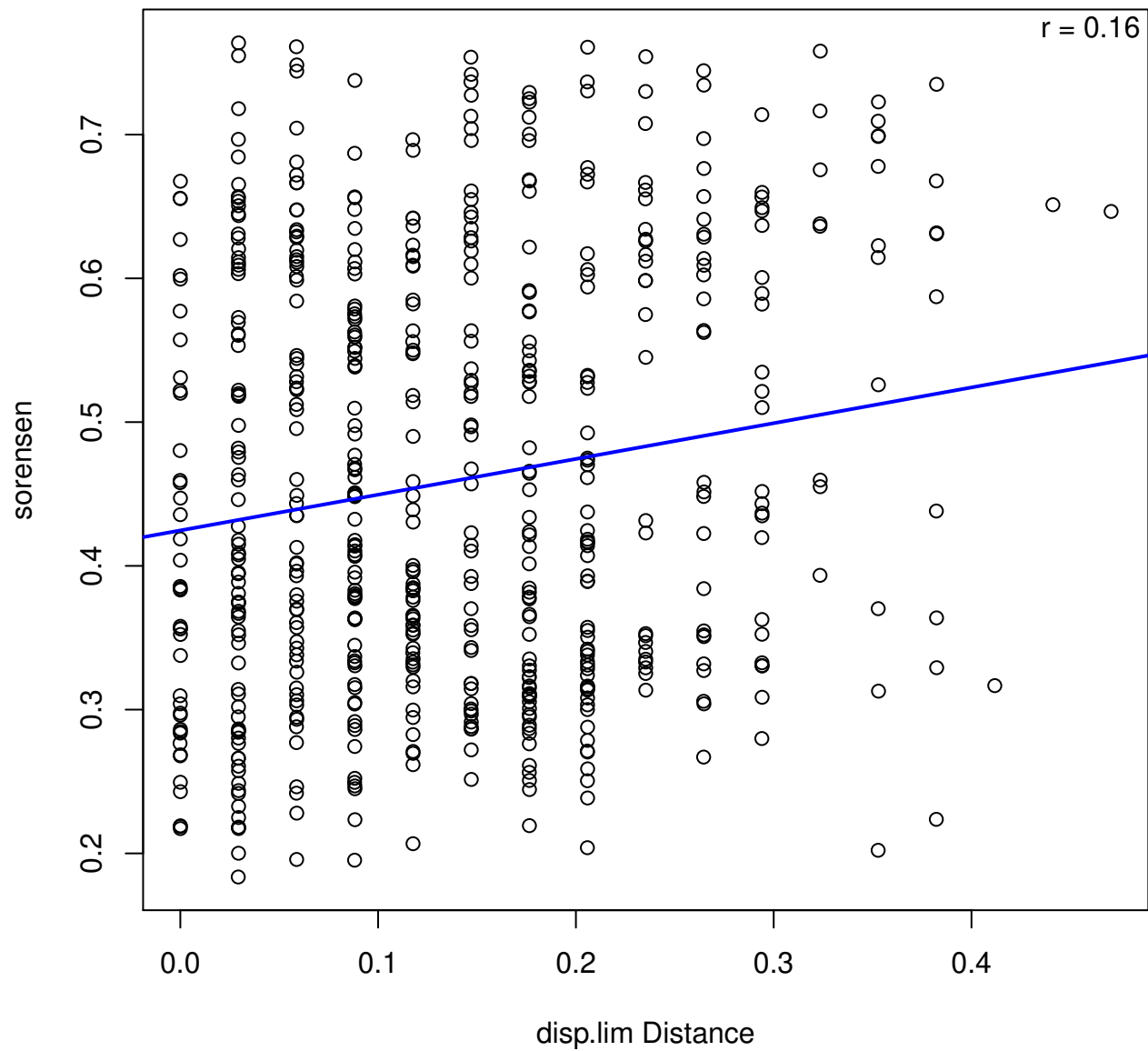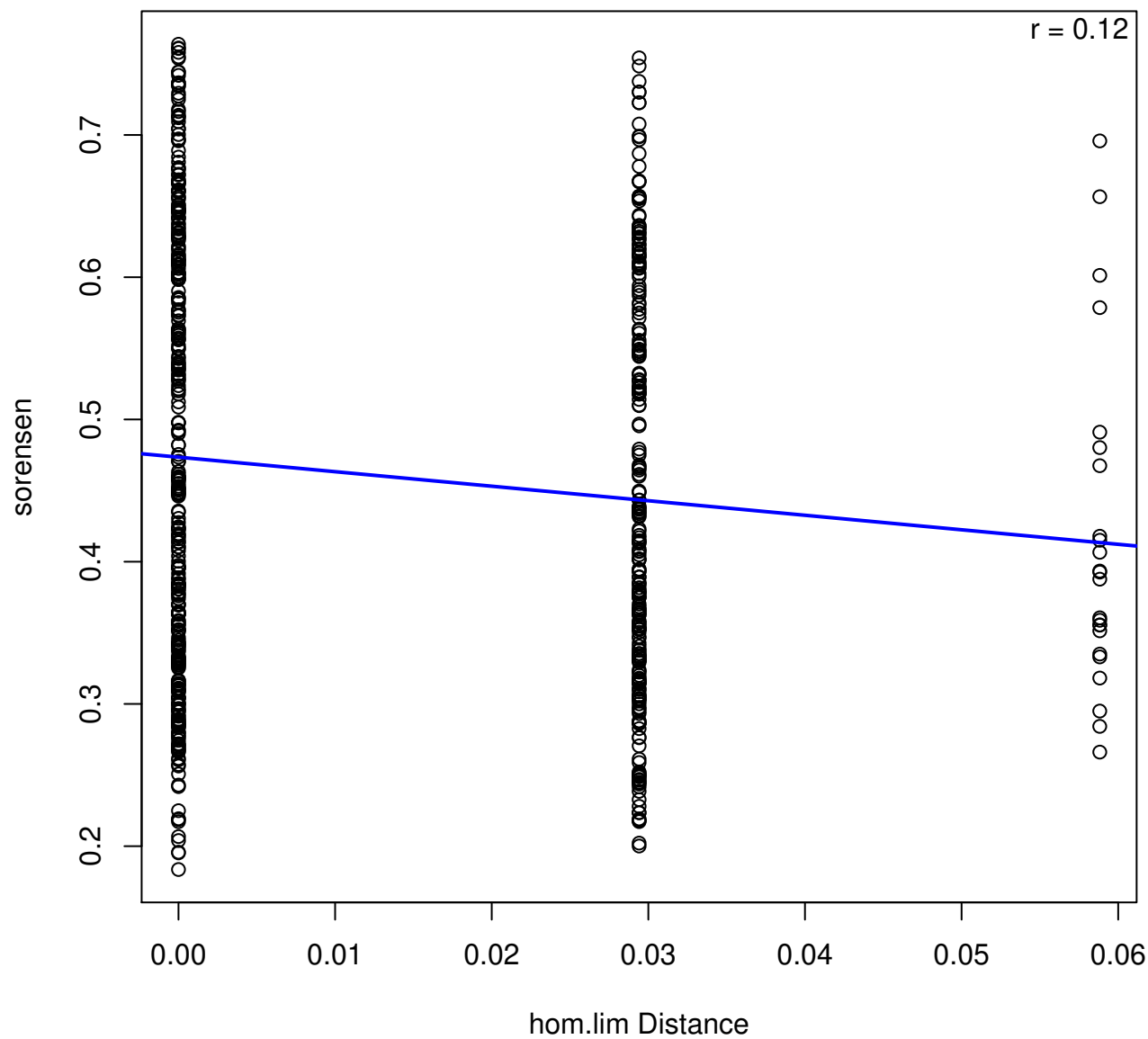
Table S1 Literature listing field-based natural salinity gradient studies, long-term field manipulations of salinity exposure, and lab-based incubation studies subjecting soils to varying levels of salinity

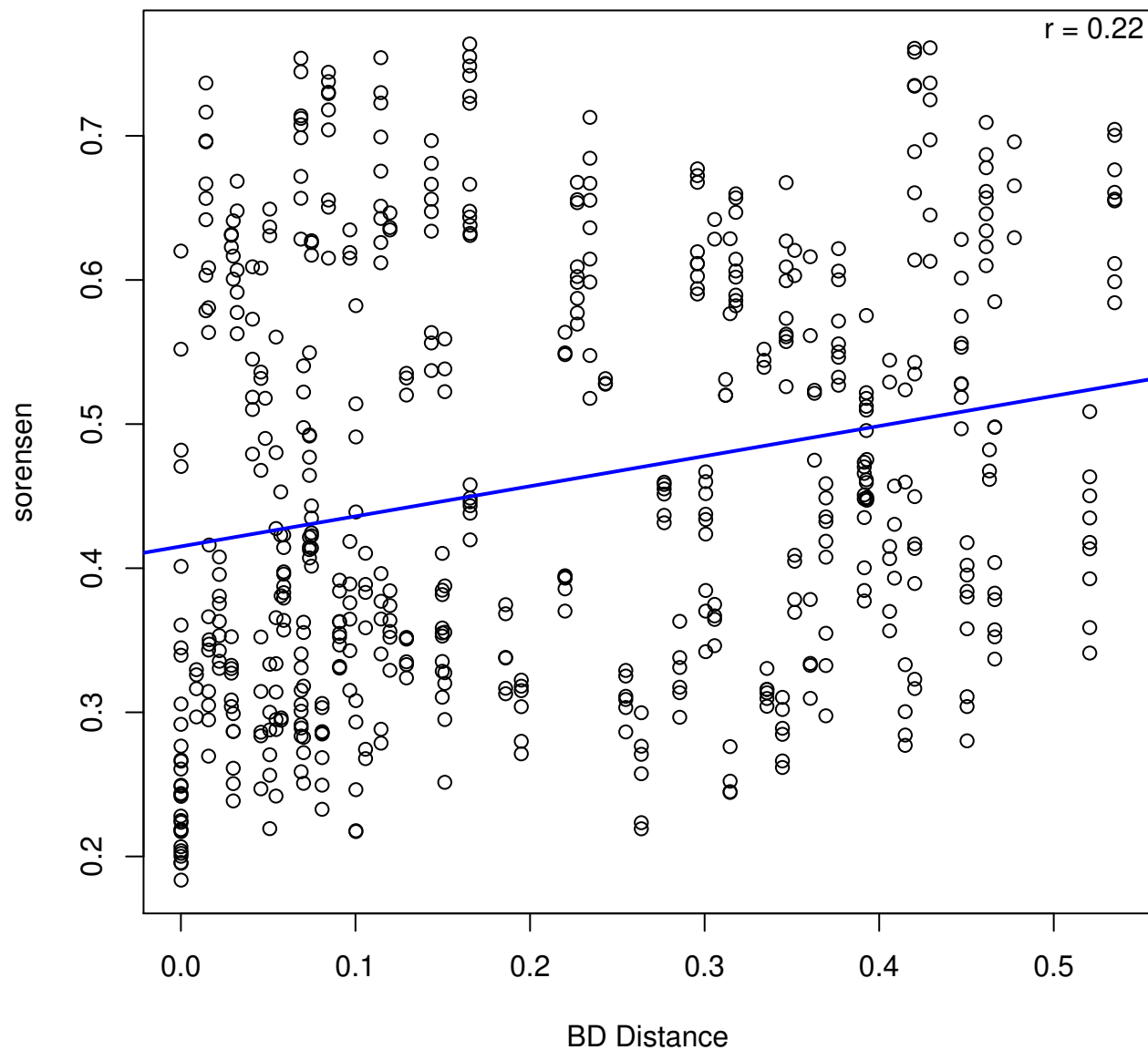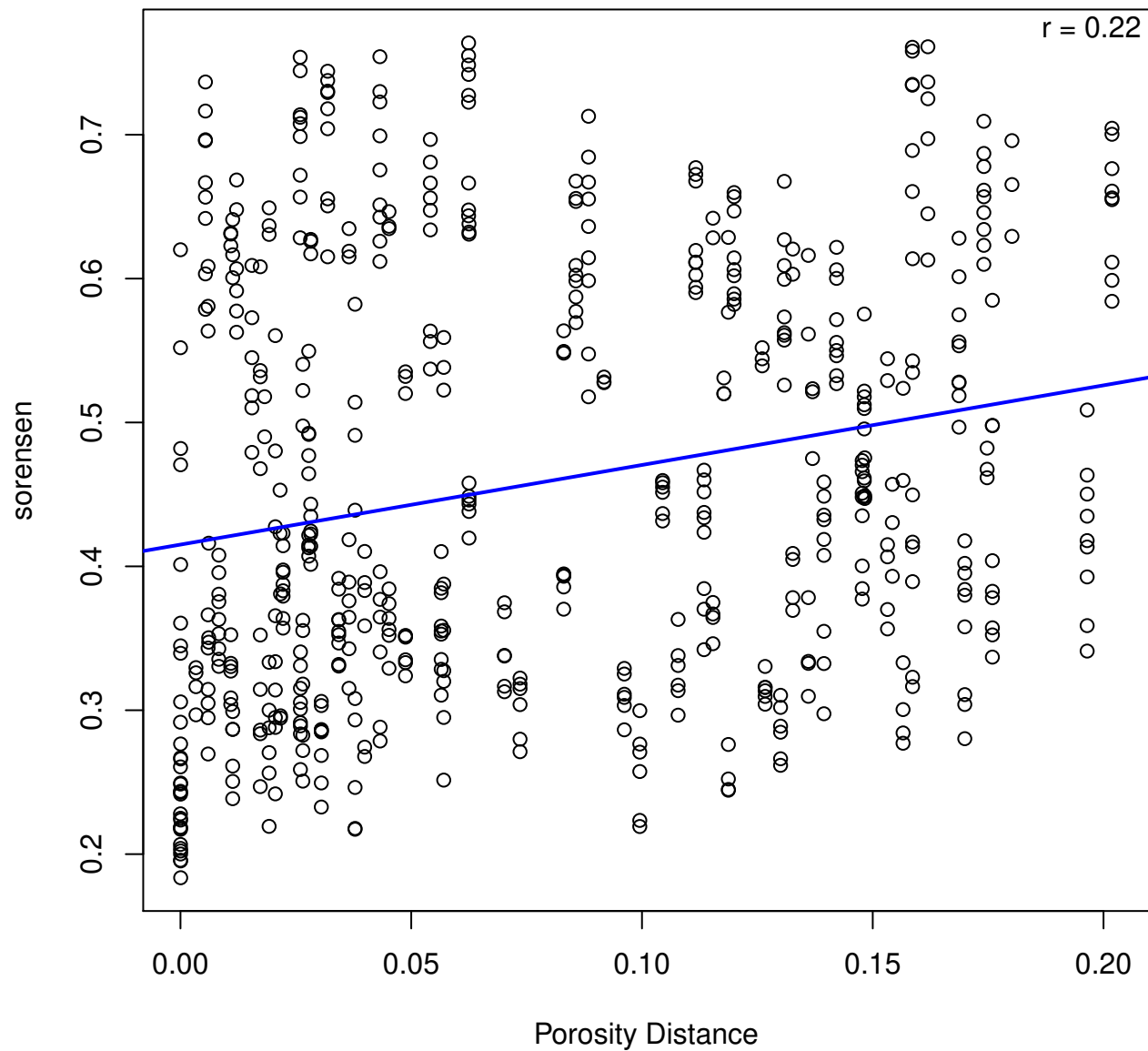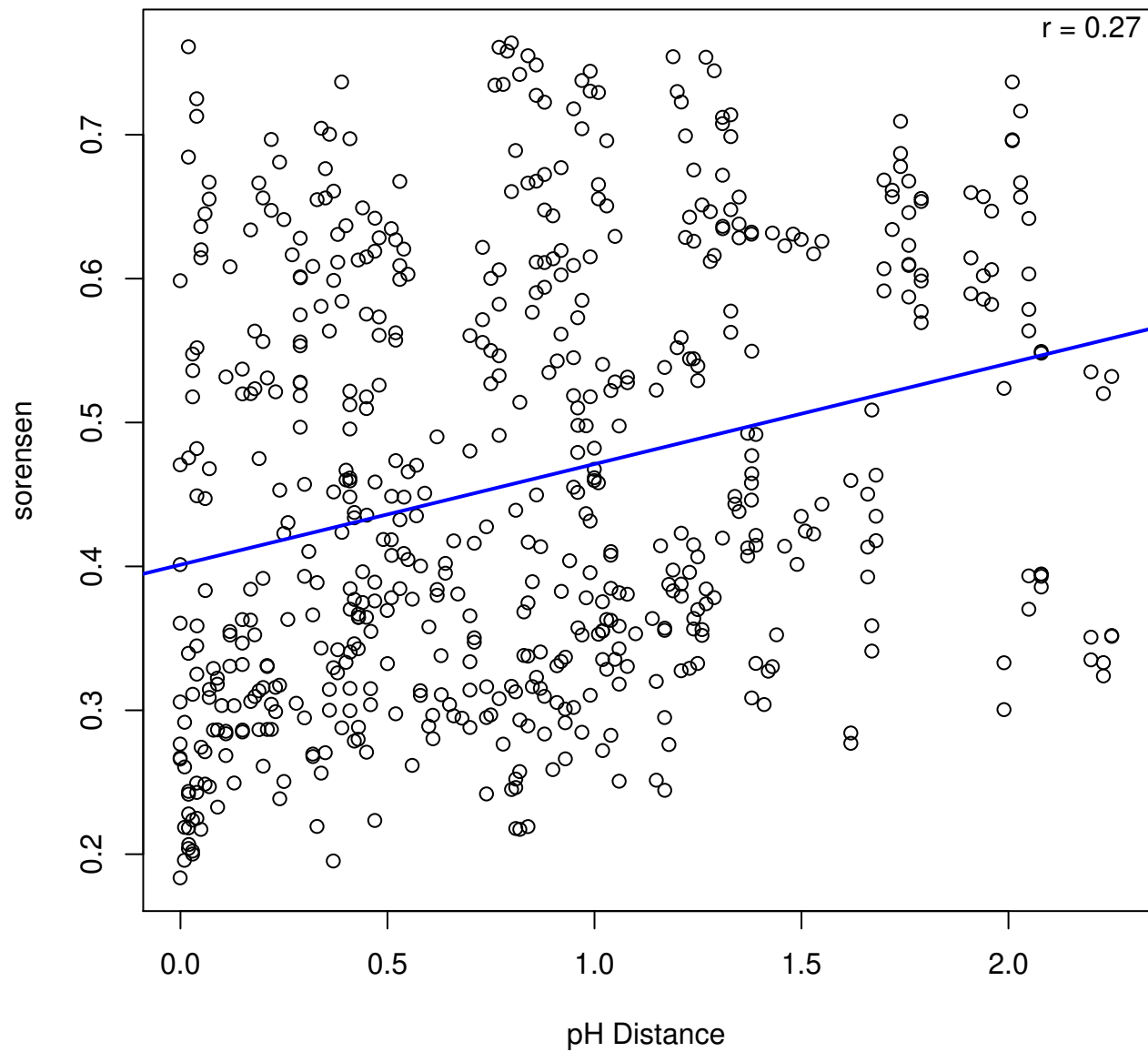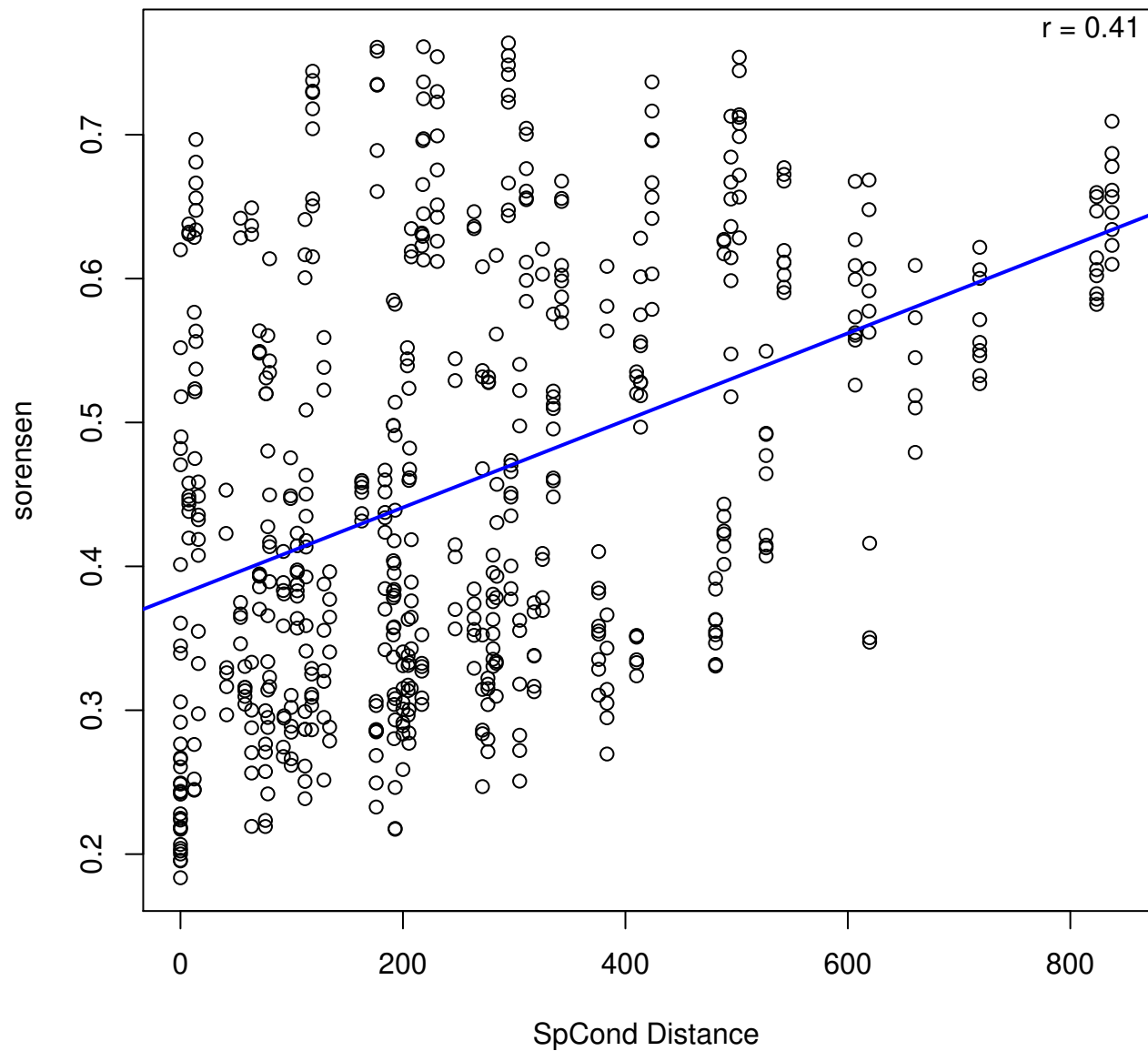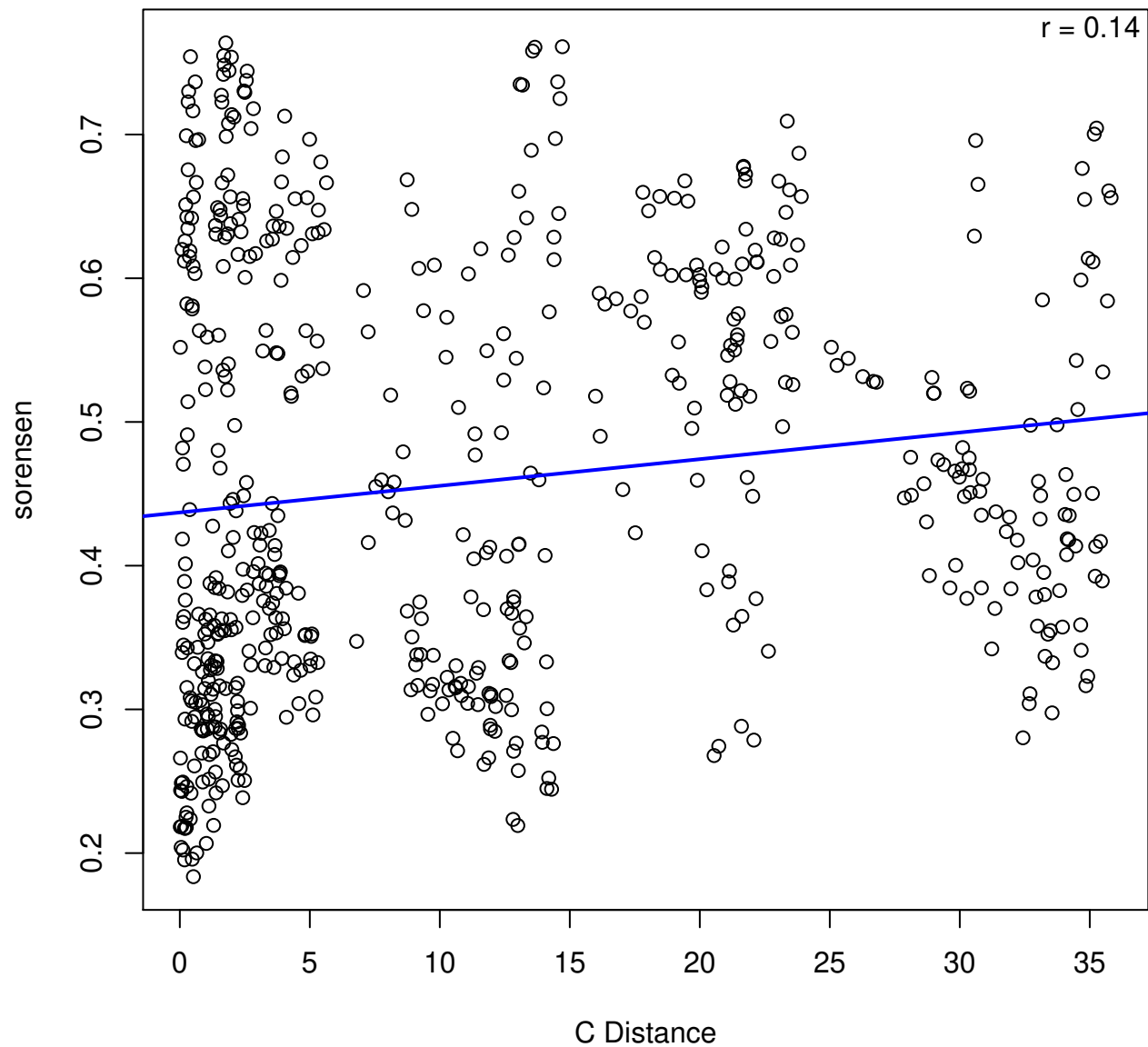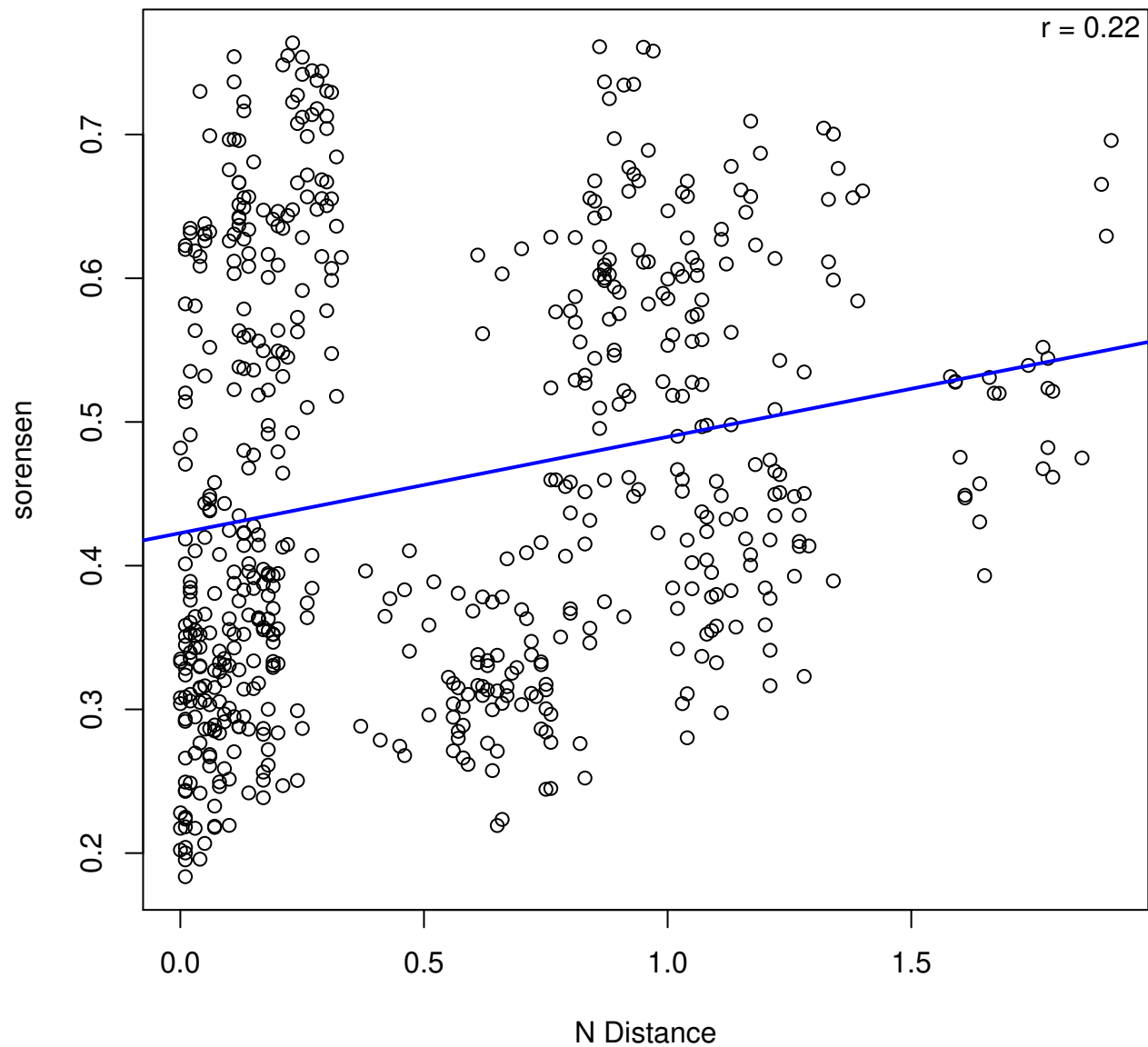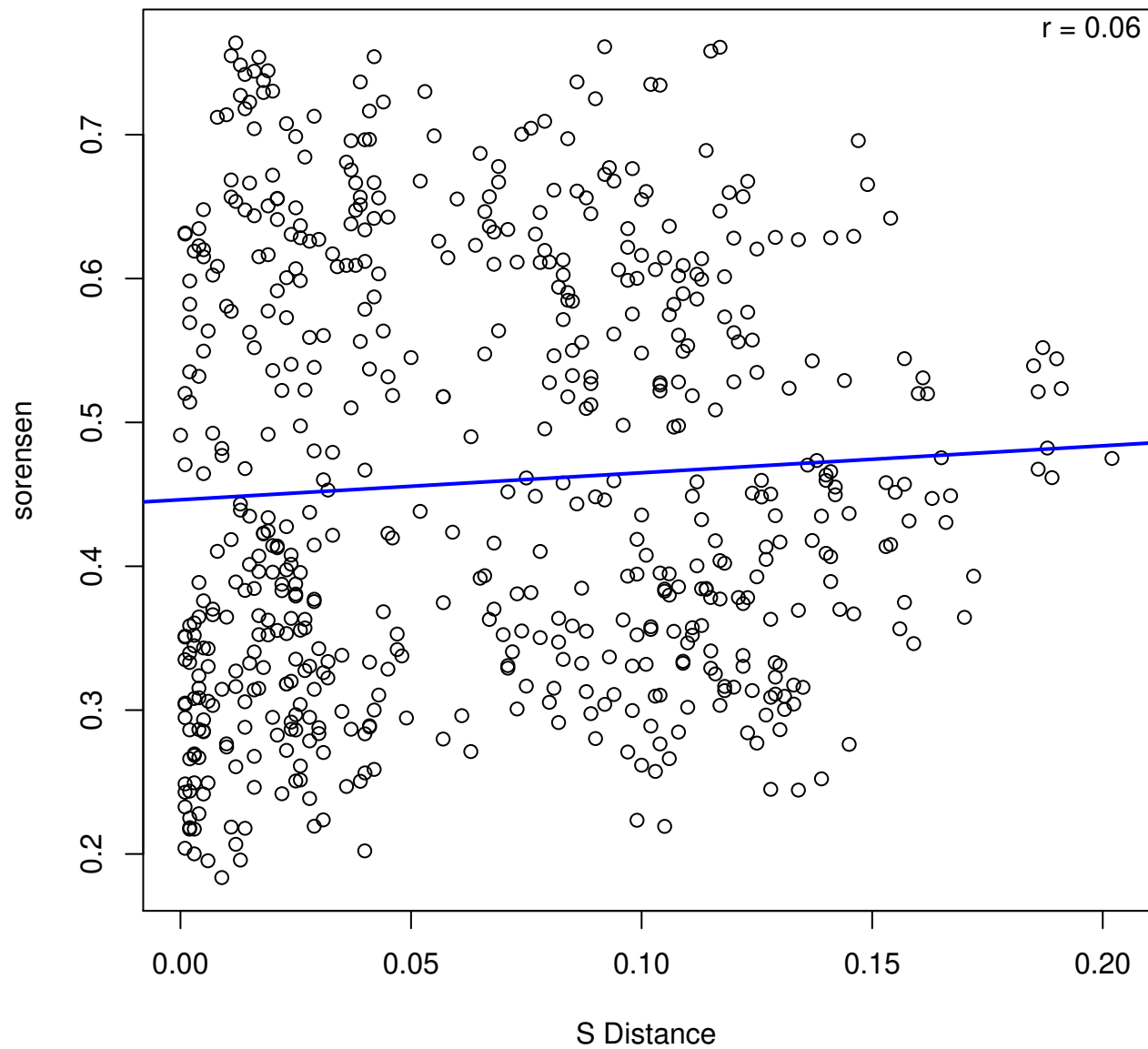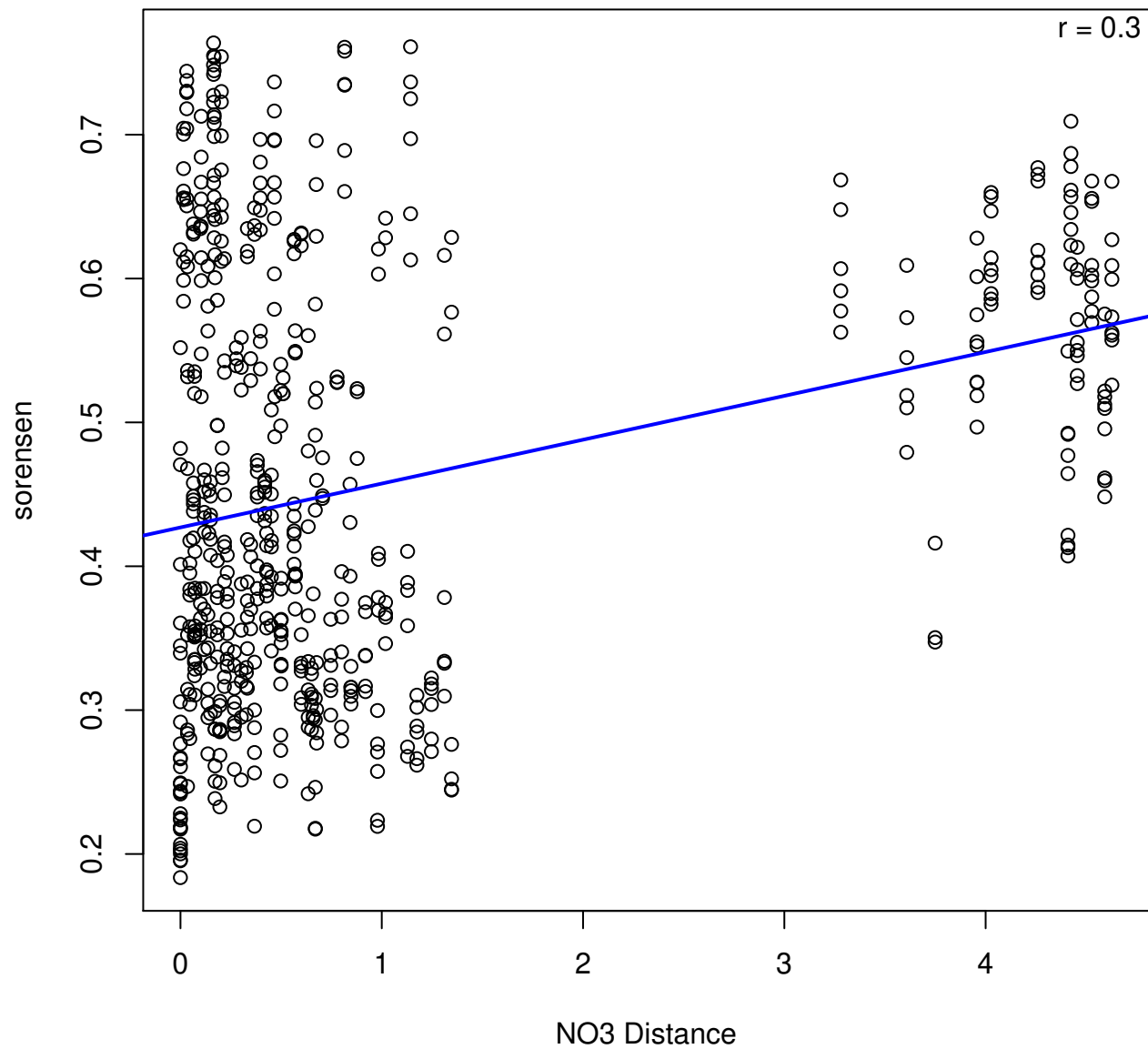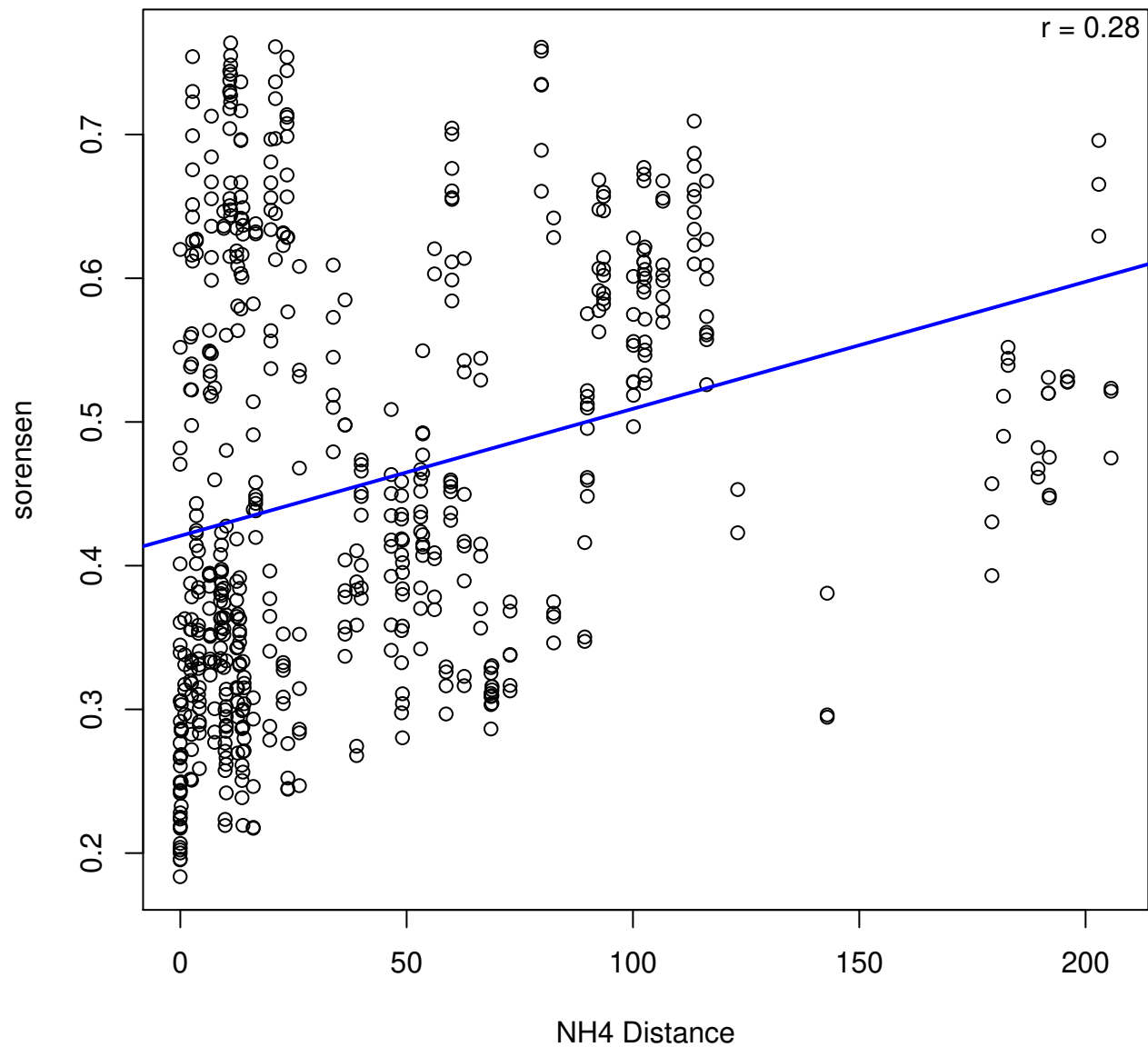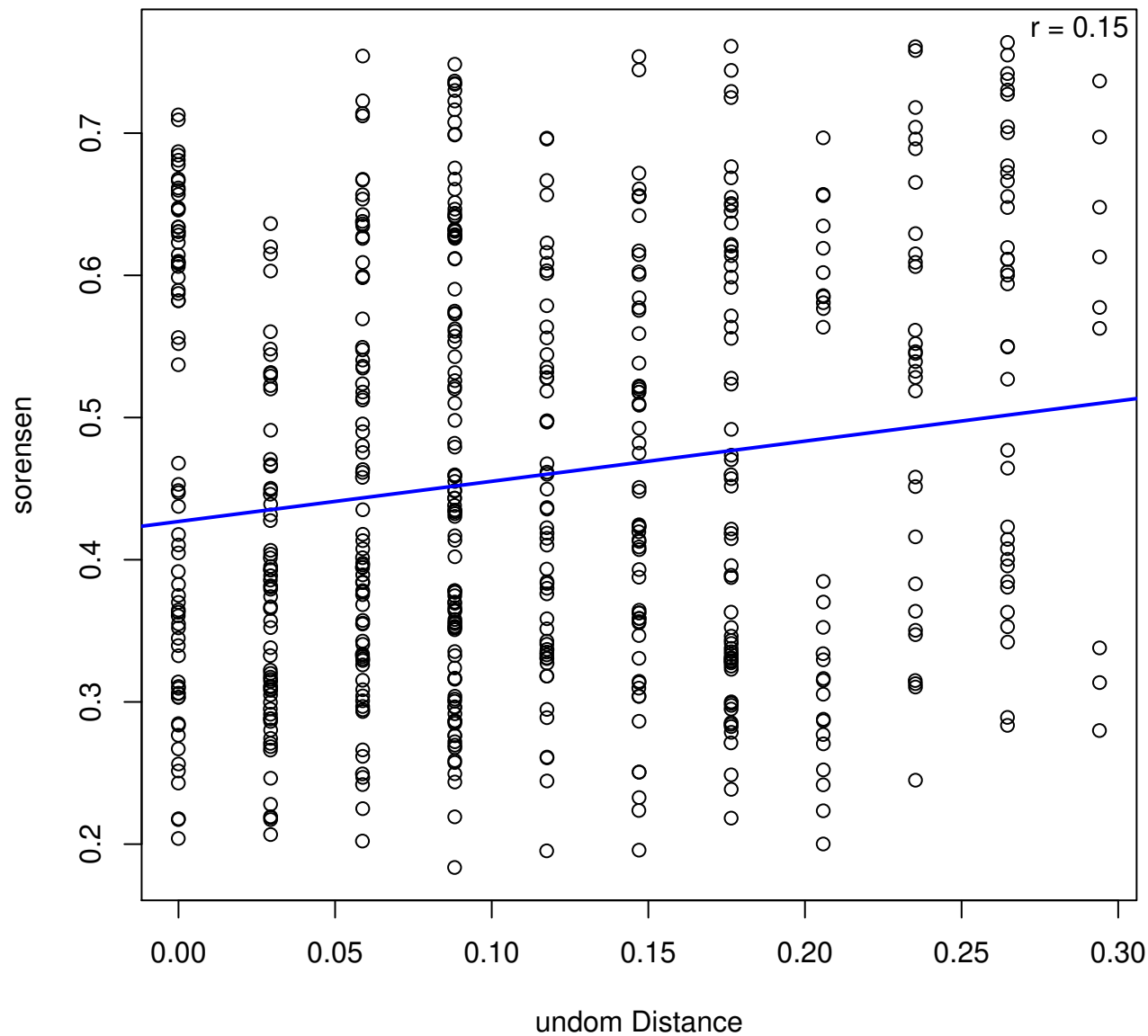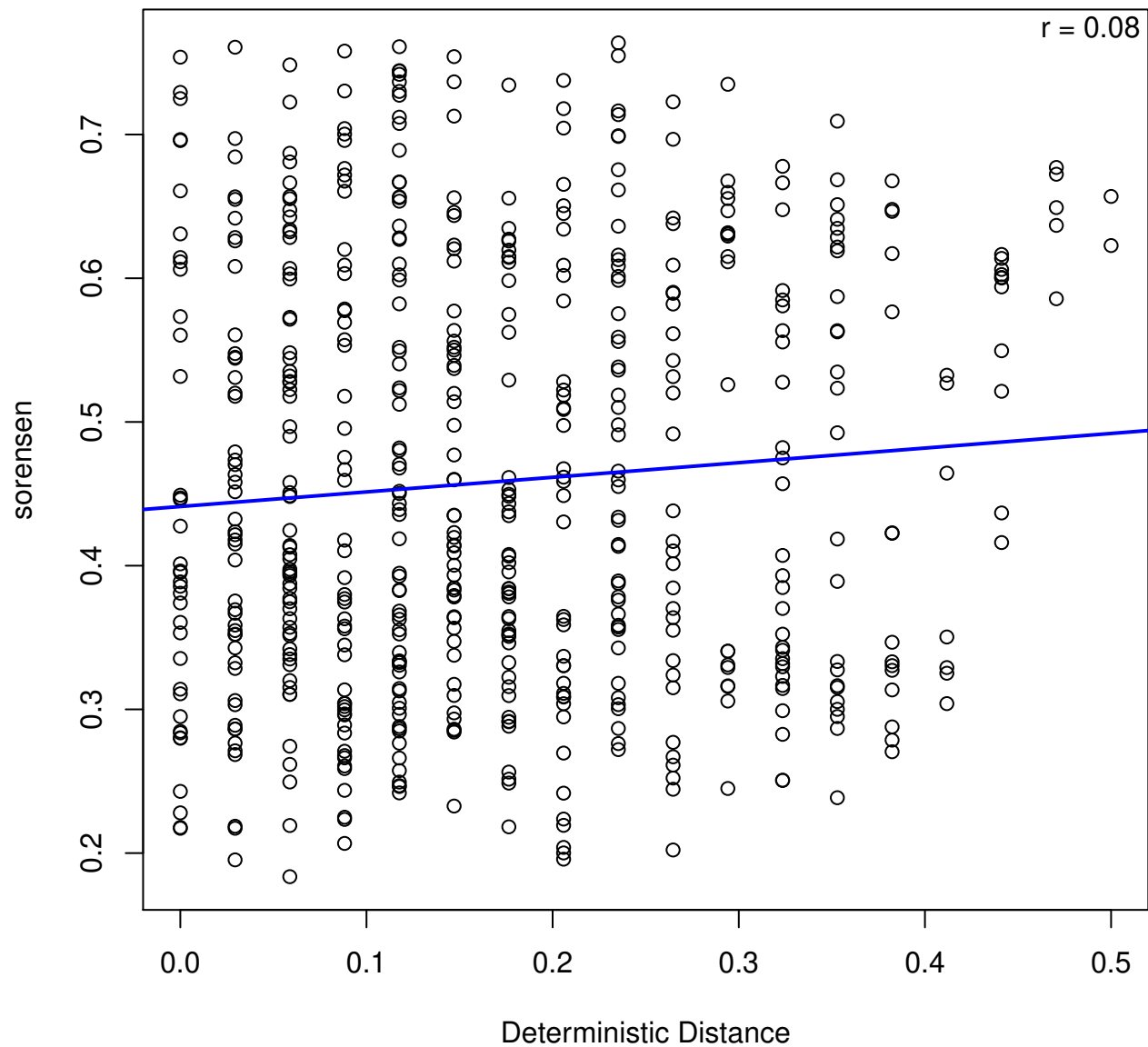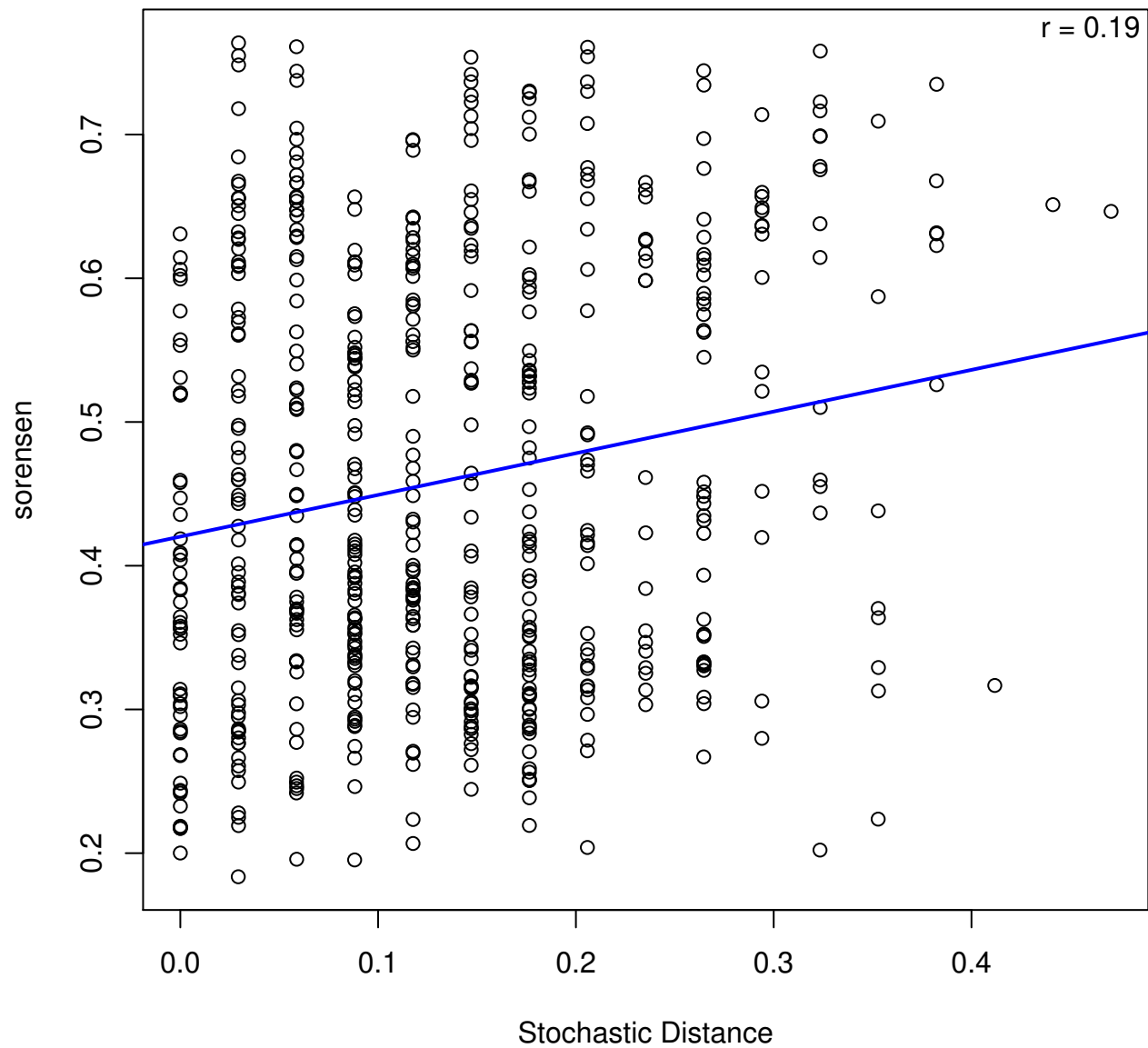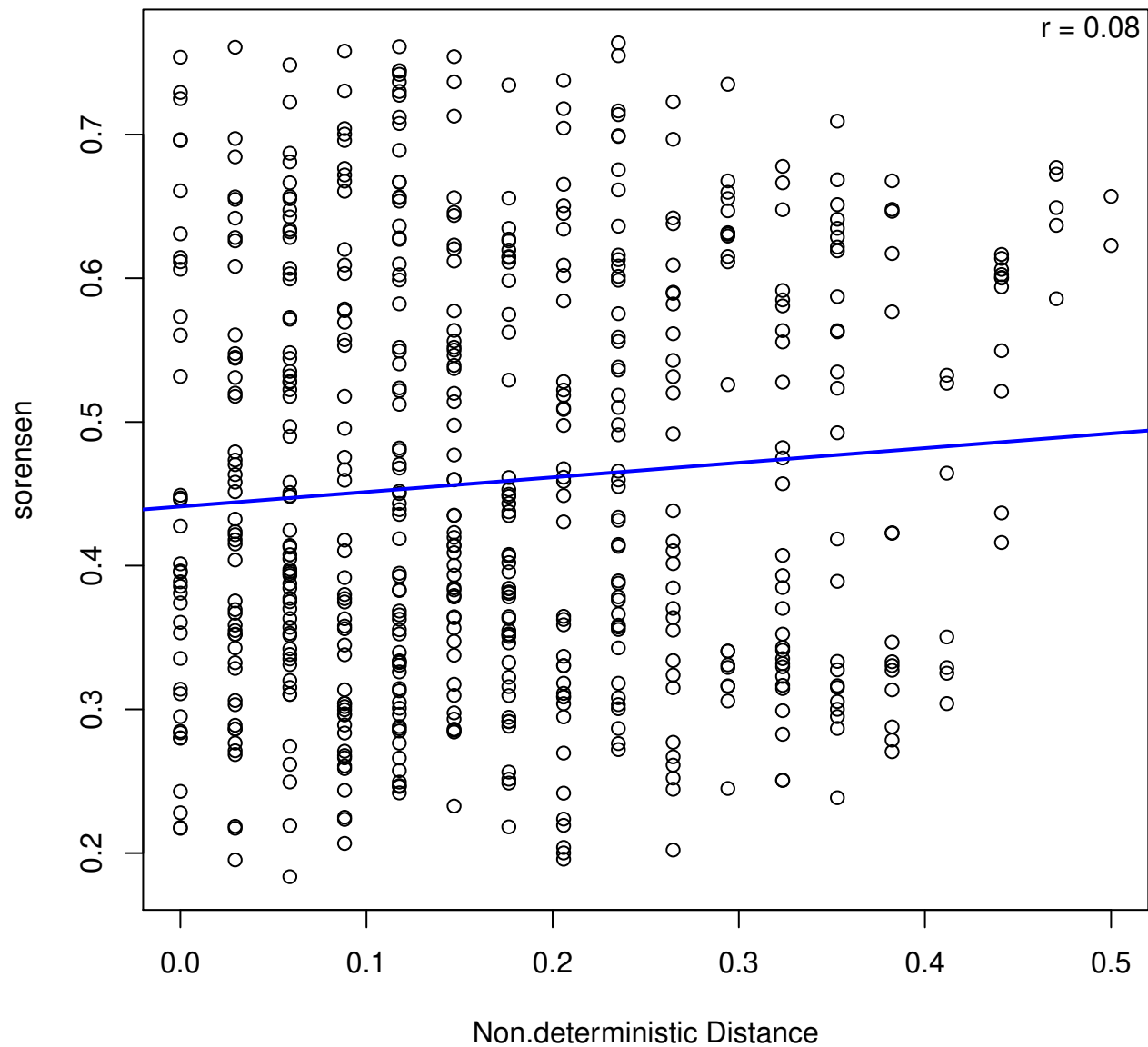| Study	Year	Experiment	Carbon variables measured	Observation	DOI
Smith et al.	1983	Field measurement of CO2 flux in salt, brackish, freshwater marshes in Loiusiana	CO2	Decreased with increasing salinity	10.1016/0272-7714(83)90042-2
Nyman and DeLaune	1991	Effect of water table depths on CO2 emissions were examined in intact fresh, brackish, and saline marsh soil cores	CO2	Emissions greatest in fresh cores followed by brackish and then saline cores	10.4319/lo.1991.36.7.1406
Chmura et al.	2003	Global carbon sequestration in tidal, saline wetland soils. 154 global datasets in mangroves and salt marshes were compiled.	Soil carbon density	In contrast to peatlands, salt marshes and mangroves release neglible amounts of GHG and store more carbon per unit area	10.1029/2002GB001917
Choi and Wang	2004	Metaanalysis of carbon sequestration in coastal wetlands using radiocarbon measurements of field soil along a soil chronosequence in coastal wetland in north Florida	CO2	Saltmarshes sink of CO2	10.1029/2004GB002261
Neubauer et al.	2005	Brackish and freshwater marsh (Jug Bay), and tidal brackish high salinity marsh (Jack Bay) soil cores were collected for measurements.	CH4,CO2	CO2 and CH4 decreased at high salinity marsh site	10.1890/04-1951
Weston et al.	2006	Sediments from tidal freshwater portion of Altamaha River subjected to salinity gradient in flow-through sediment reactors in the lab (0.063 vs 9.9 psu)	CO2, CH4, DOC	CO2 increased, CH4 decreased, DOC and DON concentration did not change with increasing salinity.	10.1029/2005JG000071
Baldwin et al.	2006	Never impacted freshwater sediment collected from non-salt imapacted freshwater wetland subjected to NaCl treatment in lab incubations	CO2, CH4	No noticeable effect of NaCl load on CO2 production,CH4 decreased with increasing NaCl conc	10.1672/0277-5212(2006)26[455:tseoso]2.0.cc
Chambers et al.	2011	Short term response to salinity pulse in freshwater wetland soils exposed to seawater and NaCl pulsing in a batch incubation studies	CO2, CH4, TOC, OC, Microbial Biomass C	CO2 increased and CH4 decreased in response to seawater. NaCl treatment reduced CH4, no effect on CO2	10.2136/sssaj2011.0026
Weston et al.	2011	Tidal-freshwater marsh soils incubated in lab to tidal cycle of freshwater and dilute seawater	CO2, CH4	CO2 and CH4 increased	10.1007/s10533-010-9427-4
Tzortziou et al.	2011	Brackish and freshwater marsh soil subjected to tidal upwelling at the Rhode River estuary-marsh in Chesapeake Bay	DOC, DIC, DOM, and CO2 calculated from total DIC	DIC, DOC, pCO2 was higher at marsh than estuary	10.3354/meps09017
Marton et al.	2012	Tidal freshwater forest soil cores collected along a organic matter gradient in Altamaha River>Ogeechee>Satilla in southeastern Georgia. These systems have not been exposed to prolonged saline water. Incubations were performed by adjusting salinity to 0,2, or 5 psu	CH4, CO2	CO2 increased (overall for Altamaha, treatment level 2 for Ogeechee, no effect in Satilla), CH4 decreased with increasing salinity for all three rivers.	10.1007/s13157-012-0270-3
Neubauer et al.	2013	Tidal freshwater marsh soil with 3.5 year in situ salt manipulation (either increasing freshwater inputs or adding seawater) and short term lab incubations	CO2, CH4,	CO2 increased and CH4 decreased short term with salinity, but CO2 and CH4 decreased long-term with salinity (was higher in the control and freshwater plots)	10.5194/bg-10-8171-2013
Chambers et al.	2013	Intact soil cores from freshwater tidal, brackish and salt marsh exposed to 3 salinity pulses during 53 day lab experiment	CO2, CH4, Total C, DOC, TOC	CO2 from freshwater marsh increased, CO2 from brackish and salt marsh decreased	10.1007/s10533-013-9841-5
Chambers et al.	2014	Increased salinity (15 psu) and inundation (-8 c) and their combination on soil organic C loss mangrove peat soil that was collected and brought back outdoor tidal mesocosm facility	CO2, CH4, DOC	No significant impact on soil organic C mineralizaiton, though CO2 increased in control water_elevated salinity than inundated_elevated salinity. No significant differences in CH4 flux.	10.1007/s10750-013-1764-6
Weston et al.	2014	Saltwater marsh, Oligohaline and tidal freshwater coastal marshes along a salinity gradient at Delaware River Estuary over four years	CO2, CH4, C sequestration with radiodating of soils	Saltwater marsh was C, CH4, GHG sink. Tidal freshwater marsh source of CH4, Oligohaline saline source of CO2 and CH4. No difference in DOC	10.1007/s10533-014-9989-7
Liu et al.	2017	Freshwater forest wetland not affected by saltwater intrusion incubated in lab to water change (0.4-3.0 g/g) and salinity changes (0, 1, 5 ppt NaCl)	CH4, CO2, DOC	Wet-dry cycles decreased DOC, increased CO2, decreased CH4. CO2-C vs DOC linear increase, CH4-C exponential increase. Cumulative emission of gases increased over time.	10.1016/J.SOILBIO.2017.04.002
Steinmuller & Chambers	2018	Intact freshwater wetland soil cores with site gradient (cypress dome, bayhead swamp, mineral marsh selected to capture variaton in soil organic matter) brought back to lab and exposed to salinity gradient (5 and 15 psu)	DOC, total C, Microbial biomass C, CO2 and CH4 flux	CO2 increased with increasing salinity in swamp soil with no change in CH4 wrt salinity. DOC unaffected	10.2136/sssaj2017.05.0162
Ardon et al.	2018	Intact soil core from coastal forested wetland collected in 2010, subjected to marine salt treatment (5psu) and hydrologic treatment (flooded or water table kept 20 cm below surface) in lab.	DOC, CO2, CH4	No change in DOC. Increased salinity decreased CO2 flux, CH4 flux increased in salt treatments relative to control. (Both results were surprising, given the general trend from other studies and lit review).	https://doi.org/10.1007/s10533-018-0486-2
Hebert et al.	2018	Chronic (15 psu) and acute (2 months of brackish) simulated seawater intrusion on tidal freshwater marsh	CO2, CH4, DOC	Press(constant/chronic) reduced CO2 and CH4 emissions, led to reduced carbon fixation, while acute pulses did not lead to lasting effects on porewater chemistry or ecosystem carbon balance. Gross ecosystem productivity, net ecosystem productivity, and ecosystem respiration was lower in press plots than control. Porewater DOC decreased in both press and pulse following seawater addition but increae 3-4 months afterwards (perhaps due to rapid increase in C mineralization via sulfate reduction, DOC flocculation or stress-induced reductions in C inputs from plant)	https://doi.org/10.1007/s10533-018-0436-z
Yang et al.	2018	Soil cores from brackish wetland incubated in lab with salinity gradient (fresh, 3, 5, and 10‰)	DOC, CO2	High salinity treatments decreased soil respiration rates while for freshwater while for freshwater control and level 3 salinity, CO2 first increased and then decreased), decreased DOC concentrations.	https://www.sciencedirect.com/science/article/pii/S0048969718321971?via%3Dihub

Table S2 Soil Chemistry Data (values are average of three replicates)

Sample	Location_depth	Transect	% Carbon	% Nitrogen	% Sulfur	NO3-N (mg kg^{-1})	NH4-N (mg kg^{-1})	pH	Sp. conductivity (µs/cm)	Bulk density (g cc^{-1})	Porosity	Volumetric water content	% Sand	% Silt	% Clay
BC2-10	Floodplain_shallow	High-salt	25.1	1.33	0.19	4.97	121	6.56	867	0.17	0.93	79.6	31.8	3.41	64.8
BC2-30	Floodplain_deep	High-salt	2.70	0.30	0.08	1.01	20.4	6.85	453	0.62	0.77	38.2	37.0	34.4	28.6
BC3-10	Floodplain_shallow	High-salt	31.0	2.04	0.37	2.24	299	6.18	794	0.12	0.95	85.2	24.9	41.5	33.6
BC3-25	Floodplain_deep	High-salt	4.03	0.44	0.10	0.37	30.6	6.15	532	0.57	0.79	55.0	6.3	54.6	39.0
BC4-10	Inland_shallow	High-salt	16.8	1.05	0.21	1.69	28.0	4.98	248	0.21	0.92	78.9	40.9	24.1	35.0
BC4-30	Inland_deep	High-salt	6.18	0.49	0.17	0.44	13.9	4.79	524	0.40	0.85	66.1	8.8	50.5	40.8
BC12-10	Floodplain_shallow	Moderate-salt	37.4	1.53	0.21	0.56	67.0	5.19	340	0.10	0.96	77.2	38.9	22.1	33.0
BC12-30	Floodplain_deep	Moderate-salt	2.42	0.27	0.08	0.34	4.29	6.06	260	0.52	0.80	42.4	4.1	54.0	42.0
BC13-10	Floodplain_shallow	Moderate-salt	33.5	2.05	0.27	1.22	210	5.84	247	0.16	0.94	81.1	20.0	38.0	42.0
BC13-19	Floodplain_deep	Moderate-salt	4.72	0.47	0.10	0.51	17.9	5.82	148	0.55	0.79	47.5	4.4	47.8	47.8
BC14-10	Inland_shallow	Moderate-salt	15.6	1.13	0.23	1.36	86.8	5.63	206	0.21	0.92	78.7	46.6	21.4	32.0
BC14-25	Inland_deep	Moderate-salt	3.78	0.41	0.11	0.71	18.1	5.68	324	0.47	0.82	58.1	12.0	46.0	42.0
BC15-10	Upland_shallow	Terrestrial	7.41	0.31	0.08	0.94	27.0	4.63	43.0	0.49	0.81	44.8	14.1	54.0	32.0
BC15-30	Upland_deep	Terrestrial	2.14	0.18	0.12	0.54	7.00	4.83	29.2	0.63	0.76	42.7	12.2	57.9	29.9

Table S3 FTICR peaks of Water Soluble Organic Fraction (WSOC) processed through FREDA to obtain Gibbs Free Energy (GFE), relative abundance of compound classes and heteroatoms, and biochemical transformations

Sample	Depth	Location	avgGFE (kJ mol C-1)	Protein	Amino Sugar	Lipid	Lignin	ConHC	Tannin	Other	Carb	UnsatHC	CHO	CHNO	CHOP	CHOS	CHNOS	CHNOP	CHNOSP	CHOSP	Total Transformations	Total Nitrogen transformations	Relative Nitrogen transformation	Relative Nitrogen contaning formula
BC2-10-1	Shallow	BC2	64.93705	18.3	3.8	9.4	30	20	14	0.8	2.5	1.1	86	14	8.4	7.0	3.6	2.1	1.1	0.24	2293	86	0.04	0.17
BC2-10-2	Shallow	BC2	63.61414	16.4	3.4	8.2	31	23	13	0.6	2.0	1.4	87	13	7.8	6.3	2.9	2.0	0.8	0.33	3234	159	0.05	0.16
BC2-10-3	Shallow	BC2	64.22539	16.9	2.7	10.9	32	24	12	0.2	0.8	1.2	87	13	2.9	5.2	2.7	1.0	0.7	0.05	2685	145	0.05	0.15
BC3-10-1	Shallow	BC3	66.48832	20.8	3.6	11.0	30	22	10	0.4	1.2	1.2	85	15	6.0	7.2	1.4	1.7	0.3	0.11	2755	169	0.06	0.16
BC3-10-2	Shallow	BC3	66.80659	22.4	4.1	12.1	25	24	9	0.4	1.8	1.1	87	13	8.8	6.1	0.9	2.0	0.2	0.14	2063	93	0.05	0.13
BC4-10-1	Shallow	BC4	53.69184	1.6	0.6	0.2	46	30	20	0.0	0.9	0.2	86	14	0.1	1.0	9.1	0.3	4.8	0.03	4144	164	0.04	0.24
BC4-10-2	Shallow	BC4	53.46295	1.5	0.6	0.3	45	33	19	0.0	0.8	0.3	83	17	0.2	1.4	10	0.8	5.5	0.09	4373	218	0.05	0.28
BC4-10-3	Shallow	BC4	53.59828	1.7	0.7	0.3	45	33	18	0.1	0.8	0.2	82	18	0.2	1.7	11	0.7	6.4	0.11	4822	273	0.06	0.30
BC12-10-1	Shallow	BC12	57.81569	8.0	2.5	4.3	37	32	14	0.2	1.4	0.8	88	12	2.5	1.9	6.2	0.6	2.4	0.12	3494	104	0.03	0.19
BC12-10-2	Shallow	BC12	58.02936	7.9	1.8	4.3	39	30	15	0.1	1.2	0.6	86	14	2.1	2.0	7.1	0.9	3.4	0.04	3691	148	0.04	0.22
BC12-10-3	Shallow	BC12	56.53031	7.0	1.1	3.3	39	32	17	0.1	0.9	0.6	83	17	1.3	1.1	7.3	0.9	3.6	0.12	5063	313	0.06	0.25
BC13-10-1	Shallow	BC13	58.11019	11.5	2.3	5.3	33	30	16	0.1	0.9	1.0	83	17	2.4	2.5	3.6	1.1	1.2	0	3157	255	0.08	0.21
BC13-10-2	Shallow	BC13	59.44556	14.0	2.8	5.4	34	27	15	0.2	1.0	0.8	79	21	2.6	4.3	5.2	0.8	2.5	0	3856	376	0.10	0.25
BC13-10-3	Shallow	BC13	61.09489	14.6	2.2	7.1	33	28	13	0.2	0.7	1.0	81	19	2.0	3.4	4.1	1.1	1.8	0.04	4368	393	0.09	0.23
BC14-10-1	Shallow	BC14	53.89356	6.4	1.8	1.9	37	36	16	0.1	0.9	0.5	79	21	1.3	5.9	7.4	0.8	3.9	0.06	5406	486	0.09	0.28
BC14-10-2	Shallow	BC14	52.9046	6.0	1.7	1.3	37	36	17	0.3	0.7	0.4	77	23	0.5	6.6	8.3	1.2	4.5	0.14	5461	509	0.09	0.31
BC14-10-3	Shallow	BC14	53.26191	5.9	1.6	1.8	37	35	17	0.2	0.7	0.6	77	23	0.5	7.7	7.3	1.2	3.5	0.03	5510	580	0.11	0.29
BC15-10-1	Shallow	BC15	67.32013	3.3	1.5	1.3	52	18	21	0.2	1.5	0.6	82	18	3.0	1.4	12	1.0	8.3	0.25	4434	163	0.04	0.31
BC15-10-2	Shallow	BC15	68.81556	4.4	2.0	1.3	51	18	21	0.3	1.7	0.6	83	17	3.0	2.3	13	1.0	8.4	0.26	4281	116	0.03	0.31
BC15-10-3	Shallow	BC15	70.52464	3.4	1.0	1.2	52	19	21	0.2	1.2	0.3	82	18	1.4	1.4	13	1.2	9.1	0.39	4397	154	0.04	0.33
BC2-30-1	Deep	BC2	51.96419	2.1	0.7	1.4	39	31	25	0.2	1.1	0.1	78	22	1.0	1.8	10	0.8	6.3	0.41	4333	350	0.08	0.33
BC2-30-2	Deep	BC2	53.09664	2.3	0.2	1.8	41	25	28	0.1	1.0	0.5	89	11	0.4	1.3	7.2	0.5	4.0	0.22	1733	28	0.02	0.20
BC2-30-3	Deep	BC2	53.94344	2.5	0.4	1.4	44	26	24	0.2	1.2	0.2	83	17	0.6	1.3	9.8	0.6	5.5	0.16	3160	143	0.05	0.28
BC3-25-1	Deep	BC3	52.32721	3.7	0.2	3.8	32	34	25	0.4	0.7	0.4	89	11	0.6	1.4	6.4	0.5	3.1	0.19	1360	28	0.02	0.19
BC3-25-2	Deep	BC3	53.08825	3.7	0.4	3.2	36	32	23	0.3	1.0	0.2	82	18	0.6	1.4	7.8	0.4	3.9	0.13	2958	186	0.06	0.27
BC3-25-3	Deep	BC3	51.0188	2.3	0.4	2.3	34	35	25	0.3	1.0	0.1	78	22	0.8	1.1	10	1.0	5.9	0.04	3579	268	0.07	0.33
BC4-30-1	Deep	BC4	54.51698	2.4	0.8	0.6	48	31	16	0.3	0.8	0.3	81	19	0.6	9.0	8.9	0.9	5.5	0.24	5515	363	0.07	0.27
BC4-30-2	Deep	BC4	56.75285	3.1	0.7	0.6	54	24	16	0.2	0.7	0.3	85	15	1.9	8.7	6.8	0.3	4.1	0.15	5309	331	0.06	0.21
BC4-30-3	Deep	BC4	55.50154	2.8	0.9	0.7	50	28	17	0.2	0.6	0.2	83	17	1.3	9.6	6.8	0.5	4.3	0.11	5628	407	0.07	0.23
BC12-30-1	Deep	BC12	52.65896	1.8	0.5	1.3	42	31	22	0.2	1.2	0.2	79	21	0.6	0.9	9.8	0.5	5.7	0.17	3840	301	0.08	0.32
BC12-30-2	Deep	BC12	54.73211	3.3	0.2	2.0	45	24	24	0.2	1.1	0.4	88	12	0.4	1.1	8.2	0.2	4.8	0.20	1257	25	0.02	0.22
BC12-30-3	Deep	BC12	52.90291	1.8	0.5	1.0	43	30	22	0.1	1.3	0.3	77	23	0.5	1.0	11	0.8	6.2	0.17	4704	369	0.08	0.34
BC13-19-1	Deep	BC13	53.4101	2.9	0.5	1.9	41	33	20	0.2	0.8	0.2	79	21	0.6	1.5	7.9	0.5	4.6	0.24	4899	418	0.09	0.29
BC13-19-2	Deep	BC13	53.21399	3.5	0.7	1.7	40	33	19	0.2	0.8	0.2	77	23	0.6	2.2	9.8	0.9	5.9	0.28	5279	510	0.10	0.33
BC13-19-3	Deep	BC13	53.58759	4.0	0.6	2.4	38	35	18	0.3	0.8	0.4	77	23	1.0	2.3	9.5	1.0	6.2	0.39	4682	405	0.09	0.33
BC14-25-1	Deep	BC14	52.63258	1.5	0.7	0.5	43	33	20	0.1	1.2	0.2	79	21	0.6	3.7	9.3	0.7	5.5	0.14	5110	405	0.08	0.30
BC14-25-2	Deep	BC14	53.146	1.7	0.7	0.5	44	32	19	0.2	1.0	0.2	78	22	0.5	4.6	11	1.1	6.8	0.37	4907	394	0.08	0.33
BC14-25-3	Deep	BC14	53.41649	1.9	0.8	0.8	44	32	19	0.3	0.9	0.3	75	25	0.6	4.9	11	1.4	7.4	0.33	5090	451	0.09	0.36
BC15-30-1	Deep	BC15	67.32013	7.9	1.9	4.1	63	7.1	12	0.7	0.9	2.6	86	14	11.5	2.9	4.9	0.9	1.4	0.28	2824	118	0.04	0.19
BC15-30-2	Deep	BC15	68.81556	8.7	2.0	4.2	68	4.1	9	0.9	0.6	2.4	84	16	12.4	3.3	5.0	1.1	1.4	0.39	2016	92	0.05	0.16
BC15-30-3	Deep	BC15	70.52464	11.9	3.7	5.8	61	4.0	8	0.6	1.6	2.8	86	14	13.0	3.9	3.8	1.1	0.5	0.27	1888	52	0.03	0.33

Abbreviations: Condensed hydrocarbon (ConHC), Carbohydrates (Carb), Unsaturated hydrocarbon (UnsatHC)

Table S4 FTICR peaks of CHCl3 fraction processed through FREDA to obtain Gibbs Free Energy (GFE), relative abundance of compound classes and heteroatoms, and biochemical transformations

Sample	Depth	Location	avgGFE (kJ mol C-1)	Lipid	Protein	Lignin	Carb	AminoSugar	UnsatHC	ConHC	Other	Tannin	CHO	CHOS	CHOP	CHNOS	CHNO	CHNOP	CHNOSP	CHOSP	Total transformations	Total Nitrogen transformations	Relative Nitrogen transformations	Relative Nitrogen containing formula
BC2-10-1	Shallow	BC2	108	100	0	0	0	0	0	0	0	0.00	92.3	23.1	7.7	0.0	7.7	0.0	0.0	0.0	1.0	20	0.11	0.06
BC2-10-2	Shallow	BC2	104	88.8	4.20	3.03	0.47	0.00	2.56	0.93	0	0.00	77.9	19.6	12.8	8.4	22.1	5.8	0.7	1.6	186	31	0.12	0.25
BC2-10-3	Shallow	BC2	106	96.3	0.61	0.61	0.00	0.00	2.13	0.30	0	0.00	88.1	27.4	7.9	5.5	11.9	1.8	0.6	0.6	111	17	0.08	0.14
BC3-10-1	Shallow	BC3	105	92.5	3.73	1.36	0.00	0.00	2.03	0.34	0	0.00	87.8	10.5	12.9	4.1	12.2	3.4	0.0	1.7	249	1.0	0.17	0.15
BC3-10-2	Shallow	BC3	105	94.4	1.39	1.05	0.00	0.00	2.44	0.70	0	0.00	83.3	13.2	11.8	3.8	16.7	3.5	0.0	1.0	326	0	0.00	0.18
BC3-10-3	Shallow	BC3	105	92.5	3.76	1.25	0.00	0.00	1.88	0.63	0	0.00	84.3	14.7	11.9	5.6	15.7	1.9	0.3	1.6	347	1.0	0.02	0.17
BC4-10-1	Shallow	BC4	102	82.0	7.52	5.64	0.19	0.38	3.01	0.94	0	0.38	71.8	12.0	18.2	10.3	28.2	8.1	0.6	0.6	316	19	0.10	0.31
BC4-10-2	Shallow	BC4	103	88.1	5.54	3.48	0.00	0.16	2.06	0.47	0	0.16	77.4	15.8	12.5	7.0	22.6	7.4	0.2	0.8	334	8.0	0.05	0.26
BC4-10-3	Shallow	BC4	104	93.4	2.13	2.98	0.00	0.00	0.64	0.21	0	0.21	80.4	24.9	4.9	8.7	19.6	3.6	0.2	2.3	223	6.0	0.07	0.22
BC12-10-1	Shallow	BC12	105	91.4	5.17	1.44	0.00	0.00	2.01	0.00	0	0.00	83.0	16.4	13.2	4.6	17.0	5.5	0.6	1.4	144	3.0	0.03	0.19
BC12-10-2	Shallow	BC12	104	87.6	6.75	2.83	0.00	0.00	2.40	0.44	0	0.00	73.2	13.3	14.2	8.7	26.8	8.1	0.0	0.7	324	8.0	0.04	0.30
BC12-10-3	Shallow	BC12	104	89.1	4.77	2.52	0.00	0.13	3.18	0.26	0	0.00	78.9	15.8	13.9	5.4	21.1	7.8	0.1	0.7	451	13	0.06	0.24
BC13-10-1	Shallow	BC13	105	91.5	4.48	0.64	0.21	0.00	2.56	0.64	0	0.00	80.8	17.3	14.7	5.8	19.2	6.0	0.0	1.1	174	31	0.08	0.21
BC13-10-2	Shallow	BC13	105	91.7	3.67	1.22	0.00	0.00	3.18	0.24	0	0.00	81.2	13.9	12.5	6.4	18.8	5.4	0.0	1.0	257	31	0.12	0.22
BC13-10-3	Shallow	BC13	104	92.9	2.53	1.01	0.34	0.00	2.69	0.34	0	0.17	83.2	16.3	12.1	4.7	16.8	5.6	0.3	1.0	368	12	0.08	0.20
BC14-10-1	Shallow	BC14	105	90.3	4.12	0.97	0.24	0.00	2.91	1.21	0.24	0.00	78.0	16.7	17.4	9.4	22.0	6.3	0.5	1.5	195	5.0	0.05	0.25
BC14-10-2	Shallow	BC14	105	88.7	6.05	1.01	0.25	0.00	3.27	0.50	0.25	0.00	74.8	14.9	13.9	9.1	25.2	9.1	0.3	1.3	219	14	0.09	0.29
BC14-10-3	Shallow	BC14	105	94.4	2.65	0.53	0.00	0.00	2.25	0.13	0.00	0.00	76.6	14.9	14.4	6.0	23.4	8.3	0.3	0.8	349	0	0.00	0.26
BC15-10-1	Shallow	BC15	104	90.8	3.90	2.51	0.56	0.00	1.67	0.28	0.00	0.28	83.6	10.6	15.3	6.1	16.4	3.9	1.1	0.6	145	15	0.07	0.20
BC15-10-2	Shallow	BC15	103	90.3	3.23	2.93	0.00	0.00	1.76	0.29	1.17	0.29	85.3	10.6	9.7	5.9	14.7	2.9	0.6	0.9	118	10	0.04	0.18
BC15-10-3	Shallow	BC15	104	93.4	1.62	2.36	0.44	0.00	1.47	0.29	0.44	0.00	86.1	10.3	13.6	3.5	13.9	4.1	0.3	0.4	266	0.0	0.00	0.16
BC2-30-1	Deep	BC2	103	88.1	6.11	2.25	0.64	0.32	1.29	0.64	0.64	0.00	72.7	14.8	17.0	11.6	27.3	5.5	1.6	2.9	182	20	0.11	0.30
BC2-30-2	Deep	BC2	105	92.6	2.81	0.66	0.66	0.17	2.48	0.33	0.17	0.17	82.5	16.2	16.0	5.3	17.5	8.1	0.5	1.2	251	31	0.12	0.21
BC2-30-3	Deep	BC2	104	91.3	3.52	2.35	0.23	0.47	1.17	0.70	0.00	0.23	77.5	15.0	17.1	8.2	22.5	8.5	0.7	1.6	204	17	0.08	0.26
BC3-25-1	Deep	BC3	97	77.8	4.44	6.67	2.22	2.22	2.22	0.00	2.22	2.22	77.8	22.2	4.4	15.6	22.2	2.2	4.4	2.2	6.0	1.0	0.17	0.29
BC3-25-2	Deep	BC3	101	89.1	1.82	5.45	0.00	0.00	0.00	0.00	3.64	0.00	89.1	9.1	7.3	7.3	10.9	1.8	3.6	0.0	15	0	0.00	0.18
BC3-25-3	Deep	BC3	103	88.9	4.17	0.69	0.69	0.00	4.17	0.00	1.39	0.00	71.5	18.1	6.9	10.4	28.5	6.9	2.8	3.5	65	1.0	0.02	0.33
BC4-30-1	Deep	BC4	103	89.5	2.81	4.68	0.47	0.78	1.09	0.31	0.16	0.16	83.5	18.6	12.8	3.6	16.5	5.3	0.3	1.1	194	19	0.10	0.18
BC4-30-2	Deep	BC4	101	75.7	8.37	5.70	2.28	1.14	4.18	1.52	1.14	0.00	74.1	16.0	17.9	11.4	25.9	5.7	3.4	3.0	172	8.0	0.05	0.29
BC4-30-3	Deep	BC4	104	91.3	3.79	2.62	0.29	0.00	0.87	0.58	0.29	0.29	82.5	19.2	8.7	5.2	17.5	4.1	0.6	1.2	88	6.0	0.07	0.20
BC12-30-1	Deep	BC12	102	79.6	5.97	3.48	2.49	1.00	4.48	1.99	1.00	0.00	82.1	14.4	22.9	6.5	17.9	3.0	2.0	2.0	103	3.0	0.03	0.19
BC12-30-2	Deep	BC12	101	78.9	7.75	4.23	1.76	0.70	4.23	1.41	1.06	0.00	72.9	14.4	20.4	12.3	27.1	4.2	3.9	3.9	184	8.0	0.04	0.30
BC12-30-3	Deep	BC12	101	77.5	10.18	3.92	2.09	1.04	2.61	2.09	0.26	0.26	79.4	12.0	20.1	7.6	20.6	6.5	2.1	1.6	214	13	0.06	0.25
BC13-19-1	Deep	BC13	104	88.2	6.90	1.81	0.00	0.18	2.00	0.73	0.18	0.00	73.7	13.4	18.1	6.9	26.3	10.3	0.2	0.9	368	31	0.08	0.29
BC13-19-2	Deep	BC13	104	88.7	5.86	2.60	0.00	0.22	1.74	0.65	0.22	0.00	74.8	14.5	16.3	8.2	25.2	7.6	0.4	1.5	260	31	0.12	0.28
BC13-19-3	Deep	BC13	105	88.5	6.73	1.25	0.00	0.00	2.74	0.50	0.25	0.00	76.1	15.0	17.7	7.7	23.9	8.0	0.2	1.5	144	12	0.08	0.27
BC14-25-1	Deep	BC14	106	91.7	3.21	1.60	0.32	0.00	1.92	0.32	0.32	0.64	79.2	15.1	16.3	8.7	20.8	4.8	0.6	0.3	95	5.0	0.05	0.24
BC14-25-2	Deep	BC14	106	91.1	3.51	1.17	0.23	0.00	2.81	0.47	0.47	0.23	79.6	22.0	14.8	9.4	20.4	5.2	0.9	2.6	152	14	0.09	0.23
BC14-25-3	Deep	BC14	106	93.9	1.52	0.00	1.52	0.00	1.52	0.00	1.52	0.00	75.8	12.1	13.6	12.1	24.2	4.5	0.0	0.0	14	0	0.00	0.29
BC15-30-1	Deep	BC15	104	89.8	3.79	3.45	0.52	0.17	0.86	0.86	0.17	0.34	86.0	8.4	14.7	3.4	14.0	3.8	0.9	0.5	210	15	0.07	0.17
BC15-30-2	Deep	BC15	101	75.7	9.91	4.80	3.00	0.90	2.70	2.10	0.90	0.00	76.3	11.1	23.7	7.2	23.7	4.5	3.3	2.1	224	10	0.04	0.25
BC15-30-3	Deep	BC15	104	85.7	5.71	2.86	0.00	0.00	5.71	0.00	0.00	0.00	100	11.4	17.1	0	0	0	0	2.9	6.00	0	0	0

Abbreviations: Condensed hydrocarbon (ConHC), Carbohydrates (Carb), Unsaturated hydrocarbon (UnsatHC).

Table S5 Regression of WEOC and CHCl3 fraction compound classes with specific conductivity

Regression of WEOC compound classes with specific conductivity

Shallow	R2	P	Deep	R2	P
AminoSuga	0.5539	0.000101	AminoSugar	0.06437	0.729993
Carb	0.4767	0.001293	Carb	0.03364	0.5134
ConcHC	0.773	2.05E-06	ConcHC	0.0456	0.6321
Lignin	0.4356	0.00235	Lignin	0.05919	0.8258
Lipid	0.7203	1.01E-05	Lipid	0.05361	0.718101
Other	0.5287	0.000568	Other	0.06515	0.1588
Protein	0.6135	0.000121	Protein	0.0627	0.9371
Tannin	0.4701	0.001427	Tannin	0.03662	0.5034
UnsatHC	0.6035	0.000148	UnsatHC	0.05848	0.8085

Regression of CHCl3 fraction compound classes with specific conductivity

Shallow	R2	P	Deep	R2	P
AminoSuga	0.01224	0.2875	AminoSugar	0.00245	0.4029
Carb	0.0654	0.663	Carb	0.0564	0.70386
ConHC	0.0788	0.947	ConHC	0.07725	0.1391
Lignin	0.003	0.3429	Lignin	0.07082	0.14924
Lipid	0.1854	0.0423	Lipid	0.06781	0.9069
Other	0.0666	0.1563	Other	0.1157	0.09143
Protein	0.2402	0.02254	Protein	0.06499	0.1468
Tannin	0.07467	0.1431	Tannin	0.02427	0.2503
UnsatHC	0.1154	0.09176	UnsatHC	0.00544	0.3552