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Supplemental Material

METHODS

Reflection seismic processing sequence

The multichannel reflection seismic (MCS) profiles have been processed following the traditional sequence of MCS processing including time migration using the Echos software of Emerson Paradigm. However, time varying amplitude scaling processes, such as Automatic Gain Control, were not applied in order to preserve seismic amplitudes. Within the shallow water depths of the continental shelf (Fig. 1A) seafloor multiple reflections are common elements in the seismic records of the Ross Sea. Multiples were suppressed from the MCS profiles by means of Surface Related Multiple Elimination and Wave Equation Multiple Attenuation (Verschuur et al., 1992). In addition, the seafloor multiples in the single channel reflection seismic (SCS) profiles have been suppressed through careful application of predictive deconvolution and bandpass filters. Moreover, the seafloor multiples were predicted by applying a simple water bottom dependent time static. The results were further improved by applying an adaptive subtraction between the original reflection and the multiple reflection. A matching filter of 60 ms length was applied which minimizes the result of the subtraction over rectangular time windows of 5 traces x 600 ms. However, the seafloor multiples have not been completely eliminated, particularly on the SCS profiles.

Drill-Site Measurements and Corrections

The relation between wireline downhole logged density (ρ_p , in g/cm^3) and wet bulk density (ρ_b , in g/cm^3) in data sets from Site U1521 corresponds to the linear relation: $\rho_p = 1.02101 \cdot \rho_b + 0.207547$ [$r = 0.83$]. The regression line has been calculated through cross-plot with least squares regression and normalized error [0.09] including values between 1 and 2.4 g/cm^3 (Supplemental Fig. S1). Wet-bulk density values measured in the Deep Sea Drilling Project (DSDP) Sites 272 and 273 cores are anomalously low. The linear regression relationship between core and wireline logged density in the International Ocean Discovery Program (IODP) Site U1521 is used to correct the wet bulk densities of the DSDP sites, making the density values comparable among the three sites.

For comparison, density values for the DSDP sites have been calculated from core-log velocities following Gardner's Law ($\rho = 0.31 \cdot V_p^{0.25}$) (Gardner et al., 1974). Corrected density values, calculated with the Site U1521 linear regression, are higher than wet bulk density values from GRAPE measurements ($\sim 0.24 \text{ g/cm}^3$), but show the same trend (Fig. 5A, 5B). The general trend of the density from Gardner's relationship is significantly offset from the trend of the

measured and corrected densities (Fig. 5A, 5B). The corrected densities fit better in the range of expected values according to densities from wireline downhole logging at Site U1521.

Corrected and measured densities in DSDP Sites 272 and 273 are used to calculate porosities (ϕ) according to (Fig. 5A, 5B): $\phi = [\rho_{ma} - \rho] / [\rho_{ma} - \rho_f]$, where ρ_{ma} is the density of the sediment matrix considered as the mean density of the sediments recovered at ANDRILL Site AND-2A (2.6 g/cm³) (Niessen et al., 2013) and ρ_f is the fluid density considered as a default brine (1.09 g/cm³). The acoustic impedance (I_p , in kg/m²s) was also calculated from density values as $I_p = V_p * \rho$ (Fig. 5).

Water saturation (S_w) along the stratigraphic column is calculated at Site U1521 on the basis of porosity (ϕ) and resistivity (R_t) measurements in Ohm·m following Archie's empirical relationship (Archie, 1942): $S_w^n = [a / \phi^m] * [R_w / R_t]$, where a is the cementation factor taken as 1, m is the cementation exponent taken as 1.8, n is the saturation exponent equal to 2 and R_w is the resistivity of the formation water taken as 0.04.

Core-Log-Seismic Ties

At Site U1521 check-shots were obtained with a seismic source consisting of two 4.1 l (250 in³) Sercel G guns in parallel array and a sonic tool string lowered into the hole with eighteen recording stations (average spacing 33 m) matching with the main lithologic boundaries. Sixteen out of the eighteen stations were successful (details in McKay et al., 2019). The logging curves were depth-matched using the total gamma ray log from the main pass of the triple combo tool string as the reference. Depth offsets between core and wireline logs are usually small (<2 m) (McKay et al., 2019).

The core-log-seismic correlations with the DSDP sites have been done through the core velocity measurements. MCS time-depth correlation synthetic seismograms were constructed in Hampson Russell software (Supplemental Fig. S2). The synthetic seismograms were generated from the 5 m resampled velocity logs after applying, in the time domain, a high-pass frequency filter at 50 Hz and a low-pass frequency filter at 60 Hz. Estimated source wavelets were obtained from the corresponding SCS profiles (PD90_34 for DSDP Site 272 and PD90_37 for DSDP Site 273) by statistical analysis using the e-Log function of the Hampson Russell software which combines seismic and well data. A representative seismic trace near the sites was obtained by averaging the five nearest traces (Taner et al., 1979). Finally, visual adjustment on the time-depth correlation was performed to find the best possible fit to a 0.5 correlation.

Spatial Velocity Distribution

The 2D velocity distribution along the composite SCS profile formed by lines PD90_34, PD90_35, PD90_36 and PD90_37 has been obtained through extrapolation of the compressional velocity measurements from the wireline and core logging of the three sites in Hampson Russell software (Fig. 3C). Seismic attributes are the quantitative measure of a seismic characteristic (e.g., Chopra and Marfurt, 2005). The multi-attribute analysis allows the prediction of petrophysical parameters along the seismic profiles, with compressional velocity being predicted in the case of this work. The analysis considers the compressional velocities at the sites: wireline P-wave measurements resampled at 5 m intervals by a running average for IODP Site U1521 and core-log P-wave measurements resampled to 5 m for DSDP Sites 272 and 273. Previously obtained time-depth correlations were applied, as detailed in the core-log-seismic ties section.

Processes to attenuate seafloor multiple reflections were previously applied to the seismic data, but amplitude has not been further adjusted since seismic and log correlation has proved to be very sensitive to the amplitude of the seismic signal (Volpi et al., 2009). A linear regression is performed between pairs of seismic attributes and petrophysical parameters (Coren et al., 2001; Volpi et al., 2009). Convolution of seismic attributes and petrophysical parameters is determined by an operator length of 5 units. Accordingly, the compressional velocity is modeled as a polynomial combination of several seismic attributes by step-wise regression of a maximum of 11 attributes (amplitude weighted frequency, cosine instantaneous phase, second derivative, instantaneous phase, amplitude weighted phase, filter 15/20–25/30 Hz, reflection strength, second derivative instantaneous amplitude, derivative instantaneous amplitude, filter 45/50–55/60 Hz, and filter 55/60–65/70 Hz). The polynomial combination is used to invert the seismic signal and predict the spatial distribution of the compressional velocities along the seismic profile. The uncertainty (here given by standard deviation) of the quantitative velocities obtained from the multi-attribute analysis oscillates between 323 and 367 m/s in this work (~14% uncertainty). Due to the questionable acoustic continuity along some parts of the composite SCS profile and the large error, we consider the 2D spatial velocity distribution as a qualitative result.

Reflection Tomography

Travel-time inversion tomography has been performed along the MCS profile IT94AR126 between shot points 3400 and 8000 (Supplemental Fig. S3), providing a large-scale velocity field in depth in the surroundings of IODP Site U1521. The input horizons of the tomography model correspond to seafloor, RSU4, RSU4a and RSU5, downwards in stratigraphic order. The images of the input time horizons have been obtained from the interpolation of all the reflected arrivals picked in the pre-stack data. The tomographic software CAT3D (Böhm et al., 2009) is based on Simultaneous Iterative Reconstruction Technique - SIRT method (Stewart, 1993) and the minimum time ray tracing (Böhm et al., 1999). The velocity field is inferred from the inversion of the picked reflected travel times from normal move-out measurements. The structure of the units and horizons is inferred in sequence from the shallowest to the deepest. For each horizon the iterative procedure starts from constant velocity within the sequence and horizontally flat lower interface (Böhm et al., 2009). Each iteration inverts the picked travel-times and updates the velocity model. The new interface (output horizon) is estimated following the principle of minimum dispersion of the reflected points (Carrion et al., 1993). The residual travel-time associated with each reflected event is converted to depth, by using the velocity field updated in the first step of any iteration, and used to update the corresponding reflected point (Carrion et al., 1993).

STRATIGRAPHIC RECORD

The major stratigraphic discontinuities interpreted in this work, i.e., RSU4 and RSU5 (Fig. 3, 7), are reinterpretations of the surfaces with the same names defined in the Scientific Committee on Antarctic Research (SCAR) Antarctic Offshore Stratigraphy Project (ANTOSTRAT) (Brancolini et al., 1995; Cooper et al., 1995), after consideration of more recently acquired data and updated age models (Table 2). In general, the RSU4 surface presented in this work is shallower over the banks and deeper along the northeast modern continental shelf edge of Iselin Bank than in the ANTOSTRAT interpretation (Supplemental Fig. S4). The

reinterpreted RSU5 surface is markedly shallower than the discontinuity mapped in ANTOSTRAT particularly in the western Ross Sea (Supplemental Fig. S4).

In addition, a reinterpretation of the acoustic basement below the sedimentary record have been conducted based on the updated database as a lower constraint for the stratigraphic interpretation presented in this work (Fig. 7). The basement is locally identified as a major reflection in the MCS profiles (Fig. 8). It is deeper in the eastern Ross Sea (>4 s two-way travel-time TWTT) forming three isolated depressions in the Joides and Central basins and southern Crary-Mawson Bank (Fig. 7). The shallowest acoustic basement depths (<1 s TWTT) occur over the southwestern part of Glomar Challenger Basin, Ross, Pennell, and Iselin banks (Fig. 7). Major differences, of up to 1 s TWTT for the basement depth mapped in this work with respect to the ANTOSTRAT surface, are most notable in Glomar Challenger Basin and landwards of Iselin Bank (Supplemental Fig. S4).

Seafloor, RSU4, RSU5 and basement surfaces define three major seismic packages in the stratigraphic record. While Package B, constrained between RSU4 and RSU5, is the main focus of this work and fully described on the main manuscript, the detailed mapping within Package A and Package C is beyond the scope of this study. Thus, the general description of the thickness distribution, seismic facies and physical properties of the sedimentary record contained in Package A and Package C is included below for reference.

Package A: Seafloor to RSU4

Package A is bounded by the seafloor and RSU4. As the uppermost seismic package, it is widely truncated by the present-day seafloor (Fig. 3B, 6). It has an irregular distribution, forming a sediment wedge thickening to the northeast, up to 2.4 s TWTT at the continental shelf edge of Houtz Bank, Whales Basin and Hayes Bank (Fig. 7). In Little America, Glomar Challenger, Pennell and Joides basins, Package A is thin or absent. Accordingly, its record is thin at all three drilled sites (Fig. 3B, 4, 7), but this package thickens in the northeastern Glomar Challenger Basin and northern Joides Basin. Both of these basins register covers in excess of 0.5 s TWTT, that thickens oceanwards up to 1.2 s TWTT. Isolated depocenters (<0.4 s TWTT) are located in Ross, Pennell and Crary-Mawson banks, whereas a homogeneous thickness of 0.2 – 0.4 s TWTT covers Iselin Bank (Fig. 7).

In general, Package A is formed by relatively high amplitude reflections of low lateral continuity, with different dip orientation in the Glomar Challenger and Whales basins (Fig. 2, 3B, 6). Major discontinuities are identified regionally within the package, e.g., at 44 and 62 mbsf at DSDP Site 272 and IODP Site U1521, respectively (Fig. 5). These discontinuities form the boundaries of the sequences RSS8 to RSS5 previously identified in the ANTOSTRAT study (Fig. 2). Broadly, the uppermost seismic sequences are characterized by chaotic seismic facies bounded by high amplitude tilted reflections. The lower seismic sequence is locally formed by stratified reflections of high amplitude and high lateral continuity (Fig. 3B, 6).

In the drill site records of the Glomar Challenger (DSDP Site 272), Pennell (IODP Site U1521) and Joides basins (DSDP Site 273), the P-wave velocity oscillates within a wide range of values with a general decreasing downhole trend (Fig. 4, 5). The 2D distribution of velocities shows continuous layers with high to very high P-wave values (>2350 m/s), interbedded with layers of low or moderate values (<2100 m/s) in the Ross Bank and Glomar Challenger Basin (Fig. 3C).

Density values have an overall decreasing trend downward (Fig. 5). The porosity minimum occurs at ~23 mbsf and ~65 mbsf in DSDP Site 272 and IODP Site U1521, respectively. Average porosity of Package A is higher in Glomar Challenger Basin relative to Pennell Basin. At Site U1521, resistivity and magnetic susceptibility decrease downwards, respectively. Natural gamma radiation reaches maximum values around 75 mbsf. The water saturation reaches maximum values around 66 mbsf but has fairly constant values underneath (Fig. 5).

Package C: RSU5 – Basement

Underlying RSU5 down to the acoustic basement, Seismic Package C encompasses ANTOSTRAT seismic sequences RSS2 and RSS1 (Fig. 2). Package C is widely distributed across the Ross Sea, with maximum thicknesses corresponding with the main depressions of the basement (Fig. 3B, 6, 7). Depressions in the basement of the Ross Sea continental shelf are primarily related to horst-graben features associated with the Cretaceous to Eocene rifting (DeSantis et al., 1995; Decesari et al., 2007; Eagles et al., 2004; Wilson and Luyendyk, 2009; Wobbe et al., 2012; Tinto et al., 2019). These basement structures are infilled by sediments that constitute the lower part of Package C (RSS1) which lacks accurate age control. The seismic signal attenuation leads to low reflectivity in the lower part of Package C, limiting detailed interpretation (Fig. 3A, 3B, 6). These sediments likely vary from fluvial in the lower and deepest depressions, to glacial-related in the upper part according to previous interpretations (Luyendyk et al., 2001; Wilson and Luyendyk, 2009; Galeotti et al., 2016). Beyond the basement depression infill, the sedimentary distribution of Package C across the continental shelf shows thicker records in the inner part where main depocenters reach 3.5 s TWTT. A very thin record (<0.4 s TWTT) is identified along a SE-NW fringe crossing Pennell Basin to Pennell Bank (Fig. 7). The upper part of the package is well-imaged in the seismic profiles and contains medium amplitude, high lateral continuity and stratified reflections (Fig. 2, 3A, 3B).

The drill sites studied in this work only recovered the uppermost intervals (<100 m) of Package C (Fig. 4). The measured P-wave values are relatively high with general downwards decreasing trend. A maximum value at the top of Package C occurs over more uniform values downwards in IODP Site U1521 and DSDP Site 273, whereas in DSDP Site 272 the maximum P-wave value is recorded toward the lower part of the core-log record (Fig. 4, 5). The spatial velocity distribution shows several layers of high P-wave values (2600 m/s) in the central part of Joides Basin embedded in average P-wave value record (Fig. 3C). Due to the limited drill site data in this package, the velocity distribution of this sequence is mainly determined by the seismic record.

Density is relatively high throughout, but generally decreases downwards. The porosity presents relatively constant values within each basin, but is low in Pennell Basin and high in the Glomar Challenger and Joides basins. Resistivity and magnetic susceptibility keep constant values along Package C (Fig. 5). The latter presents maximum values (~2315 SI) near the bottom, which could be an artifact related to the drill-bit. Natural gamma radiation values slightly decrease downwards as well as the water saturation (Fig. 5).

DEPTH VELOCITY MODEL FROM REFLECTION TOMOGRAPHY

A low-resolution velocity model results from the reflection tomography over MCS profile IT94AR126 (Supplemental Fig. S3). From the tomographic inversion of the reflected arrivals, four horizons are distinguished. They roughly match with the seafloor, RSU4, RSU4a and RSU5. No inversion has been attempted below RSU5, due to the low confidence in the seismic data picking. Between the seafloor and RSU4, Package A constitutes a layer of P-wave velocities between 1750 and 2000 m/s with slightly higher velocities toward Glomar Challenger Basin and lower velocities in Pennell Basin. Between RSU4 and RSU5, Package B presents two different P-wave velocity trends. They are bounded by a picked horizon that roughly correlates with RSU4a. In RSS4, P-wave velocity values increase toward the shelf edge in the Glomar Challenger Basin to a maximum of ~2600 m/s. Very low velocities (1450–1750 m/s) are derived in this seismic sequence to the southwest of Ross Bank, with minimum values in Pennell Basin (Supplemental Fig. S3). RSS3 is characterized by highly variable P-wave velocity values. Beneath the central part of Glomar Challenger Basin there are slightly higher P-wave velocity values in RSS3 than in RSS4, with exceptionally high values of 2600 – 3000 m/s near Ross Bank, while low values are distinguished beneath the bank itself (<2000 m/s). Much higher velocity values occur in RSS3 beneath the Pennell Basin and Pennell Bank with respect to RSS4. Maximum values of ~2600 m/s are reached near to Pennell Bank (Supplemental Fig. S3).

DIAGENETIC OPAL FRONT

Silica diagenetic reactions occur typically within the first 1000 m of burial of biosiliceous sediment (Isaacs, 1981; Williams et al., 1985). RSS3-Ia is related to diagenetic opal presently buried at ~325 mbsf at Site U1521 (Fig. 2B, 3B, 4B). Yet the large number of erosional surfaces identified in the overlying record point to potentially thicker sedimentary cover during several periods of its stratigraphic history. The seismic-stratigraphy shows at least 110 m (~0.20 s TWT) of sediment associated with RSS4-I have been eroded by the RSU4 discontinuity from the upper part of Lithostratigraphic Unit III in IODP Site U1521 (Fig. 3B). In addition to the burial depth, a determining factor for the formation of silica diagenesis fronts is the geothermal gradient (Davies and Cartwright, 2002). The formation of the opal A/CT diagenetic fronts occurs within ~10 Myr at subsurface temperatures of 25 – 50 °C (Hein et al., 1978). However, the diagenetic process is highly influenced by local factors such as the near-bottom water temperature and tectonic processes, and it could occur at temperatures as low as 8 – 15 °C (Davies and Cartwright, 2002). In the Ross Sea, a few sparse downhole temperature measurements have been performed in deep and shallow boreholes offshore and onshore (<http://www.heatflow.und.edu/index2.html>). They show strong variability in the geothermal gradient, particularly in the western Ross Sea (e.g., Begeman et al. 2017; Giustiniani et al., 2017). The broad range of geothermal gradients is largely related to the fluctuating magnitude and spatial variability of the heat flow, which may be enhanced by temporal shifts in magmatism or advection of crustal fluids (e.g., Begeman et al. 2017; <http://www.heatflow.und.edu/index2.html>). In addition, as the continental shelf of the Ross Sea is structurally complex (e.g., Davey and Brancolini, 1995), the tectonic faults may act as advection pathways for the geothermal heat, adding heterogeneity to the heat flow distribution. A wide range of geothermal gradient values should therefore be considered, from 24 – 40 °C/km in the southern Victoria Land Basin (Bücker et al., 2001, Geletti and Busetti, 2011) to 103 °C/km in

McMurdo Sound area (Risk and Hochstein, 1974). Assuming these end-member scenarios of geothermal gradient, the 25 °C threshold is placed between 1040 and 243 mbsf (Supplemental Fig. S5), a range that spans the present-day stratigraphic position of RSS3-Ia. Measured heat flow ranges from 160 – 250 mW/m² in McMurdo Sound (Risk and Hochstein, 1974) to 63 – 73 mW/m² in the Drygalski Basin (Blackman et al., 1987). Considering the average geothermal gradient of 50 °C/km for West Antarctica (Begeman et al., 2017), subsurface temperatures of 25 – 50 °C would be reached between 500 and 1000 mbsf (Supplemental Fig. S5). Thus, the present-day stratigraphic position of RSS3-Ia is shallower than the depth required for chert formation (Supplemental Fig. S5).

The geothermal gradient (GG) in Pennell Basin can be calculated out of local heat flow (HF) and thermal conductivity (TK) values as $GG = HF/TK$ (Horai and Nur, 1970). Thermal conductivity measurements were taken during IODP Expedition 374 at Site U1521 (McKay et al., 2019). However, no heat flow values were obtained at this site. The closest heat flow measurement to Site U1521 was obtained from HF305 located at 602 m wd and 115 km southeast of the site in Glomar Challenger Basin (Fig. 1A) (Sato et al., 1984). The heat flow value at HF305 is 114 mW/m², which lies within the range of regional heat flow values on the southern part of the Ross Bank 91 – 120 mW/m² (<http://www.heatflow.und.edu/index2.html>). Considering the heat flow in HF305 and the thermal conductivity obtained in U1521, the geothermal gradient in Pennell Basin would be between 83 and 216 °C/km with an average of 139 °C/km (Supplemental Fig. S5). The local geothermal gradient of Pennell Basin would place the 25 °C threshold between 300 and 115 mbsf. These depths are shallower than the present emplacement of RSS3-Ia, which could indicate that the opal layer has been buried by sediment ranging in thickness from between 25 and 210 m since the timing of the diagenetic front formation occurred. However, the 50 °C threshold is located between 600 and 230 mbsf, range which spans the present-day emplacement of RSS3-Ia. Thus, distinct plausible scenarios could be correlated to the present-day buried depth of RSS3-Ia in terms of erosional-depositional patterns across the Ross Sea continental shelf.

Along the middle continental shelf of the western Ross Sea, the 2D velocity distribution reveals additional high velocity layers along the middle continental shelf (Fig. 3C), which could be related to localized chert layers. The identification of chert layers through geophysical methods has been previously used as indicator of basin-wide biogenic silica abundance, i.e., in the northeast Atlantic (Davies and Cartwright, 2002; Neagu, 2011); the Pacific Margin of the Antarctic Peninsula (Volpi et al., 2003); New Caledonia and the southwest Pacific (Nouzé et al., 2009); and Mauritania (Ireland et al., 2010).

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SUPPLEMENTAL FIGURE CAPTIONS

Supplemental Figure S1. Cross-plot between downhole logging density (ρ_p) and core logged wet bulk density (ρ_c) at Site U1521. ρ_c Values below 1 and over 2.4 g/cm³ are in gray and excluded from the least squares regression that yields the linear relation: $\rho_p = 1.02101 \cdot \rho_c + 0.207547$ [$r = 0.83$]. mbsf, meters below seafloor.

Supplemental Figure S2. Synthetic seismograms (red wiggle traces) for drilled sites DSDP 272, IODP U1521 and DSDP 273 obtained from Hampson Russell – Emerge plotted over single channel seismic profiles PD90_34, PD90_36 and PD90_37, respectively.

Supplemental Figure S3. (A) Multi-channel seismic profile IT94AR126 between shot points 8000 and 3500. See location in Figure 1B (orange line). TWTT, two-way travel-time. Zooms on the seafloor and RSU4a reflections are shown, highlighting that they exhibit the same polarity. Automatic Gain Control (<500 ms) was applied to enhance the stratigraphic discontinuities. The crossing line points and the projected location of the Site U1521 are marked. (B) Tomography model and line drawing along the depth-converted multi-channel seismic profile. The four distinguished layer boundaries correspond to the seafloor, RSU4, RSU4a and RSU5 from top to bottom. The lower layer beneath RSU5 has not been inverted in the tomographic model.

Supplemental Figure S4. Ross Sea continental shelf maps of the major interpreted surfaces depth with respect to ANTOSTRAT (Cooper et al., 1995) stratigraphic position in two-way travel-time (TWTT). Modern continental shelf edge is marked by the thick black line and the thin black lines outline banks and basins as in Figure 1B. Note green colors denote positive values where the reinterpreted surface is below the ANTOSTRAT surface, whereas pink colors denote negative values where the reinterpreted surface is above the ANTOSTRAT surface.

Supplemental Figure S5. (A) Depths where the threshold temperatures for formation of opal A/CT diagenetic front are reached according to several regional geothermal gradients (GG) (°C/km) as discussed in the Supplemental Material. (B) Temperature variation with depth along the upper 500 m below seafloor (bsf) according to several regional geothermal heat flow values, see discussion in the Supplemental Material. The arrow marks the position of Seismic Subunit RSS3-Ia. (C) The table shows the average, median, mode, minimum and maximum geothermal gradients in °C/km, expected in Pennell Basin considering the thermal conductivity data obtained at Site U1521 during IODP Expedition 382 (McKay et al., 2019) and the heat flow values as: mean for continental crust (CC) (65 mW/m²; Pollack et al., 1993), at HF305 (114 mW/m²), local minimum (91 mW/m²) and local maximum (120 mW/m²) (Sato et al., 1984).

Supplemental Figure S1

Supplemental Figure S3

C

Geothermal Gradients	GG CC	GG HF305	GG minimum	GG maximum
Average	79.05	138.65	110.67	145.94
Median	72.95	127.95	102.13	134.68
Mode	61.61	108.06	86.26	113.74
Minimum	47.07	82.55	65.89	86.89
Maximum	123.34	216.32	172.68	227.71

Supplemental Figure S5