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## Supplementary information

### Compilation of Jurassic-Eocene proxy data

Our compilation (Table DR4) regroups published measurements from marine biogenic carbonates (molluscs, brachiopods, corals, foraminifera, belemnites)  $\Delta_{47}$  data (Keating-Bitonti et al., 2011; Douglas et al., 2014; Petersen et al., 2016b, a; Evans et al., 2018; Wierzbowski et al., 2018; Meyer et al., 2018; Vickers et al., 2019, 2020, 2021; Price et al., 2020; Brigaud et al., 2020; Fernandez et al., 2021; de Winter et al., 2021),  $\text{TEX}_{86}^{\text{H}}$  paleothermometry data (Jenkyns et al., 2012; Lunt et al., 2012; Douglas et al., 2014; Frieling et al., 2014; Robinson et al., 2017; O'Brien et al., 2017; Cramwinckel et al., 2018; O'Connor et al., 2019; Ruebsam et al., 2020), and marine turtles phosphate  $\delta^{18}\text{O}$  data (Billon-Bruyat et al., 2005; Coulson et al., 2011; van Baal et al., 2013).

Paleolatitude of each site was reevaluated based on modern site location using the online paleolatitude calculator [paleolatitude.org](http://paleolatitude.org) (van Hinsbergen et al., 2015) computed with the model of Torsvik et al. (2012). Distinction was made between the different proxies ( $\text{TEX}_{86}$  data,  $\Delta_{47}$  data from biogenic marine carbonate, and phosphate  $\delta^{18}\text{O}$ ) as each proxy can be interpreted differently.  $\text{TEX}_{86}^{\text{H}}$  is commonly used as a SST proxy from which we chose to show published SST derived from the hyperbolic core-top calibration of Kim et al. (2010). Carbonate  $\Delta_{47}$  can both resolve calcification temperature and calcifying fluid  $\delta^{18}\text{O}$ . Most of the  $\Delta_{47}$  data in this compilation were acquired before the introduction of interlaboratory carbonate standardization of the proxy (Bernasconi et al., 2018, 2021). The data  $\Delta_{47}$  could not have been reprocessed in the I-CDES reference frame to fit with our data and other recent data, as it was done for modern biogenic carbonates and laboratory precipitated carbonates

(Anderson et al., 2021). In consequence we used the published  $\Delta_{47}$  temperature for each publication. The calcification  $\Delta_{47}$  temperature of biogenic carbonates is interpreted as marine temperature, which may be interpreted differently depending on the ecology of the calcifying organism (living depth, shell growth dynamics, locomotion...). Calcifying fluid  $\delta^{18}\text{O}$  were derived from  $\Delta_{47}$  calcifying temperatures using different isotopic fractionation equations depending on the calcifying organism, and are interpreted as representing sea water  $\delta^{18}\text{O}$  ( $\delta^{18}\text{O}_{\text{sw}}$ ), except for belemnite rostra. Belemnite calcite  $\Delta_{47}$  data yielded unrealistically high  $\delta^{18}\text{O}_{\text{sw}}$  estimates (Wierzbowski et al., 2018; Price et al., 2020; Vickers et al., 2021) using widely used fractionation equations. Using Coplen (2007) equation has resulted in the most realistic  $\delta^{18}\text{O}_{\text{sw}}$  estimates from belemnite rostra (Price et al., 2020). We followed this practice and used this equation to derive  $\delta^{18}\text{O}_{\text{sw}}$  from belemnite calcite  $\Delta_{47}$  data in our compilation, but there is no evidence that any published fractionation equation is well suited to describe belemnite rostra oxygen isotope fractionation. Therefore, belemnite-based  $\delta^{18}\text{O}_{\text{sw}}$  values should not be taken as absolute  $\delta^{18}\text{O}_{\text{sw}}$  estimates but only as recording relative changes in  $\delta^{18}\text{O}_{\text{sw}}$ . We used the equation of Erez and Luz (1983) for foraminifera data, the equation of Grossman and Ku (1986) for biogenic aragonite samples (ammonite shells, aragonite bivalves and belemnite phragmocones), and the equation of Epstein et al. (1953) for calcite bivalves. There is a linear relationship between modern aquatic turtle bone phosphate  $\delta^{18}\text{O}$  and living water  $\delta^{18}\text{O}_{\text{w}}$  (Barrick et al., 1999; Coulson et al., 2008). We derived past  $\delta^{18}\text{O}_{\text{sw}}$  from fossil marine turtle  $\delta^{18}\text{O}_{\text{p}}$  data using the equation of Barrick et al. (1999) normalized to the most recent NBS120c accepted value (Pouech et al., 2014).

These revised values were used to build Figure 5, and illustrate Jurassic-Paleocene temperature and  $\delta^{18}\text{O}_{\text{sw}}$  latitudinal gradient. For this compilation, data was time sliced in 8 intervals corresponding to chronostratigraphic epochs. Late Cretaceous data were further divided into two intervals to highlight long term difference between the “super-greenhouse” Cenomanian-Santonian interval and cooler Campanian-Maastrichtian interval. When only absolute age model was available (most  $\text{TEX}_{86}^{\text{H}}$  data), each data was arbitrarily attributed to its corresponding interval based on absolute date of stage boundaries from the International Chronostratigraphic chart v2020/03 (Cohen et al., 2013; updated). For each time interval and each proxy, we plotted mean temperature or  $\delta^{18}\text{O}_{\text{sw}}$  values for one site or a collection of nearby sites (sites from the same basin within  $0.5^\circ$  of latitude) with error bars representing the total range of the data (maximal to minimal value).

## References

- Anderson, N. T., Kelson, J. R., Kele, S., Daëron, M., Bonifacie, M., Horita, J., Mackey, T. J., John, C. M., Kluge, T., Petschnig, P., Jost, A. B., Huntington, K. W., Bernasconi, S. M., and Bergmann, K. D.: A Unified Clumped Isotope Thermometer Calibration ( $0.5\text{--}1,100^\circ\text{C}$ ) Using Carbonate-Based Standardization, *Geophys Res Lett*, 48, <https://doi.org/10.1029/2020GL092069>, 2021.
- van Baal, R. R., Janssen, R., van der Lubbe, H. J. L., Schulp, A. S., Jagt, J. W. M., and Vonhof, H. B.: Oxygen and carbon stable isotope records of marine vertebrates from the type Maastrichtian, The Netherlands and northeast Belgium (Late Cretaceous), *Palaeogeography*,

Palaeoclimatology, Palaeoecology, 392, 71–78, <https://doi.org/10.1016/j.palaeo.2013.08.020>, 2013.

Barrick, R. E., Fischer, A. G., and Showers, W. J.: Oxygen isotopes from turtle bone; applications for terrestrial paleoclimates?, *PALAIOS*, 14, 186–191, <https://doi.org/10.2307/3515374>, 1999.

Bernasconi, S. M., Müller, I. A., Bergmann, K. D., Breitenbach, S. F. M., Fernandez, A., Hodell, D. A., Jaggi, M., Meckler, A. N., Millan, I., and Ziegler, M.: Reducing Uncertainties in Carbonate Clumped Isotope Analysis Through Consistent Carbonate-Based Standardization, *Geochem Geophys Geosyst*, 19, 2895–2914, <https://doi.org/10.1029/2017GC007385>, 2018.

Bernasconi, S. M., Daëron, M., Bergmann, K. D., Bonifacie, M., Meckler, A. N., Affek, H. P., Anderson, N., Bajnai, D., Barkan, E., Beverly, E., Blamart, D., Burgener, L., Calmels, D., Chaduteau, C., Clog, M., Davidheiser-Kroll, B., Davies, A., Dux, F., Eiler, J., Elliott, B., Fetrow, A. C., Fiebig, J., Goldberg, S., Hermoso, M., Huntington, K. W., Hyland, E., Ingalls, M., Jaggi, M., John, C. M., Jost, A. B., Katz, S., Kelson, J., Kluge, T., Kocken, I. J., Laskar, A., Leutert, T. J., Liang, D., Lucarelli, J., Mackey, T. J., Mangenot, X., Meinicke, N., Modestou, S. E., Müller, I. A., Murray, S., Neary, A., Packard, N., Passey, B. H., Pelletier, E., Petersen, S., Piasecki, A., Schauer, A., Snell, K. E., Swart, P. K., Tripathi, A., Upadhyay, D., Vennemann, T., Winkelstern, I., Yarian, D., Yoshida, N., Zhang, N., and Ziegler, M.: InterCarb: A Community Effort to Improve Interlaboratory Standardization of the Carbonate Clumped Isotope Thermometer Using Carbonate Standards, *Geochem Geophys Geosyst*, 22, <https://doi.org/10.1029/2020GC009588>, 2021.

Billon-Bruyat, J.-P., Lécuyer, C., Martineau, F., and Mazin, J.-M.: Oxygen isotope compositions of Late Jurassic vertebrate remains from lithographic limestones of western Europe: implications for the ecology of fish, turtles, and crocodilians, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 216, 359–375, <https://doi.org/10.1016/j.palaeo.2004.11.011>, 2005.

Brigaud, B., Bonifacie, M., Pagel, M., Blaise, T., Calmels, D., Haurine, F., and Landrein, P.: Past hot fluid flows in limestones detected by  $\Delta 47$ –(U–Pb) and not recorded by other geothermometers, *Geology*, 48, 851–856, <https://doi.org/10.1130/G47358.1>, 2020.

Cohen, K. M., Finney, S. C., Gibbard, P. L., and Fan, J.-X.: The ICS International Chronostratigraphic Chart, 36, 199–204, 2013.

Coplen, T. B.: Calibration of the calcite–water oxygen-isotope geothermometer at Devils Hole, Nevada, a natural laboratory, *Geochimica et Cosmochimica Acta*, 71, 3948–3957, <https://doi.org/10.1016/j.gca.2007.05.028>, 2007.

Coulson, A. B., Kohn, M. J., Shirley, M. H., Joyce, W. G., and Barrick, R. E.: Phosphate–oxygen isotopes from marine turtle bones: Ecologic and paleoclimatic applications, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 264, 78–84, <https://doi.org/10.1016/j.palaeo.2008.04.008>, 2008.

Coulson, A. B., Kohn, M. J., and Barrick, R. E.: Isotopic evaluation of ocean circulation in the Late Cretaceous North American seaway, *Nature Geosci*, 4, 852–855, <https://doi.org/10.1038/ngeo1312>, 2011.

Cramwinckel, M. J., Huber, M., Kocken, I. J., Agnini, C., Bijl, P. K., Bohaty, S. M., Frieling, J., Goldner, A., Hilgen, F. J., Kip, E. L., Peterse, F., van der Ploeg, R., Röhl, U., Schouten, S., and Sluijs, A.: Synchronous tropical and polar temperature evolution in the Eocene, *Nature*, 559, 382–386, <https://doi.org/10.1038/s41586-018-0272-2>, 2018.

Douglas, P. M. J., Affek, H. P., Ivany, L. C., Houben, A. J. P., Sijp, W. P., Sluijs, A., Schouten, S., and Pagani, M.: Pronounced zonal heterogeneity in Eocene southern high-latitude sea surface temperatures, *Proceedings of the National Academy of Sciences*, 111, 6582–6587, <https://doi.org/10.1073/pnas.1321441111>, 2014.

Epstein, S., Buchsbaum, R., Lowenstam, H. A., and Urey, H. C.: Revised carbonate-water isotopic temperature scale, *Geol Soc America Bull*, 64, 1315, [https://doi.org/10.1130/0016-7606\(1953\)64\[1315:RCITS\]2.0.CO;2](https://doi.org/10.1130/0016-7606(1953)64[1315:RCITS]2.0.CO;2), 1953.

Erez, J. and Luz, B.: Experimental paleotemperature equation for planktonic foraminifera, *Geochimica et Cosmochimica Acta*, 47, 1025–1031, 1983.

Evans, D., Sagoo, N., Renema, W., Cotton, L. J., Müller, W., Todd, J. A., Saraswati, P. K., Stassen, P., Ziegler, M., Pearson, P. N., Valdes, P. J., and Affek, H. P.: Eocene greenhouse climate revealed by coupled clumped isotope-Mg/Ca thermometry, *Proc Natl Acad Sci USA*, 115, 1174–1179, <https://doi.org/10.1073/pnas.1714744115>, 2018.

Fernandez, A., Korte, C., Ullmann, C. V., Looser, N., Wohlgend, S., and Bernasconi, S. M.: Reconstructing the magnitude of Early Toarcian (Jurassic) warming using the reordered clumped isotope compositions of belemnites, *Geochimica et Cosmochimica Acta*, 293, 308–327, <https://doi.org/10.1016/j.gca.2020.10.005>, 2021.

Frieling, J., Iakovleva, A. I., Reichart, G.-J., Aleksandrova, G. N., Gnibidenko, Z. N., Schouten, S., and Sluijs, A.: Paleocene–Eocene warming and biotic response in the epicontinental West Siberian Sea, *Geology*, 42, 767–770, <https://doi.org/10.1130/G35724.1>, 2014.

Grossman, E. L. and Ku, T.-L.: Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology*, 59, 59–74, [https://doi.org/10.1016/0168-9622\(86\)90057-6](https://doi.org/10.1016/0168-9622(86)90057-6), 1986.

van Hinsbergen, D. J. J., de Groot, L. V., van Schaik, S. J., Spakman, W., Bijl, P. K., Sluijs, A., Langereis, C. G., and Brinkhuis, H.: A Paleolatitude Calculator for Paleoclimate Studies, *PLOS ONE*, 10, e0126946, <https://doi.org/10.1371/journal.pone.0126946>, 2015.

Jenkyns, H. C., Schouten-Huibers, L., Schouten, S., and Sinninghe Damsté, J. S.: Warm Middle Jurassic–Early Cretaceous high-latitude sea-surface temperatures from the Southern Ocean, *Clim. Past*, 8, 215–226, <https://doi.org/10.5194/cp-8-215-2012>, 2012.

Keating-Bitonti, C. R., Ivany, L. C., Affek, H. P., Douglas, P., and Samson, S. D.: Warm, not super-hot, temperatures in the early Eocene subtropics, *Geology*, 39, 771–774, <https://doi.org/10.1130/G32054.1>, 2011.

Kim, J.-H., van der Meer, J., Schouten, S., Helmke, P., Willmott, V., Sangiorgi, F., Koç, N., Hopmans, E. C., and Damsté, J. S. S.: New indices and calibrations derived from the distribution of crenarchaeal isoprenoid tetraether lipids: Implications for past sea surface

temperature reconstructions, *Geochimica et Cosmochimica Acta*, 74, 4639–4654, <https://doi.org/10.1016/j.gca.2010.05.027>, 2010.

Lunt, D. J., Dunkley Jones, T., Heinemann, M., Huber, M., LeGrande, A., Winguth, A., Loptson, C., Marotzke, J., Roberts, C. D., Tindall, J., Valdes, P., and Winguth, C.: A model–data comparison for a multi-model ensemble of early Eocene atmosphere–ocean simulations: EoMIP, *Clim. Past*, 8, 1717–1736, <https://doi.org/10.5194/cp-8-1717-2012>, 2012.

Meyer, K. W., Petersen, S. V., Lohmann, K. C., and Winkelstern, I. Z.: Climate of the Late Cretaceous North American Gulf and Atlantic Coasts, *Cretaceous Research*, 89, 160–173, <https://doi.org/10.1016/j.cretres.2018.03.017>, 2018.

O’Brien, C. L., Robinson, S. A., Pancost, R. D., Sinninghe Damsté, J. S., Schouten, S., Lunt, D. J., Alsenz, H., Bornemann, A., Bottini, C., Brassell, S. C., Farnsworth, A., Forster, A., Huber, B. T., Inglis, G. N., Jenkyns, H. C., Linnert, C., Littler, K., Markwick, P., McAnena, A., Mutterlose, J., Naafs, B. D. A., Püttmann, W., Sluijs, A., van Helmond, N. A. G. M., Vellekoop, J., Wagner, T., and Wrobel, N. E.: Cretaceous sea-surface temperature evolution: Constraints from TEX<sub>86</sub> and planktonic foraminiferal oxygen isotopes, *Earth-Science Reviews*, 172, 224–247, <https://doi.org/10.1016/j.earscirev.2017.07.012>, 2017.

O’Connor, L. K., Robinson, S. A., Naafs, B. D. A., Jenkyns, H. C., Henson, S., Clarke, M., and Pancost, R. D.: Late Cretaceous Temperature Evolution of the Southern High Latitudes: A TEX<sub>86</sub> Perspective, *Paleoceanography and Paleoclimatology*, 19, 2019.

Petersen, S. V., Dutton, A., and Lohmann, K. C.: End-Cretaceous extinction in Antarctica linked to both Deccan volcanism and meteorite impact via climate change, *Nat Commun*, 7, 12079, <https://doi.org/10.1038/ncomms12079>, 2016a.

Petersen, S. V., Tabor, C. R., Lohmann, K. C., Poulsen, C. J., Meyer, K. W., Carpenter, S. J., Erickson, J. M., Matsunaga, K. K. S., Smith, S. Y., and Sheldon, N. D.: Temperature and salinity of the Late Cretaceous Western Interior Seaway, *Geology*, 44, 903–906, <https://doi.org/10.1130/G38311.1>, 2016b.

Pouech, J., Amiot, R., Lécuyer, C., Mazin, J.-M., Martineau, F., and Fourel, F.: Oxygen isotope composition of vertebrate phosphates from Cherves-de-Cognac (Berriasian, France): Environmental and ecological significance, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 410, 290–299, <https://doi.org/10.1016/j.palaeo.2014.05.036>, 2014.

Price, G. D., Bajnai, D., and Fiebig, J.: Carbonate clumped isotope evidence for latitudinal seawater temperature gradients and the oxygen isotope composition of Early Cretaceous seas, *Palaeoecology*, 552, 109777, <https://doi.org/10.1016/j.palaeo.2020.109777>, 2020.

Robinson, S. A., Ruhl, M., Astley, D. L., Naafs, B. D. A., Farnsworth, A. J., Bown, P. R., Jenkyns, H. C., Lunt, D. J., O’Brien, C., Pancost, R. D., and Markwick, P. J.: Early Jurassic North Atlantic sea-surface temperatures from TEX<sub>86</sub> palaeothermometry, *Sedimentology*, 64, 215–230, <https://doi.org/10.1111/sed.12321>, 2017.

Ruebsam, W., Reolid, M., Sabatino, N., Masetti, D., and Schwark, L.: Molecular paleothermometry of the early Toarcian climate perturbation, 195, 103351, <https://doi.org/10.1016/j.gloplacha.2020.103351>, 2020.

Torsvik, T. H., Van der Voo, R., Preeden, U., Mac Niocaill, C., Steinberger, B., Doubrovine, P. V., van Hinsbergen, D. J. J., Domeier, M., Gaina, C., Tohver, E., Meert, J. G., McCausland, P. J. A., and Cocks, L. R. M.: Phanerozoic polar wander, palaeogeography and dynamics, *Earth-Science Reviews*, 114, 325–368, <https://doi.org/10.1016/j.earscirev.2012.06.007>, 2012.

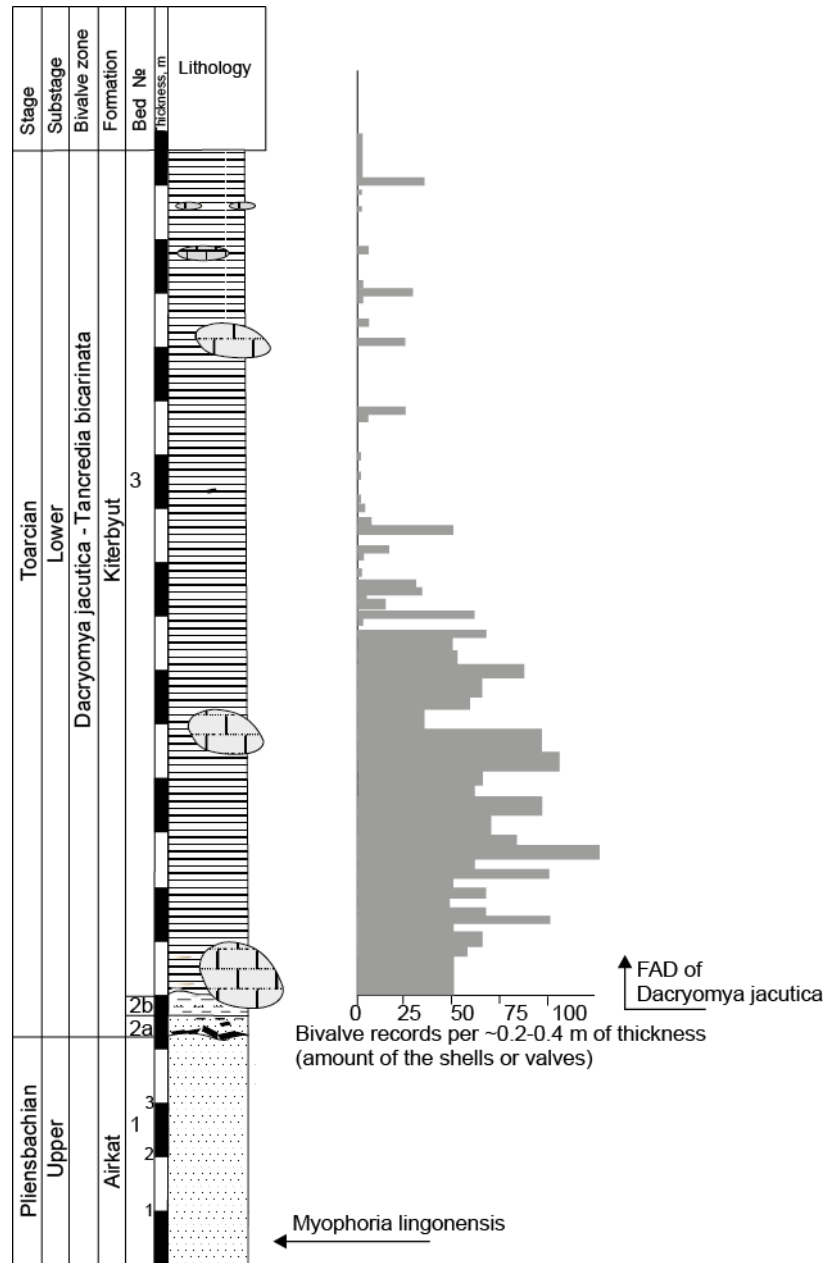
Vickers, M. L., Bajnai, D., Price, G. D., Linckens, J., and Fiebig, J.: Southern high-latitude warmth during the Jurassic–Cretaceous: New evidence from clumped isotope thermometry, *Geology*, 47, 724–728, <https://doi.org/10.1130/G46263.1>, 2019.

Vickers, M. L., Fernandez, A., Hesselbo, S. P., Price, G. D., Bernasconi, S. M., Lode, S., Ullmann, C. V., Thibault, N., Hougaard, I. W., and Korte, C.: Unravelling Middle to Late Jurassic palaeoceanographic and palaeoclimatic signals in the Hebrides Basin using belemnite clumped isotope thermometry, *Earth and Planetary Science Letters*, 546, 116401, <https://doi.org/10.1016/j.epsl.2020.116401>, 2020.

Vickers, M. L., Bernasconi, S. M., Ullmann, C. V., Lode, S., Looser, N., Morales, L. G., Price, G. D., Wilby, P. R., Hougård, I. W., Hesselbo, S. P., and Korte, C.: Marine temperatures underestimated for past greenhouse climate, *Sci Rep*, 11, 19109, <https://doi.org/10.1038/s41598-021-98528-1>, 2021.

Wierzbowski, H., Bajnai, D., Wacker, U., Rogov, M. A., Fiebig, J., and Tesakova, E. M.: Clumped isotope record of salinity variations in the Subboreal Province at the Middle–Late Jurassic transition, *Global and Planetary Change*, 167, 172–189, <https://doi.org/10.1016/j.gloplacha.2018.05.014>, 2018.

de Winter, N. J., Müller, I. A., Kocken, I. J., Thibault, N., Ullmann, C. V., Farnsworth, A., Lunt, D. J., Claeys, P., and Ziegler, M.: Absolute seasonal temperature estimates from clumped isotopes in bivalve shells suggest warm and variable greenhouse climate, *Commun Earth Environ*, 2, 121, <https://doi.org/10.1038/s43247-021-00193-9>, 2021.



**Figure S1.** Stratigraphic log of the Polovinnaya River section and the number of reported occurrences of *Dacryomya jacutica*.