Datashare 128

Oil–source correlation studies in the shallow Berea Sandstone petroleum system, eastern Kentucky

Paul C. Hackley, Thomas M. (Marty) Parris, Cortland F. Eble, Stephen F. Greb, and David C. Harris

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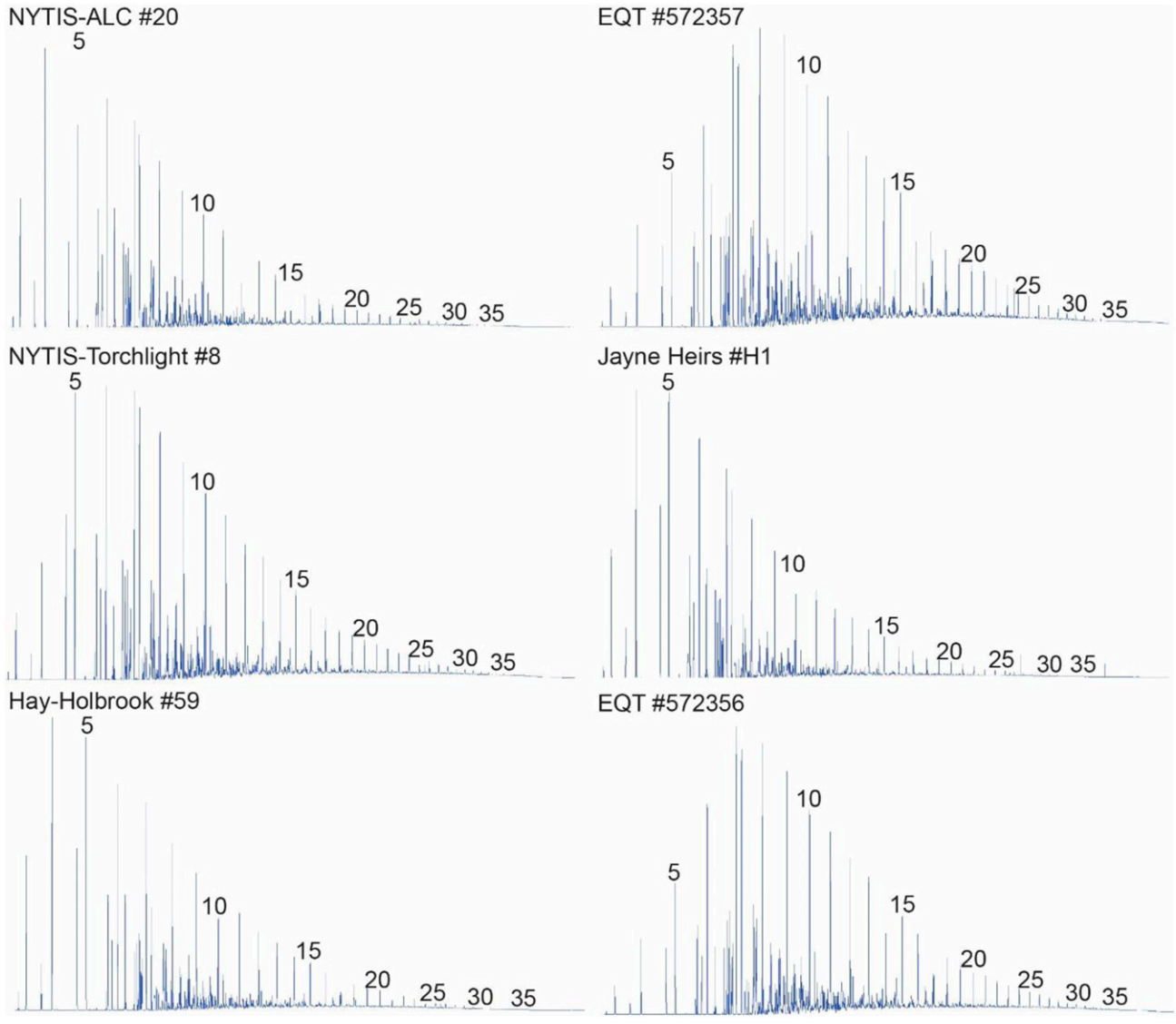

Figure S1. Gas chromatography–flame ionization detector chromatograms of whole oils. Numbers indicate number of carbon atoms for the n-alkanes. The unusual high molecular weight peaks visible in the chromatogram from sample Jayne Heirs H1 and NYTIS-Torchlight 8 probably are contamination from phthalate plasticizers. Modified from Parris et al. (2019) with permission of Kentucky Geological Survey.

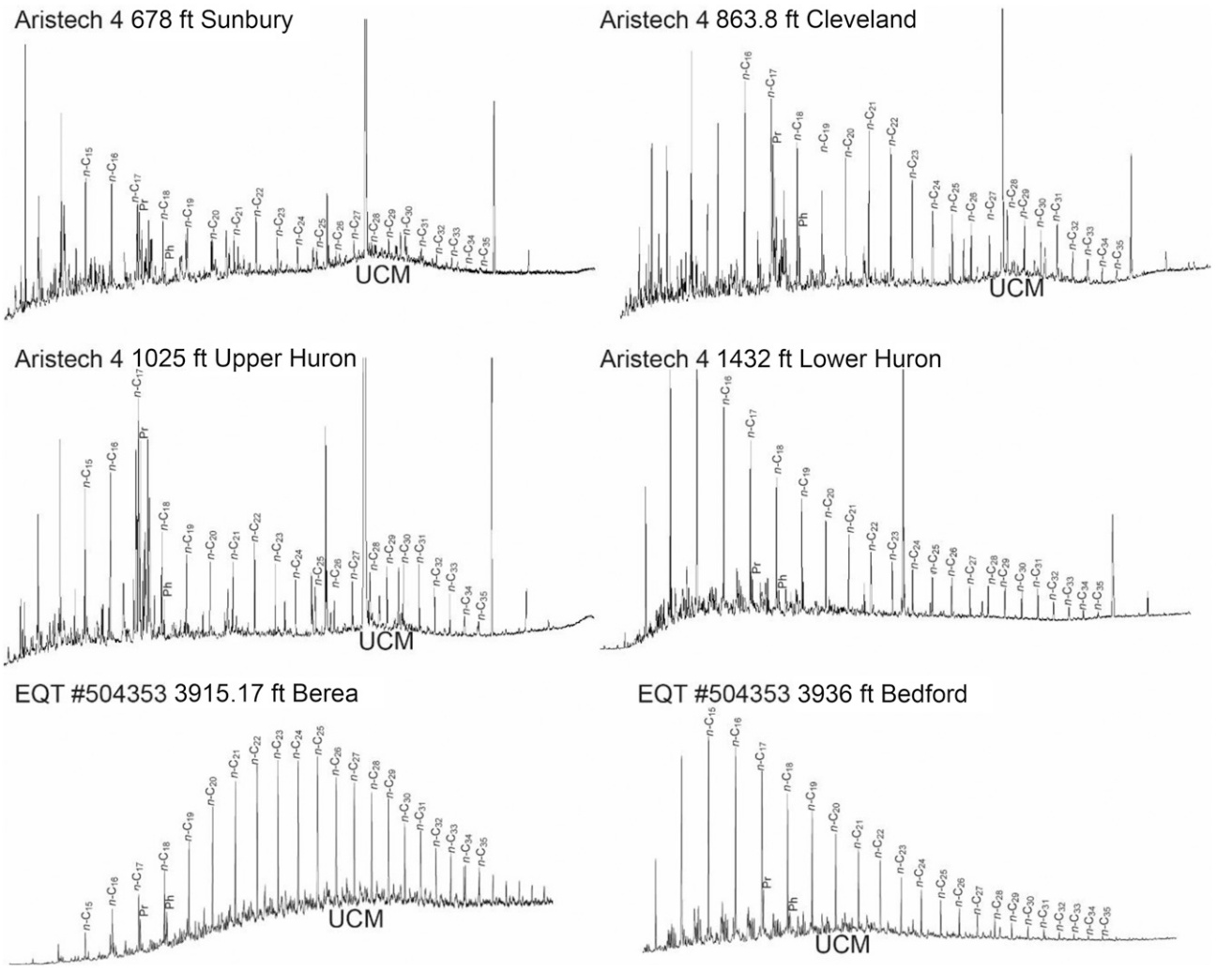

Figure S2. Solvent extract chromatograms from gas chromatography–flame ionization detection analysis of the "immature" Aristech samples and from higher-maturity Berea Sandstone and black Bedford shale in the downdip EQT 504353 well. The cluster of peaks near n-C_{17} in the Aristech 4 1025 ft upper Huron sample is possibly from an unknown contaminant, whereas the unlabeled high-molecular-weight peaks in all four chromatograms from the Aristech 4 well probably are contamination from phthalate plasticizers. Modified from Parris et al. (2019) with permission of Kentucky Geological Survey. UCM = unresolved complex mixture.

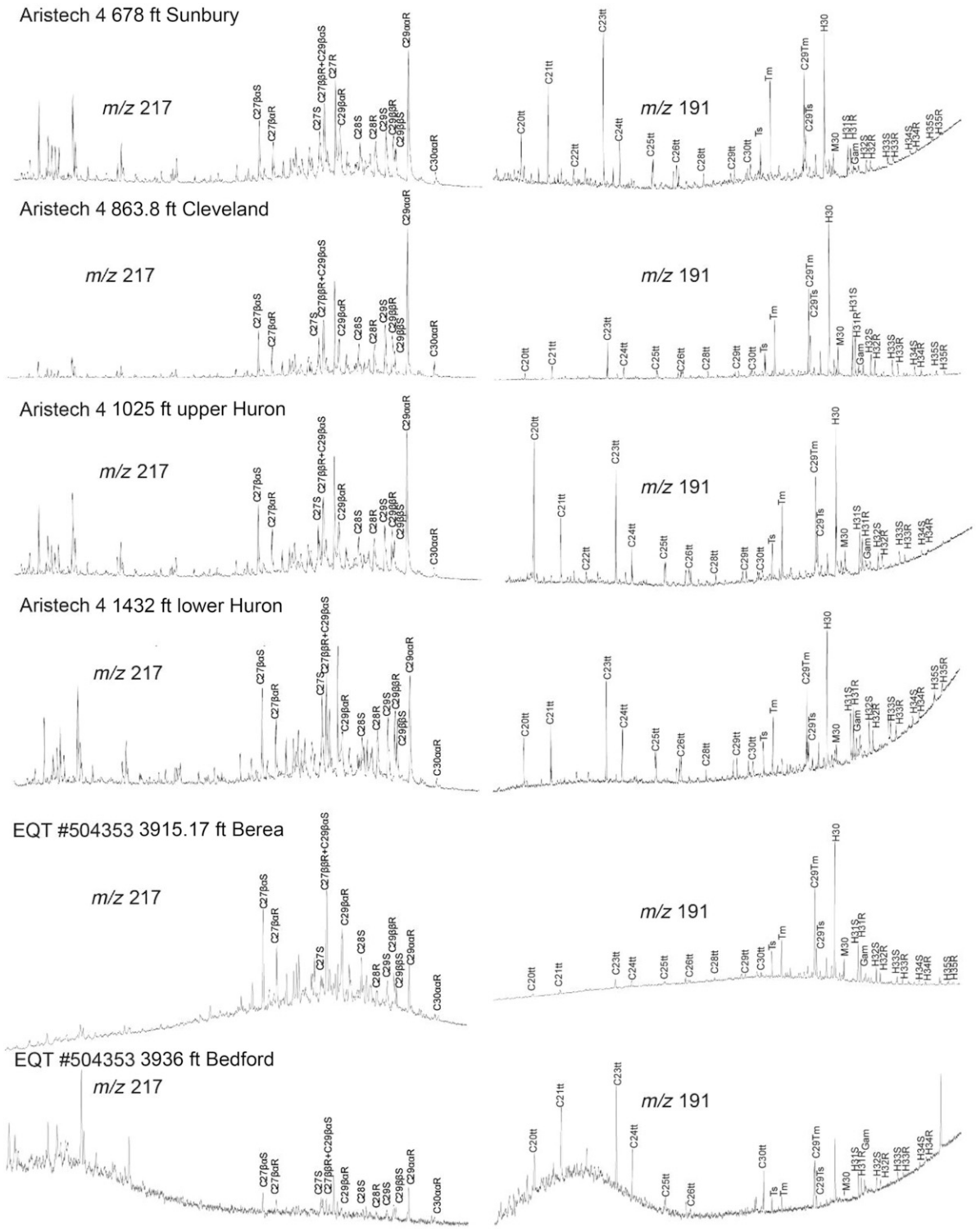

Figure S3. Gas chromatography–mass spectrometry mass-to-charge ratio (*m/z*) 191 and 217 fragmentograms for solvent extracts from core samples from the Aristech 4 well and from the EQT 504353 well. Modified from Parris et al. (2019) with permission of Kentucky Geological Survey. C20tt-C30tt (*m/z* = 191) = C_{20}-C_{30} tricyclic terpanes; C27R-C30R (*m/z* = 217) = C_{27}-C_{30} αα 20R sterane; C27βαS, C27ββS-C29S (*m/z* = 217) = C_{27}-C_{29} αα 20S sterane; C29Tm (*m/z* = 191) = C_{29} 17α(H)21β(H)-norhopane; C29Ts (*m/z* = 191) = C_{29} 18α(H)-norneohopane; Gam (*m/z* = 191) = gammacerane; H30 (*m/z* = 191) = C_{30} 17α(H)-hopane; H31S (*m/z* = 191) = C_{31} 22S 17α(H) hopane; H32R-H35R (*m/z* = 191) = C_{32}-C_{35} 22R 17α(H) hopane; H32S-H35S (*m/z* = 191) = C_{32}-C_{35} 22S 17α(H) hopane; M30 (*m/z* = 191) = C_{30} 17β(H)21α(H)-moretane; Tm (*m/z* = 191) = 17α(H)-trisnorhopane; Ts (*m/z* = 191) = 18α(H)-trisnorhopane.

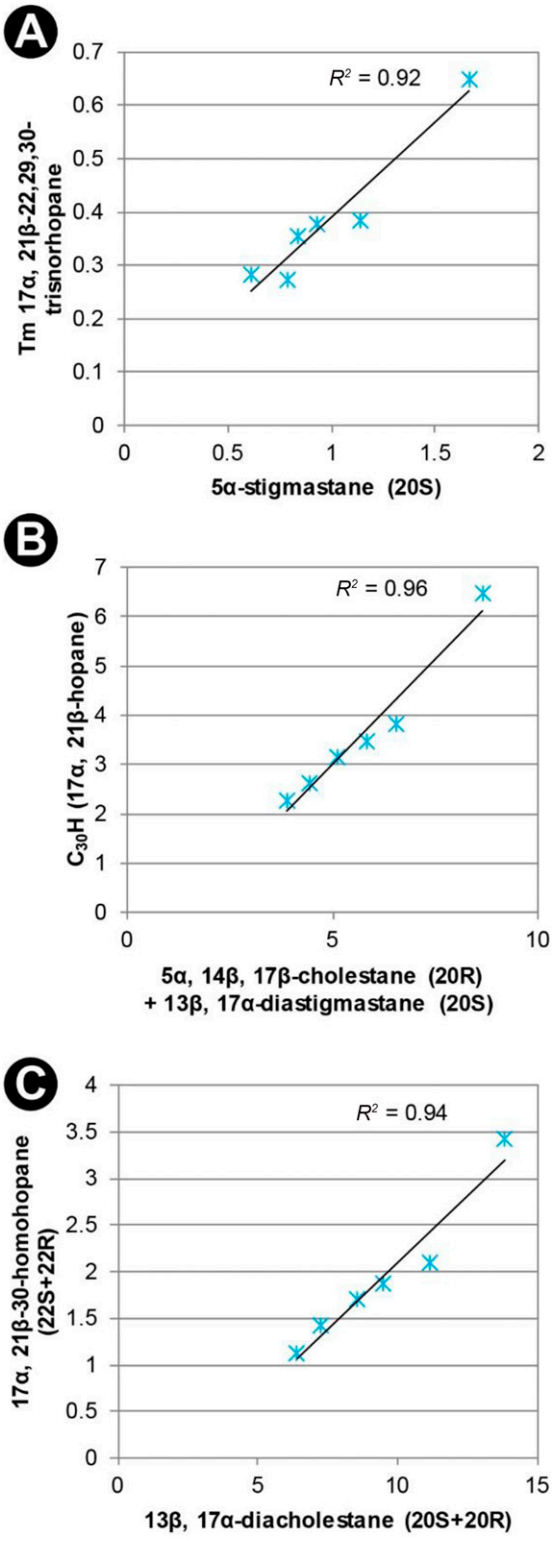

Figure S4. Relationship between concentrations (in micrograms per gram) of individual sterane and hopane compounds in Berea oil samples. (A) Tm 17α, 21β-22,29,30-trisnorhopane versus 5α-stigmastane (20S). (B) C30H (17α, 21β-hopane) versus 5α, 14β, 17β-cholestane (20R) + 13β, 17α-diastigmastane (20S).

Table S1. Concentrations (in Micrograms per Gram) of Individual Sterane and Hopane Abundances in Berea Oils

Sample ID	S4	S12	S1+S2	$C_{30}H$	Tm	$C_{31}R+S$
NYTIS-ALC 20	4.4	0.8	7.3	2.6	0.27	1.4
NYTIS-Torchlight 8	6.6	1.1	11	3.8	0.38	2.1
Hay-Holbrook 59	5.8	0.9	9.5	3.5	0.38	1.9
EQT 572357	8.7	1.7	14	6.5	0.65	3.4
Jayne Heirs H1	5.1	0.8	8.6	3.2	0.36	1.7
EQT 572356	3.9	0.6	6.4	2.3	0.28	1.1

Abbreviations: $C_{30}H$ = 17α, 21β-hopane; $C_{31}R+S$ = 17α, 21β-30-homohopane (22S+22R); ID = identifier; S1+S2 = 13β, 17α-diacholestane (20S+20R); S4 = 5α, 14β, 17β-cholestane (20R) +13β, 17α-diastigmastane (20S); S12 = 5α-stigmastane (20S); Tm = 17α, 21β-22,29,30-trisnorhopane.

Figure S4. (C) 17α, 21β-30-homohopane (22S+22R) versus 13β, 17α-diacholestane (20S+20R). Modified from Parris et al. (2019) with permission of Kentucky Geological Survey. R^2 = coefficient of determination.

REFERENCES CITED

Parris, T. M., S. F. Greb, C. F. Eble, P. C. Hackley, and D. C. Harris, 2019, Berea Sandstone petroleum system: Kentucky Geological Survey Contract Report 6, Series XIII, 342 p., accessed October 27, 2020, https://kgs.uky.edu/kgsweb/olops/pub/kgs/CNR6_13.pdf.