

Certificate of Analysis

Hydrogen and Carbon Stable Isotope Ratio Reference Materials

n-Alkane Mixture Type A8

<i>n</i> -alkane	mean $\delta^2\text{H}$ ‰	one σ ‰	range $\delta^2\text{H}$ ‰	n	mean $\delta^{13}\text{C}$ ‰	one σ ‰	range $\delta^{13}\text{C}$ ‰	n	Concentrations of individual <i>n</i> -alkanes [mg in 0.5 mL]
C-16 #2	-9.1	1.4	-7.9 to -11.1	7	-26.15	0.02	-26.13 to -26.17	5	0.70
C-17 #2	-121.2	0.5	-120.6 to -122.0	5	-31.87	0.02	-31.84 to -31.90	8	0.70
C-18 #2	-52.0	1.1	-50.6 to -53.5	5	-32.70	0.01	-32.69 to -32.72	5	0.70
C-19 #2	-56.3	1.0	-55.0 to -57.5	5	-31.99	0.01	-31.98 to -32.02	6	0.70
C-20 #4	-49.6	2.1	-47.2 to -52.3	4	-31.87	0.02	-31.85 to -31.90	5	0.70
C-21 #2	-181.6	0.6	-180.7 to -182.3	5	-28.83	0.02	-28.81 to -28.85	5	0.70
C-22 #3	-68.2	1.8	-65.7 to -70.4	5	-34.89	0.02	-34.87 to -34.92	6	0.70
C-23 #2	-67.2	1.0	-65.6 to -68.6	6	-33.37	0.03	-33.33 to -33.40	5	0.70
C-24 #2	-29.7	1.5	-28.2 to -31.8	6	-32.13	0.02	-32.11 to -32.16	6	0.70
C-25 #4	-258.9	0.8	-258.1 to -260.0	5	-28.46	0.02	-28.42 to -28.48	7	0.70
C-26 #2	-45.9	1.0	-44.4 to -46.7	5	-32.94	0.01	-32.92 to -32.95	7	0.70
C-27 #4	-205.2	1.6	-203.5 to -207.6	6	-31.11	0.01	-31.11 to -31.12	5	0.70
C-28 #2	-36.8	1.3	-35.6 to -38.9	5	-33.20	0.01	-33.20 to -33.20	5	0.70
C-29 #5	-85.4	1.4	-82.9 to -86.8	6	-31.83	0.02	-31.80 to -31.85	5	0.70
C-30 #4	-41.5	0.7	-40.9 to -42.9	6	-33.14	0.02	-33.12 to -33.16	6	0.70

Notes

Commercially available individual pure *n*-alkanes were tested for purity of each compound using gas chromatography. Stable isotope ratios of individual compounds were determined at Indiana University by combusting multiple aliquots of each pure *n*-alkane off-line according to Schimmelmann et al. (1999, *Geochimica et Cosmochimica Acta* **63**, 3751-3766). Elemental hydrogen gases were measured and reported isotopically according to Coplen's (1996) guidelines relative to VSMOW2 (zero ‰) and normalized to SLAP2 (-427.5 ‰) (Coplen, T. B., 1996. New guidelines for reporting stable hydrogen, carbon, and oxygen isotope-ratio data. *Geochimica et Cosmochimica Acta* **60**, 3359-3360). Carbon isotope ratios are reported relative to the VPDB scale where NBS 19 and LSVEC are defined as exactly +1.95 and -46.6 ‰, respectively (Coplen et al., 2006. New guidelines for $\delta^{13}\text{C}$ measurements. *Analytical Chemistry* **78** (7), 2439-2441). Mass-spectrometric data in customary δ notation have a precision of ± 1.5 ‰ for $\delta^2\text{H}$ and ± 0.05 ‰ for $\delta^{13}\text{C}$. The vial of LSVEC used for calibration was rarely opened and thus not compromised.

The data in the Table shown above represent the mean value, one σ standard deviation, the range, and the number of analyses. Concentrations of each *n*-alkane in mixture A8 are indicated in terms of milligram *n*-alkane dissolved in 0.5 milliliter chromatographically pure hexane (Honeywell Burdick & Jackson, capillary GC GC-MS solvent). Aliquots of 0.5 mL of solution are sealed under argon in glass ampoules. Primary reference materials used for isotopic characterization were VSMOW2, SLAP2, NBS 19, and LSVEC. Isotopic and statistical analyses were performed at Indiana University by Arndt Schimmelmann.

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This is a certified reference material (CRM) that can be traced to primary standards VSMOW, SLAP, NBS 19, and LSVEC.



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