

# Certificate of Analysis

Hydrogen and Carbon Stable Isotope Ratio Reference Materials

## *n*-Alkane Mixture B4

<i>n</i> -alkane	mean	one	range $\delta^2\text{H}$	<i>n</i>	mean	one	range $\delta^{13}\text{C}$	<i>n</i>	Concentrations of individual <i>n</i> -alkanes [mg in 0.5 mL]
	$\delta^2\text{H}$	$\sigma$			$\delta^{13}\text{C}$	$\sigma$			
	‰	‰	‰		‰	‰	‰		
C-16 (#2)	-9.1	1.4	-7.9 to -11.1	7	-26.15	0.02	-26.13 to -26.17	5	0.139
C-17 (#2)	-121.2	0.5	-120.6 to -122.0	5	-31.88	0.01	-31.87 to -31.90	5	0.281
C-18 (#1)	-53.8	2.1	-50.9 to -55.7	4	-31.11	0.02	-31.08 to -31.14	8	0.421
C-19 (#2)	-56.3	1.0	-55.0 to -57.5	5	-31.99	0.01	-31.98 to -32.02	6	0.562
C-20 (#2)	-89.7	1.7	-87.3 to -91.2	4	-33.97	0.02	-33.93 to -33.98	6	0.702
C-21 (#2)	-181.6	0.6	-180.7 to -182.3	5	-28.83	0.02	-28.81 to -28.85	5	0.140
C-22 (#1)	-62.8	1.6	-60.9 to -64.9	6	-32.87	0.03	-32.84 to -32.91	5	0.280
C-23 (#2)	-67.2	1.1	-65.6 to -68.6	6	-33.37	0.03	-33.33 to -33.40	5	0.422
C-24 (#1)	-53.0	1.6	-50.7 to -54.5	4	-33.34	0.02	-33.32 to -33.36	6	0.559
C-25 (#3)	-254.1	1.5	-252.0 to -256.1	5	-28.48	0.02	-28.45 to -28.51	7	0.701
C-26 (#2)	-45.9	1.0	-44.4 to -46.7	5	-32.94	0.01	-32.92 to -32.95	8	0.140
C-27 (#3)	-172.8	1.6	-170.6 to -175.1	6	-30.49	0.01	-30.47 to -30.50	5	0.281
C-28 (#1)	-49.0	1.5	-46.7 to -50.0	4	-32.21	0.03	-32.16 to -32.24	8	0.422
C-29 (#3)	-178.2	1.3	-176.1 to -179.7	6	-29.10	0.01	-29.08 to -29.11	5	0.561
C-30 (#3)	-213.6	2.4	-210.5 to -216.1	6	-29.84	0.01	-29.82 to -29.85	5	0.699

### Notes

A set of commercially available individual *n*-alkanes was tested for purity of each compound using GC-mass spectrometry at Woods Hole Oceanographic Institution. Over time, new batches of *n*-alkane mixtures required several replacement *n*-alkanes that were purchased from commercial sources and were tested for purity via GC at Indiana University. Stable isotope ratios 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 VSMOW (zero ‰) and normalized to SLAP (-428 ‰) (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  $\delta$  notation have a precision of  $\pm 1.5$  ‰ for  $\delta^2\text{H}$  and  $\pm 0.05$  ‰ for  $\delta^{13}\text{C}$ .

The data in the Table shown above represent the mean value, one standard deviation, the range, and the number of analyses. Concentrations of each *n*-alkane in mixture B4 are indicated in terms of milligram *n*-alkane dissolved in 0.5 milliliter chromatographically pure hexane (Burdick & Jackson, 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 VSMOW, SLAP, 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.



CERTIFIED 3 September 2024

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