

# Certificate of Analysis

Hydrogen and Carbon Stable Isotope Ratio Reference Materials

## *n*-Alkane Mixture B5

<i>n</i> -alkane	mean $\delta^2\text{H}$ ‰	one $\sigma$ ‰	range $\delta^2\text{H}$ ‰	n	mean $\delta^{13}\text{C}$ ‰	one $\sigma$ ‰	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	0.140
C-17 (#2)	-121.2	0.5	-120.6 to -122.0	5	-31.87	0.02	-31.84 to -31.90	8	0.280
C-18 (#2)	-52.0	1.1	-50.6 to -53.5	5	-32.70	0.01	-32.69 to -32.72	5	0.420
C-19 (#2)	-56.3	1.0	-55.0 to -57.5	5	-31.99	0.01	-31.98 to -32.02	6	0.560
C-20 (#3)	-177.6	1.1	-176.4 to -179.3	5	-40.91	0.02	-40.89 to -40.94	7	0.700
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 (#3)	-68.2	1.8	-65.7 to -70.4	5	-34.89	0.02	-34.87 to -34.92	6	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	0.420
C-24 (#2)	-29.7	1.5	-28.2 to -31.8	6	-32.13	0.02	-32.11 to -32.16	6	0.560
C-25 (#4)	-258.9	0.8	-258.1 to -260.0	5	-28.46	0.02	-28.42 to -28.48	7	0.700
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 (#4)	-205.2	1.6	-203.5 to -207.6	6	-31.11	0.01	-31.11 to -31.12	5	0.280
C-28 (#2)	-36.8	1.3	-35.6 to -38.9	5	-33.20	0.01	-33.20 to -33.20	5	0.420
C-29 (#4)	-162.6	2.2	-160.6 to -165.0	4	-29.30	0.02	-29.27 to -29.32	5	0.560
C-30 (#4)	-41.5	0.7	-40.9 to -42.9	6	-33.14	0.02	-33.12 to -33.16	6	0.700

### Notes

Individual *n*-alkanes with the highest commercially available purity were tested for purity using gas chromatography at Indiana University. Stable isotope ratios were determined at Indiana University by combusting multiple aliquots of each *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). Only relatively new LSVEC bottles were used that had been rarely opened. 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 B5 are indicated in terms of milligram *n*-alkane dissolved in 0.5 milliliter chromatographically pure hexane (Burdick & Jackson, capillary GC/GC-MS solvent). Aliquots of 0.5 mL of solution were 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.



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