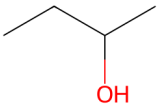
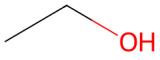
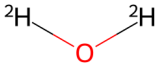
STRUCTURE CHARACTERISATION

Butan-2-ol + ethanol

REPORT ID	PROJECT	PREPARED BY	GENERATED
RPT-20261120-044551-1F3A8ABB	Nuclei Sample Dataset	admin	2026-11-20 04:45:51

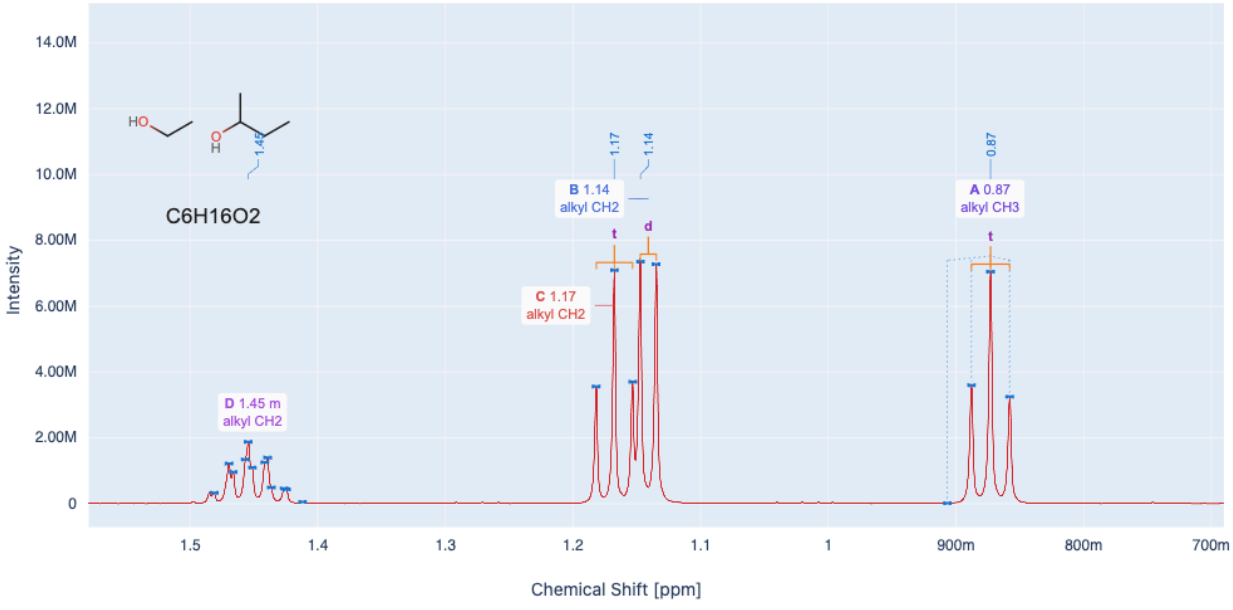
Compound

Structure	Component	Role	Formula	M (g/mol)	Monoisotopic mass	InChIKey
	Butan-2-ol	Analyte	C4H10O	74.123	74.0732	BTANRVKWQNVYAZ-UHFFFAOYSA-N
	Ethanol	Analyte	C2H6O	46.069	46.0419	LFQSCWFLJHTTHZ-UHFFFAOYSA-N
	Deuterium oxide	Solvent	D2O	20.0272	20.0231	XLYOFNOQVPJJNP-ZSJDYOACSA-N

One-dimensional NMR

^{1}H NMR — 1H

500.13 MHz, Deuterium Oxide, 298 K (24.85 °C))



^{1}H spectrum (1H).

#	δ (ppm)	Multiplicity	J (Hz)	Integration	Lines (ppm)
1F	3.77-3.71	sext	6.3	0.23	3.707, 3.719, 3.732, 3.744, 3.757, 3.769 *^{13}C satellites: 4 (3.860, 3.872, 3.885, 3.897)*
2E	3.66-3.61	q	7.1	0.52	3.615, 3.629, 3.643, 3.657 *^{13}C satellites: 6 (3.469, 3.483, 3.498, 3.512, 3.783, 3.797)*
3D	1.48-1.41	m	-	0.27	1.412, 1.425, 1.426, 1.436, 1.439, 1.442, 1.451, 1.455, 1.457, 1.466, 1.470, 1.481 *^{13}C satellites: 7 (1.324, 1.327, 1.339, 1.342, 1.563, 1.578, 1.593)*
4C	1.18-1.15	t	7.1	0.47	1.153, 1.168, 1.182 *^{13}C satellites: 6 (1.026, 1.040, 1.054, 1.277, 1.292, 1.306)*
5B	1.15-1.13	d	6.3	1.00	1.135, 1.147 *^{13}C satellites: 5 (1.008, 1.011, 1.020, 1.258, 1.271)*
6A	0.89-0.86	t	7.5	0.64	0.858, 0.873, 0.888 *^{13}C satellites: 6 (0.731, 0.746, 0.761, 0.982, 0.989, 0.996)* *Shoulders: 1 (0.907)*

Not listed: 7 minor (10.09, 3.60-3.57, 2.19, 1.51-1.50, 1.48, 1.41-1.40, 1.12-1.11); 1 artifact (4.79)

Sample

Sample name	Butan-2-ol + ethanol
Description	Butan-2-ol and ethanol in D2O at 0.5 M, 5 mm tube, 298 K, measured on a 500 MHz Bruker spectrometer (BBI probe). Sample DX-34. B. Lorandel, H. Rocha, O. Cazimajou, R. Mishra, A. Bernard, P. Bowyer, M. Nilsson, J.-N. Dumez, 10.5281/zenodo.12916108 (CC BY 4.0).

Interpretation and assignment

Summary	
Key observations	
Exceptions and limitations	
Analyst notes	

The results in this report refer only to the sample and the acquisition conditions stated above. Signal assignments and interpretation are the analyst's and are limited to the data shown.

Sign-off

ROLE	NAME	SIGNATURE	DATE
Prepared by	admin	*No signature stamp configured for this profile*	2026-11-20 04:45:51
Reviewed by			
Approved by			