

COVER PAGE OF SUPPORTING INFORMATION

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TITLE OF PRIMARY PAPER: The potential of NMR spectroscopy for the study of human amniotic fluid

ABSTRACT OF SI:

This SI section includes two figures showing 1D and 2D NMR spectra of human amniotic fluid (HAF) containing additional information on specific compound assignments. Figure S-1 shows three expansions of a 1D ^1H NMR spectrum of human amniotic fluid (HAF) where the major assignments are specified. Figure S-2 shows expansions of a TOCSY spectrum (top) and a $^1\text{H}/^{13}\text{C}$ correlation spectrum (bottom) of HAF, again showing the assignments of the major peaks. This information should be useful for the reader to interpret more fully the NMR spectra of HAF shown in the main paper.

Figure S-1. Expansions of a) high-, b) medium- and c) low-field regions of the 800MHz 1D ^1H NMR spectrum of HAF reconstituted from a freeze-dried sample, pH 9. Assignments: 1, α -hydroxybutyrate; 2, leucine; 3, isoleucine; 4, valine; 5, U8; 6, α -oxoisovalerate; 7, β -hydroxybutyrate; 8, α -hydroxyisobutyrate; 9, threonine; 10, lactate; 11, alanine; 12, lysine; 13, acetate; 14, N-acetyl groups (glycoproteins); 15, proline; 16, methionine; 17, glutamate; 18, pyruvate; 19, succinate; 20, citrate; 21, U22; 22, creatine; 23, creatinine; 24, choline; 25, carnitine; 26, β -glucose; 27, U27; 28, glycine; 29, α -glucose; 30, betaine; 31, myo-inositol; 32, U39; 33, fumarate; 34, tyrosine; 35, histidine; 36, phenylalanine; 37, formate.

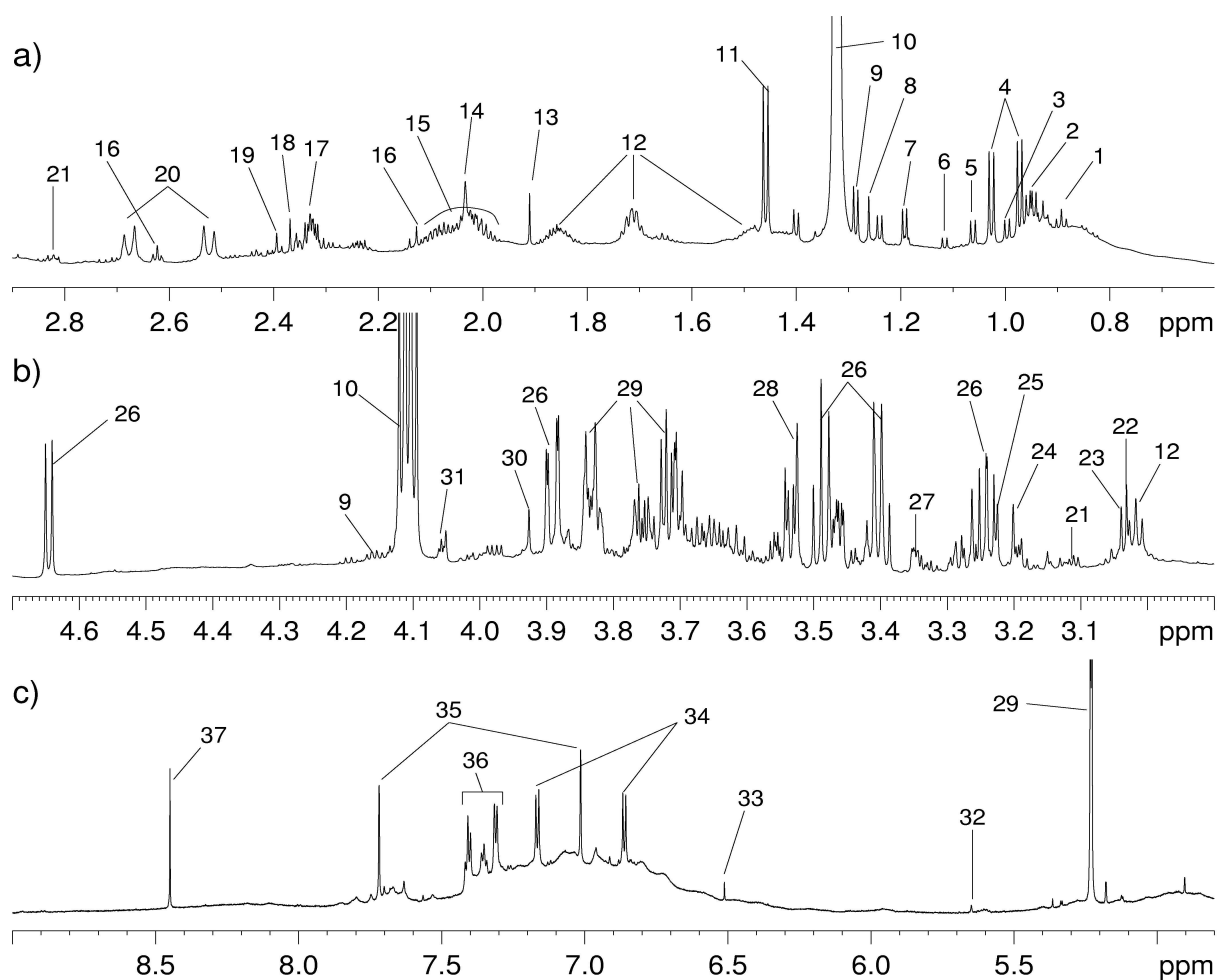
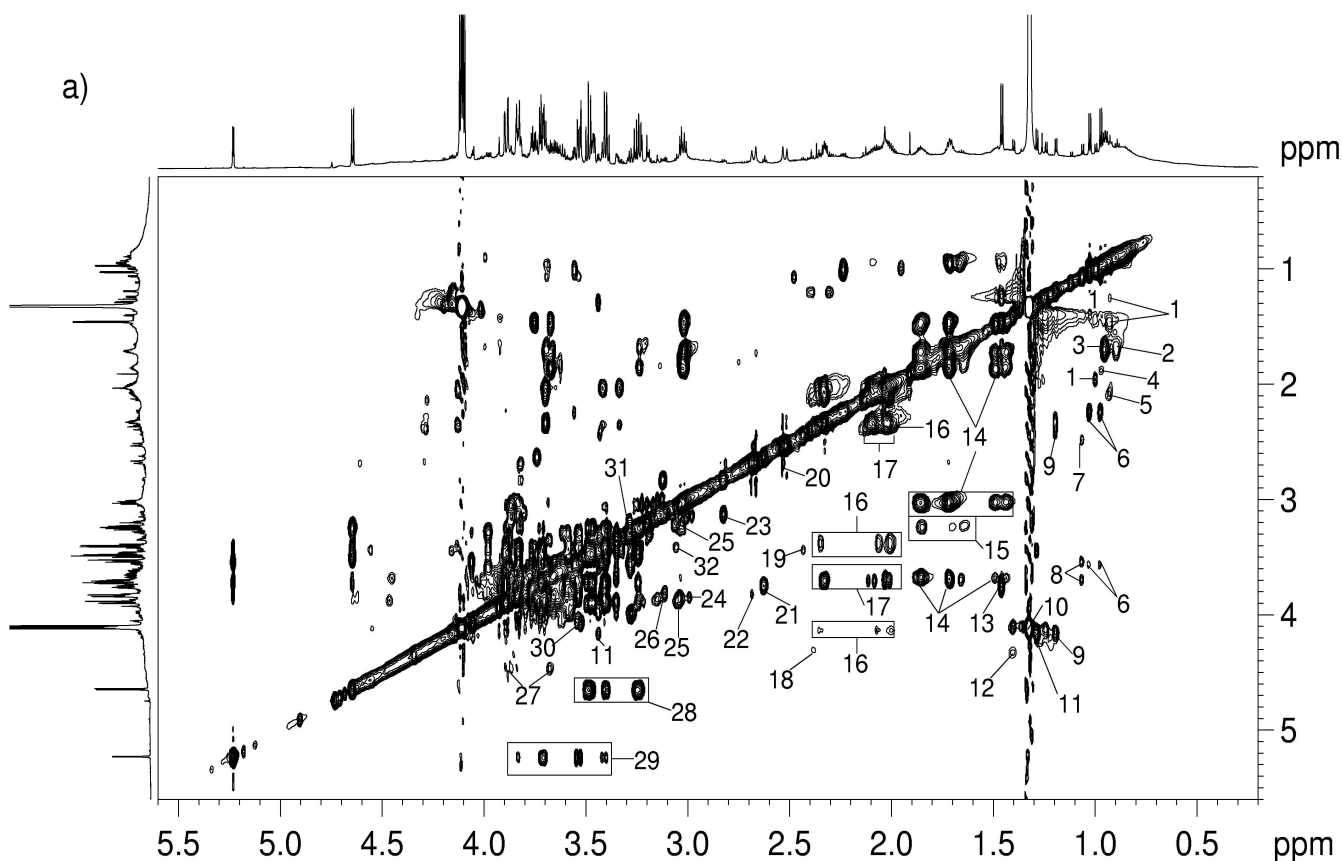


Figure S-2. Expansions of a a) TOCSY spectrum and a b) $^1\text{H}/^{13}\text{C}$ heteronuclear single quantum coherence (HSQC) correlation spectrum of HAF, at 800MHz. Assignments: 1, isoleucine; 2, α -hydroxybutyrate leucine; 3, valine; 4, α -aminobutyrate; 5, U6; 6, valine; 7, U8; 8, U9; 9, β -hydroxybutyrate; 10, lactate; 11, threonine; 12, U12; 13, alanine; 14, lysine; 15, arginine; 16, proline; 17, glutamate + glutamine; 18, hydroxyproline; 19, carnitine; 20, citrate; 21, methionine; 22, U13; 23, U22; 24, tyrosine; 25, histidine; 26, ethanolamine; 27, U27; 28, β -glucose; 29, α -glucose; 30, myoinositol; 31, taurine; 32, U24; 33, U4; 34, α -oxoisovalerate; 35, α -hydroxyisobutyrate; 36, U17; 37, U16; 38, N-acetyl groups (glycoproteins); 39, pyruvate; 40, α -ketoglutarate; 41, succinate; 42, oxaloacetate; 43, U19; 44, creatinine; 45, creatine; 46, choline; 47, betaine; 48, glycine; 49, U28; 50, U15.



b)

