Electronic Supplementary Information

GAS CHROMATOGRAPHY–FOURIER TRANSFORM INFRARED SPECTROSCOPY REVEALS DYNAMIC MOLECULAR INTERCONVERSION OF OXIMES

by

J. Shezmin Zavahir[a], Yada Nolvachai[a], Bayden R. Wood[b], Philip J. Marriott*[a]

[a] Australian Centre for Research on Separation Science, School of Chemistry, Monash University, Wellington Road, Clayton, VIC 3800, Melbourne, Australia.

[b] Centre for Biospectroscopy, School of Chemistry, Monash University, Wellington Road, Clayton, VIC 3800, Melbourne, Australia.

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Analyst

* Corresponding author: Tel. +61 3 99059630; fax. +61 3 99058501

Email: Philip.Marriott@monash.edu

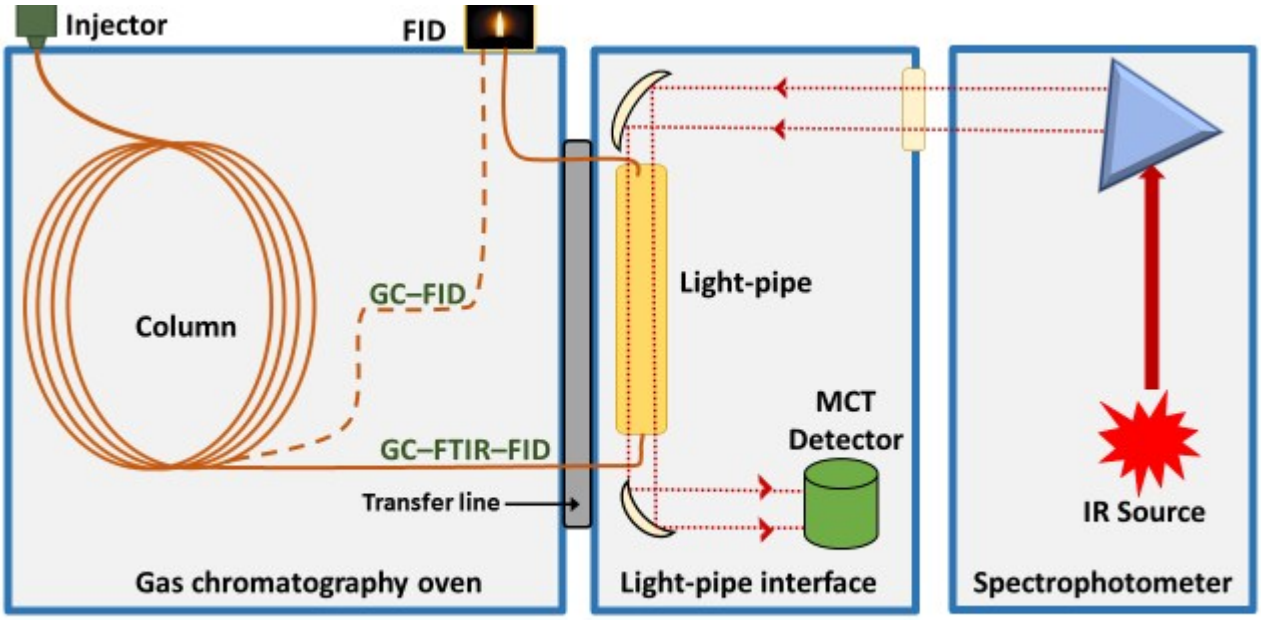

Fig. S1. Instrumental schematic for the light-pipe GC–FTIR–FID system where a GC is hyphenated to a spectrophotometer via a light-pipe interface. The dashed line represents column configuration for GC–FID setting where the sample does not travel through the light pipe.

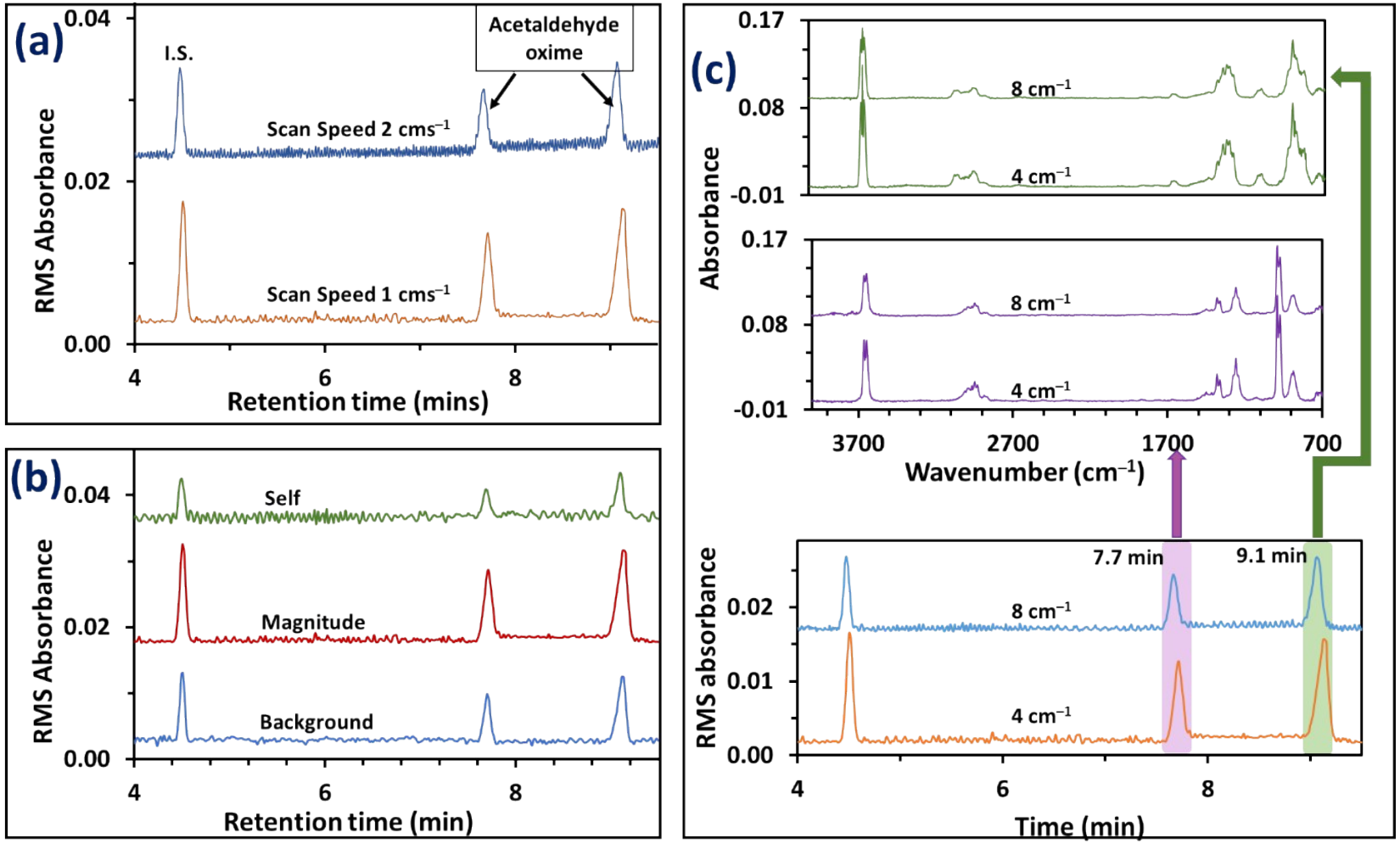

Fig. S2. Comparison of FTIR data acquisition settings (A) scan speed, (B) phase correction and (C) resolution, at isothermal oven *T* of 80 °C, flow of 3 mL min^{-1} Peaks correspond to the I.S.; internal standard and dynamic chromatographic peaks of acetaldehyde oxime. In each, better SNR was observed using a scan speed of 1 cms^{-1}, magnitude phase correction and resolution of 4 cm^{-1}.

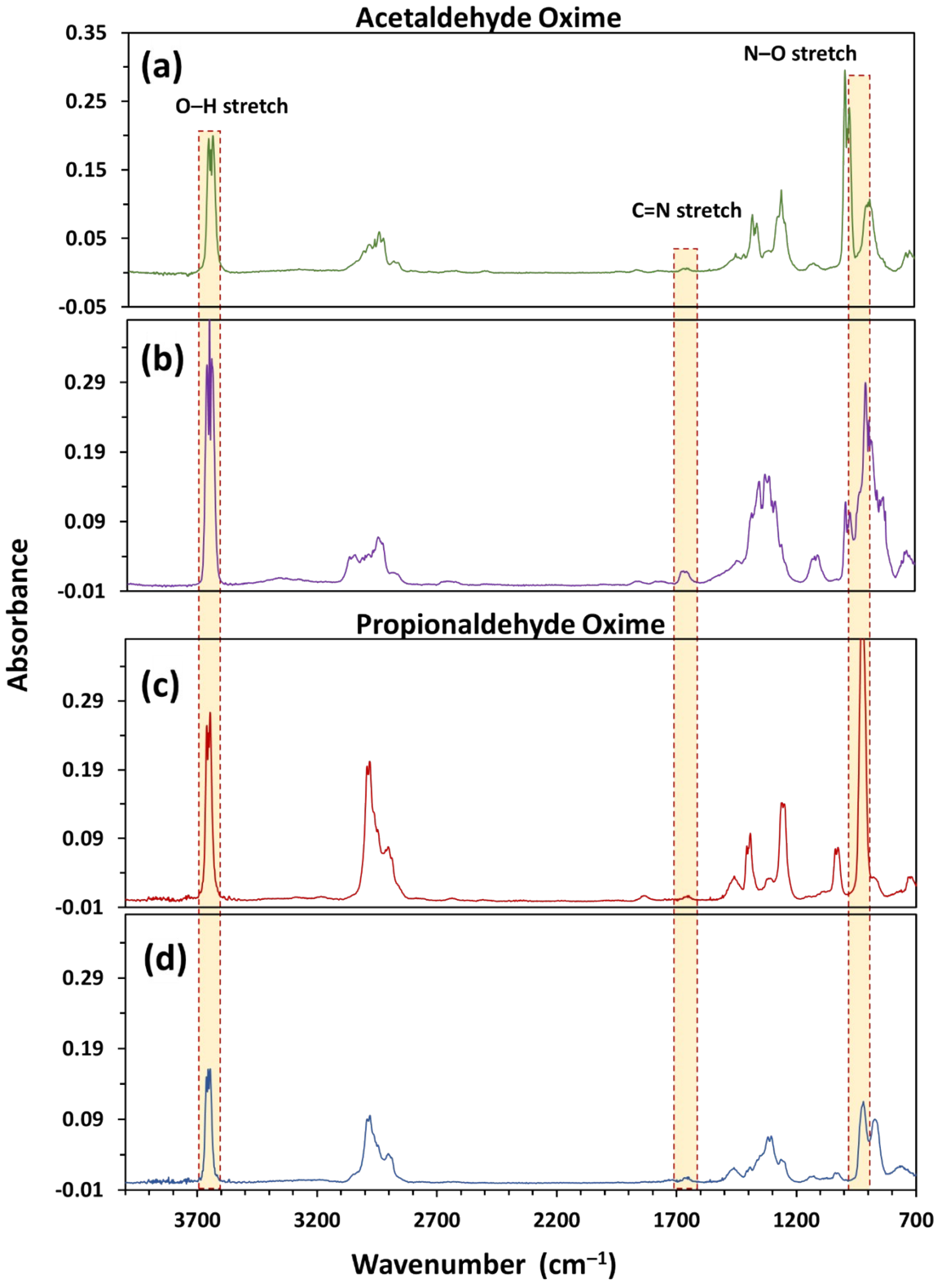

Fig. S3. Infrared spectra corresponding to the two terminal peaks of acetaldehyde oxime (a and b) and propionaldehyde oxime (c and d), demonstrating the differences in fingerprint region and absorption band intensities. Spectra were collected at T = 130 °C with a column flow of 3 mL min^{-1}. The image also shows the three bands characteristic to oximes, namely. O–H (3600 cm^{-1}), C–N (1665 cm^{-1}) and N–O (945 cm^{-1}). a and c correspond to the isomer which elutes first and b and d to the later eluting isomer for each compound.

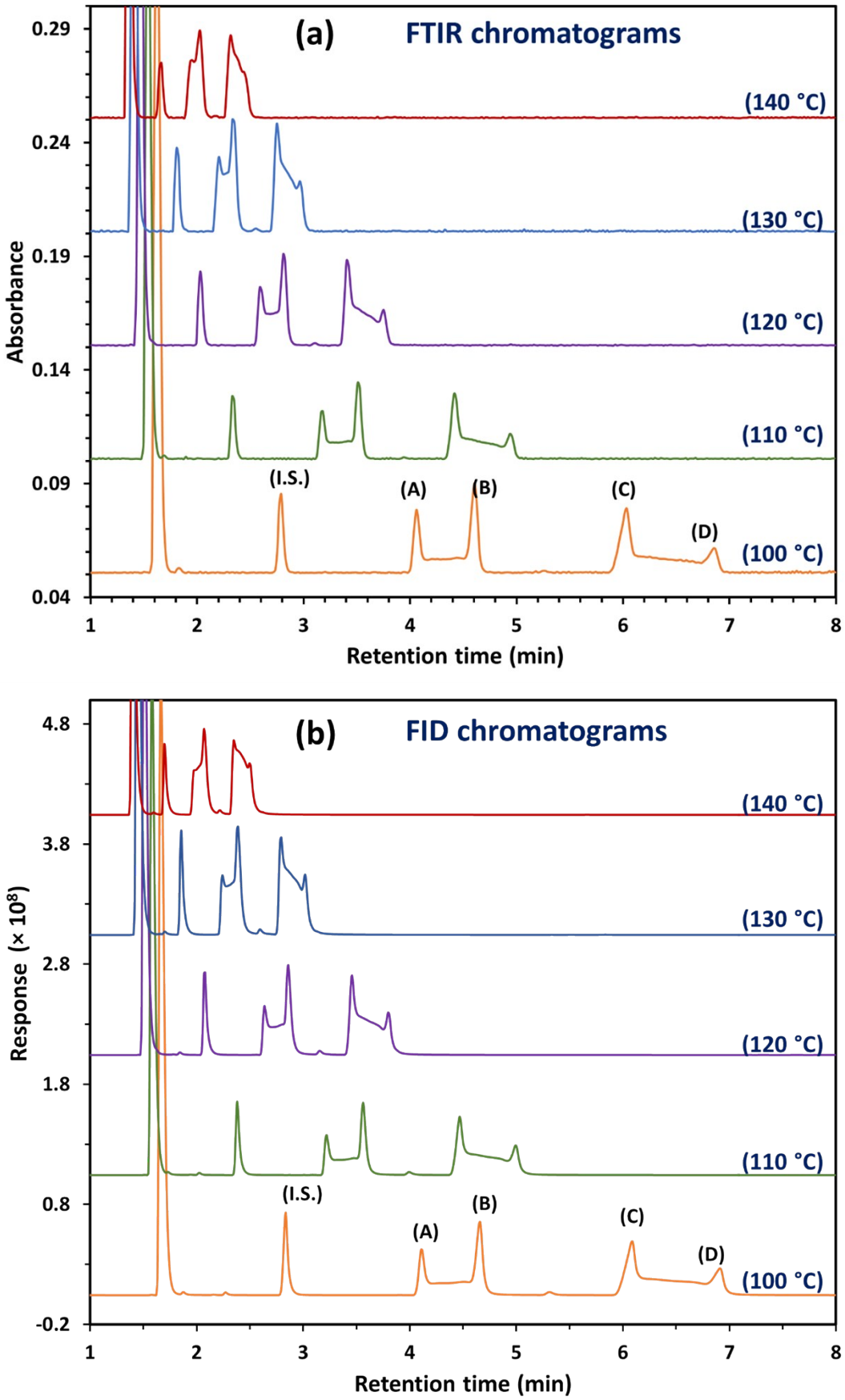

Fig. S4. GC–FTIR and GC–FID chromatograms of acetaldehyde oxime (A and B) and propionaldehyde (C and D) oxime isomer mixes at isothermal oven *T* of 100 °C, 110 °C, 120 °C, 130 °C and 140 °C. I.S.; Internal standard. Light-pipe temperature was maintained at 150 °C.

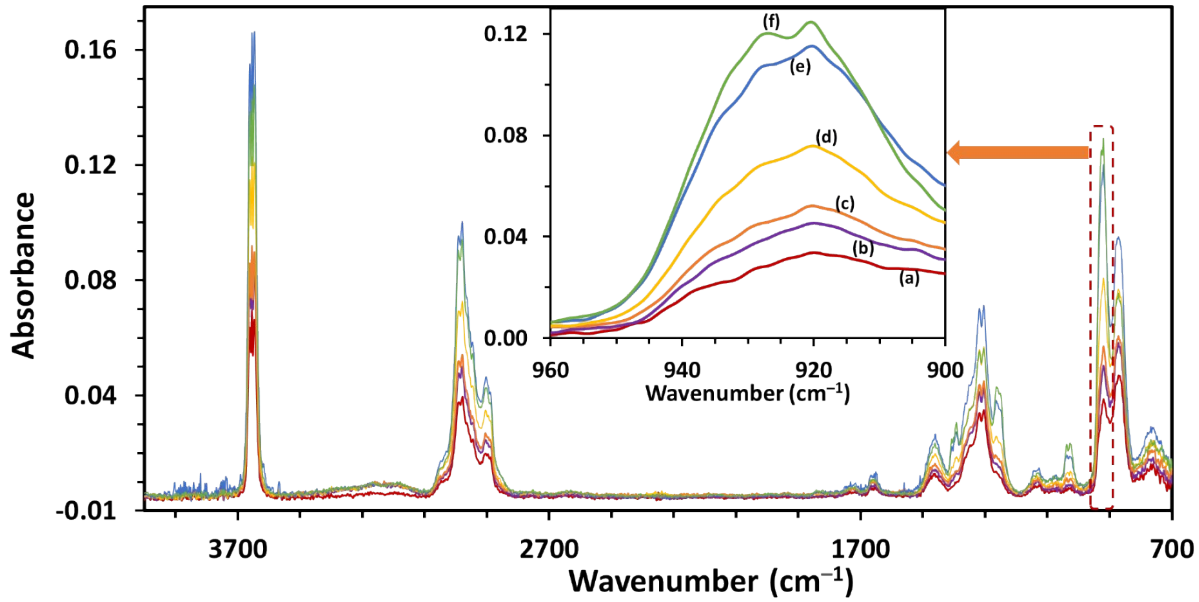

Fig. S5. Propionaldehyde oxime spectra acquired in GC–FTIR analyses with increasing isothermal temperatures of (a) 90 °C, (b) 100 °C, (c) 110 °C, (d) 120 °C, (e) 130 °C and (f) 140 °C, at a light-pipe temperature of 150 °C and column flow of 3.0 mL min^{-1}. Increased intensity of absorption bands is observed with increase in oven temperature.