Supporting Information

Optimization of Carbon-11-Carboxylate Exchange of α-Amino Acids

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1. Methodology

TE: Trapping efficiency
Decay corrected radioactivity in crude reaction mixture after He bubbling / total activity delivered to -180 ºC CO_2 trap × 100%

RCC: Radiochemical conversion
Determined by radioHPLC, fraction of integrated desired product relative all peaks, decay-corrected

RCY: Radiochemical yield
The product of TE and RCY

Analytical HPLC Method:
HPLC samples were analyzed using a Waters 2695 Alliance HPLC module with a Phenomenex Aqua C18 column (4.6 × 250 mm, 5 μm, 125 Å) and a two-component mobile phase (A – 0.1 M AMF + 1% TFA, B – ACN) with a gradient (0–4 minutes: 100% A, 4-8 minutes: from 100% to 20% A, 8-10 minutes: 20% A).

Preparative HPLC Method:
HPLC was performed onboard a Synthra MeIPlus research module with a Phenomenex Synergi Hydro-RP column (4.6 × 250 mm, 10 μm, 80 Å) and a two-component mobile phase (A – 0.1 M AMF + 1% TFA, B – ACN) with a gradient (0–2 minutes: 95% A, 2-8 minutes from 95% to 5% A, 8-12 minutes: 5% A).

2. Imine Stability

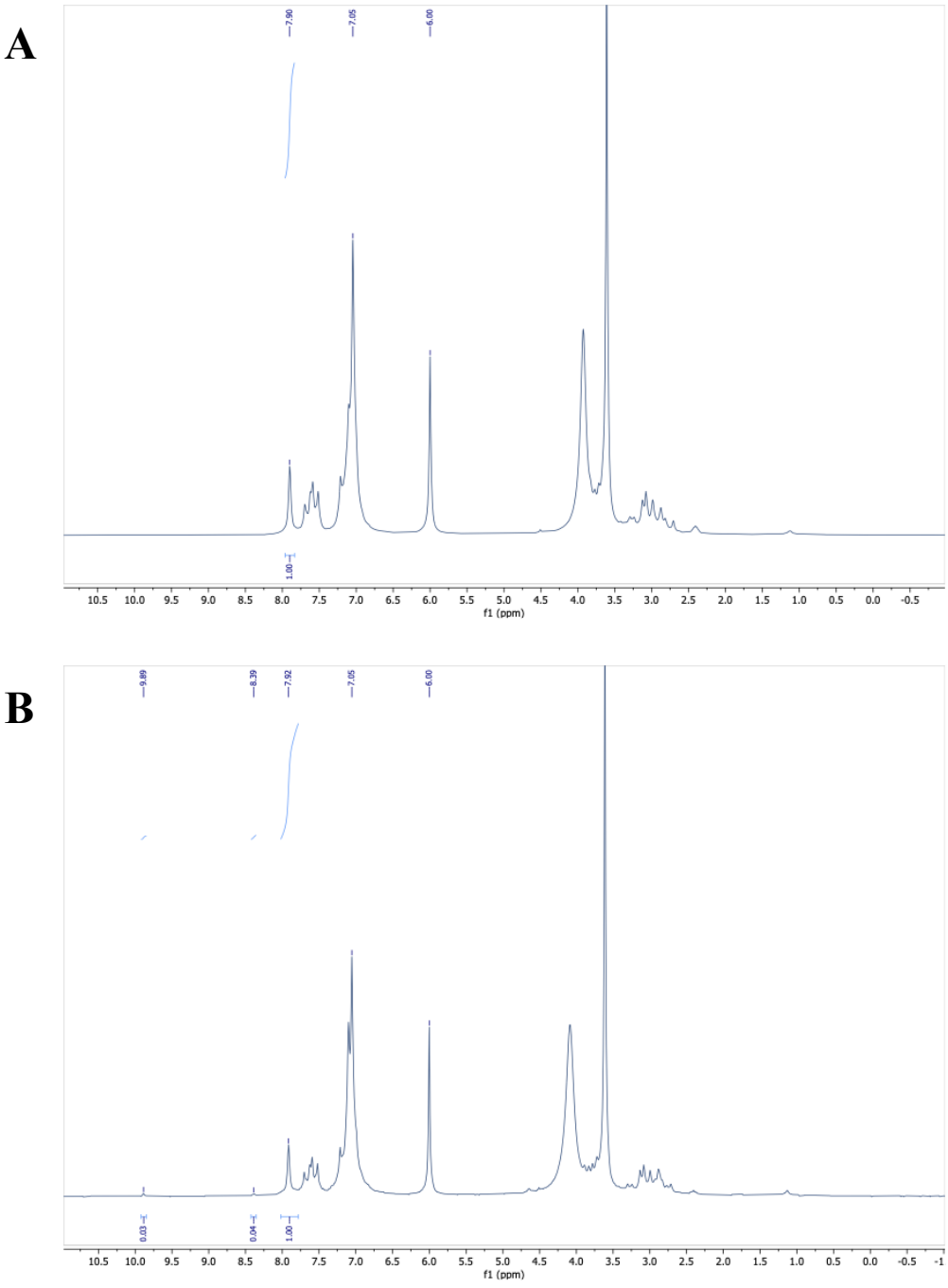


Figure S1. Stability tests with 4-fluorobenzaldehyde. *(a) ^{1}H-NMR of imine. (b) ^{1}H-NMR of imine after reaction conditions*.

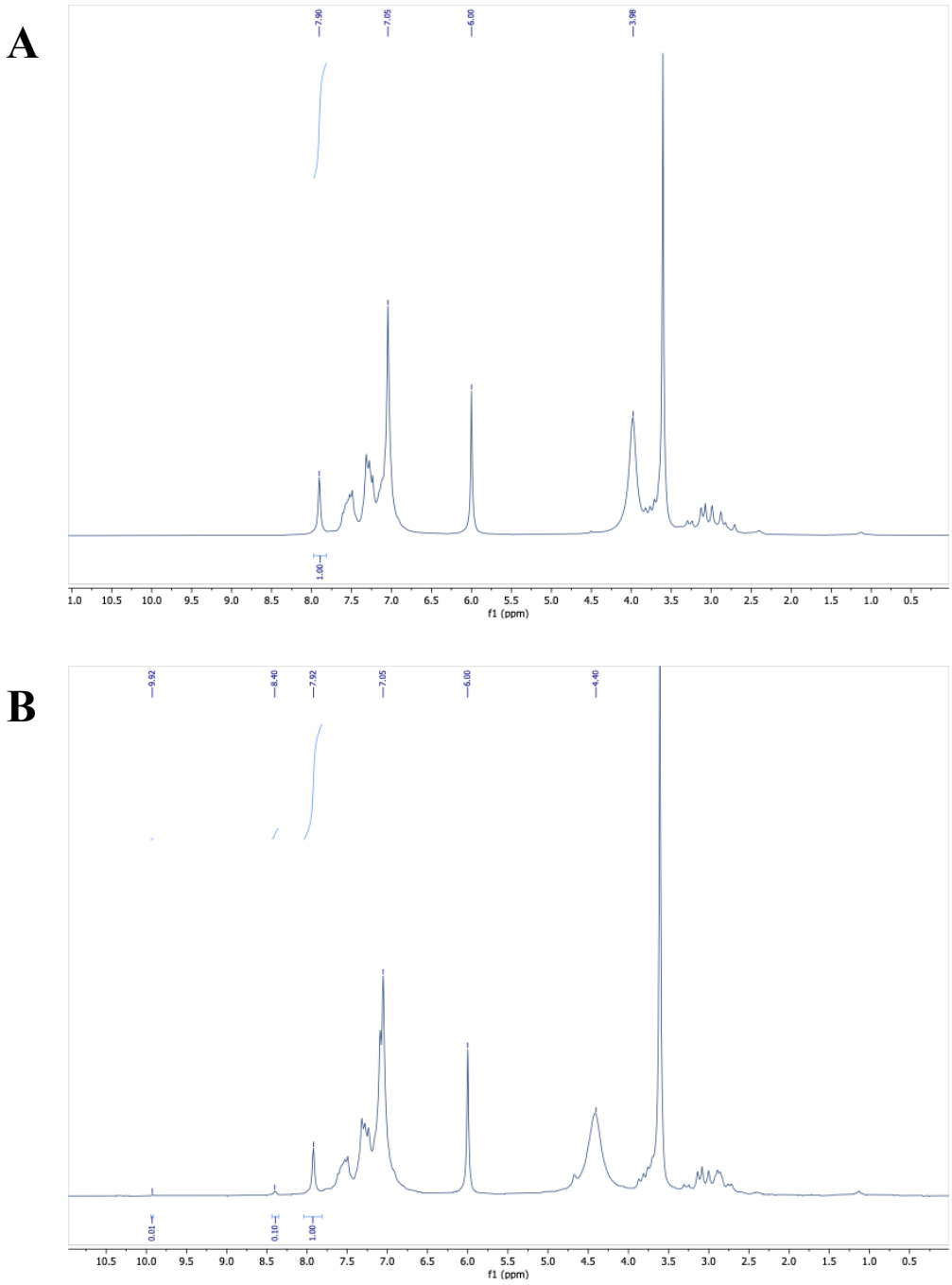


Figure S2. Stability tests with benzaldehyde. *(a) ^{1}H-NMR of imine. (b) ^{1}H-NMR of imine after reaction conditions*.

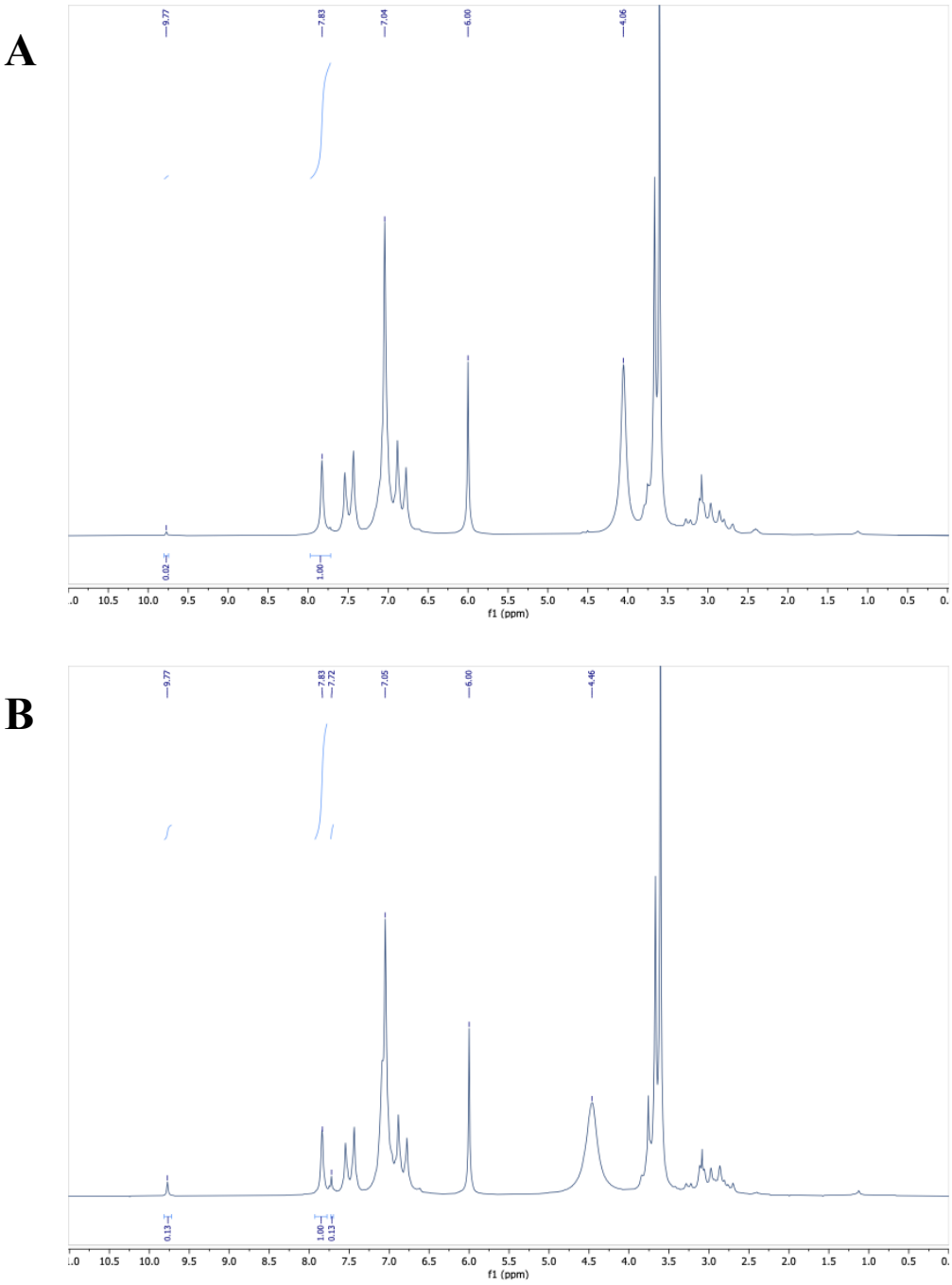


Figure S3. Stability tests with 4-methoxybenzaldehyde. *(a) ^{1}H-NMR of imine. (b) ^{1}H-NMR of imine after reaction conditions*.

3. Chiral Catalyst

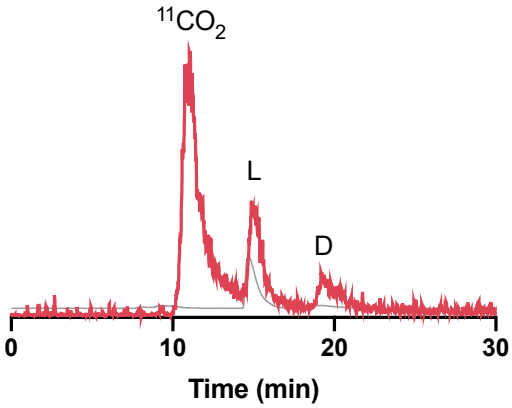


Figure S4. L- and D-[^{11}C]phenylalanine with partial L-enrichment. *Red is γ, grey is UV.*

4. Chiral Resolution

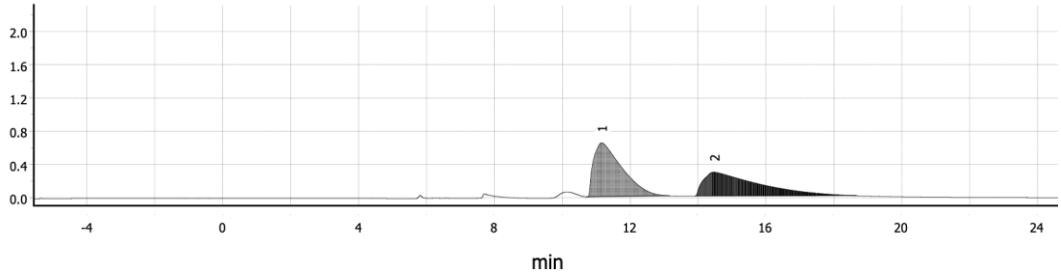


Figure S5. Preparative resolution of L- and D-leucine.

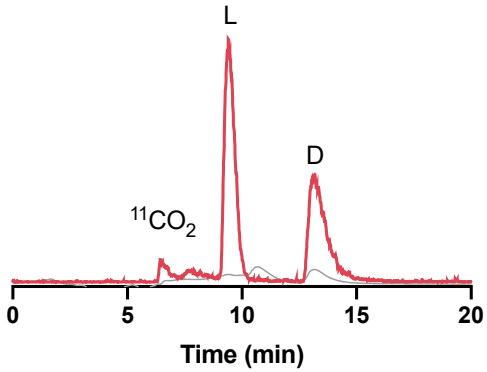


Figure S6. Analytical resolution of $^{11}CO_2$, L- and D-[^{11}C]leucine. *Red is γ, grey is UV.*

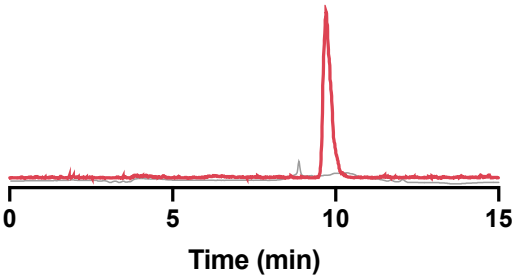
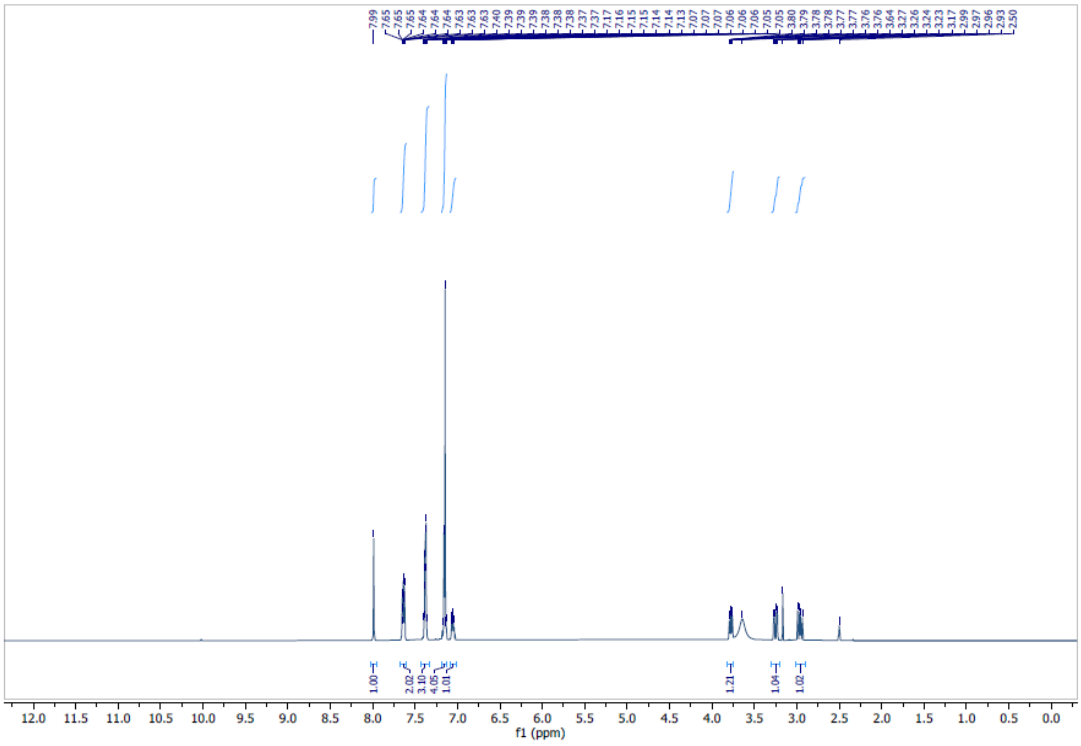
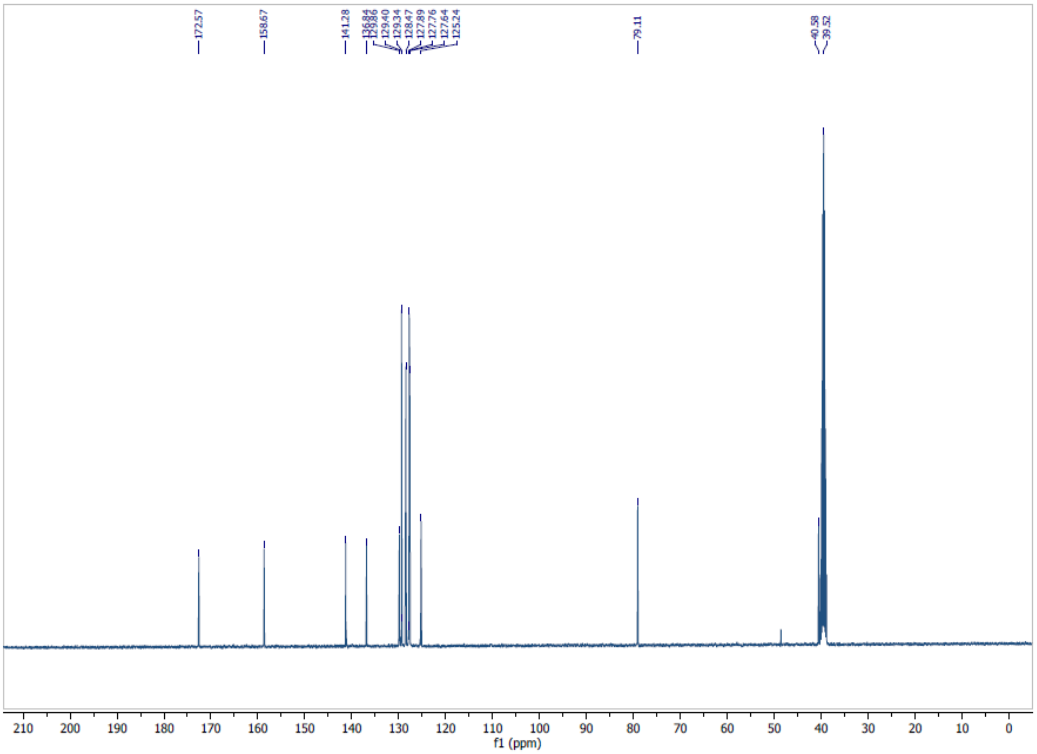


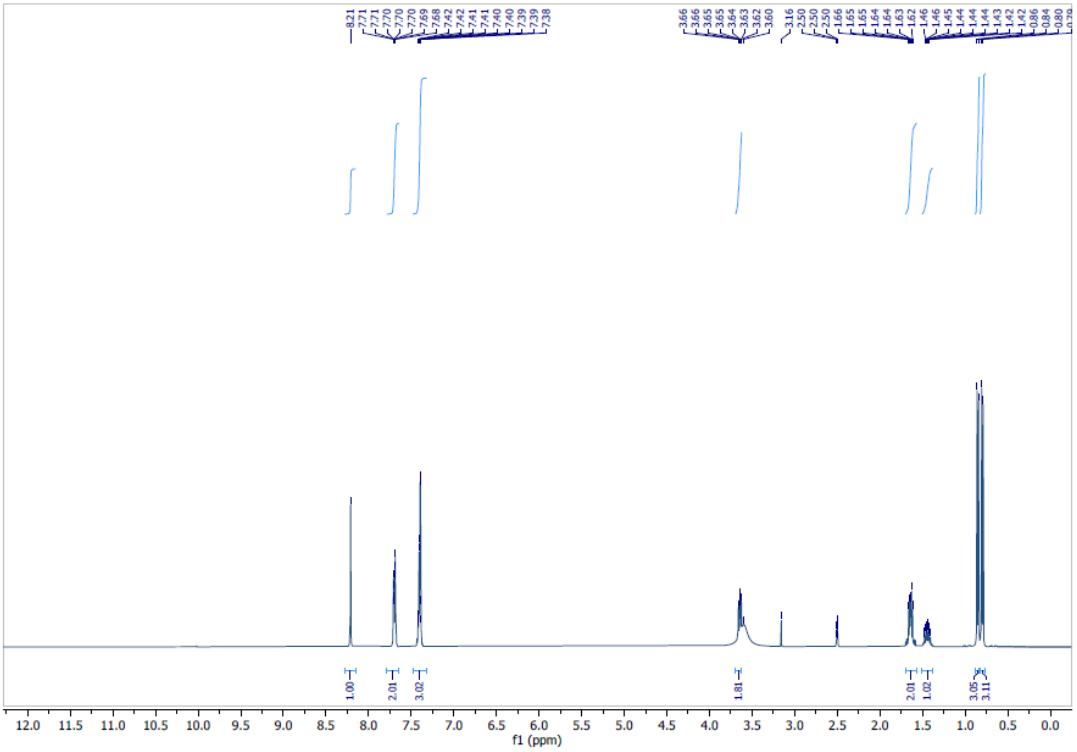
Figure S7. Isolation of [^{11}C]leucine. *Red is γ, grey is UV.***Representative NMRs**

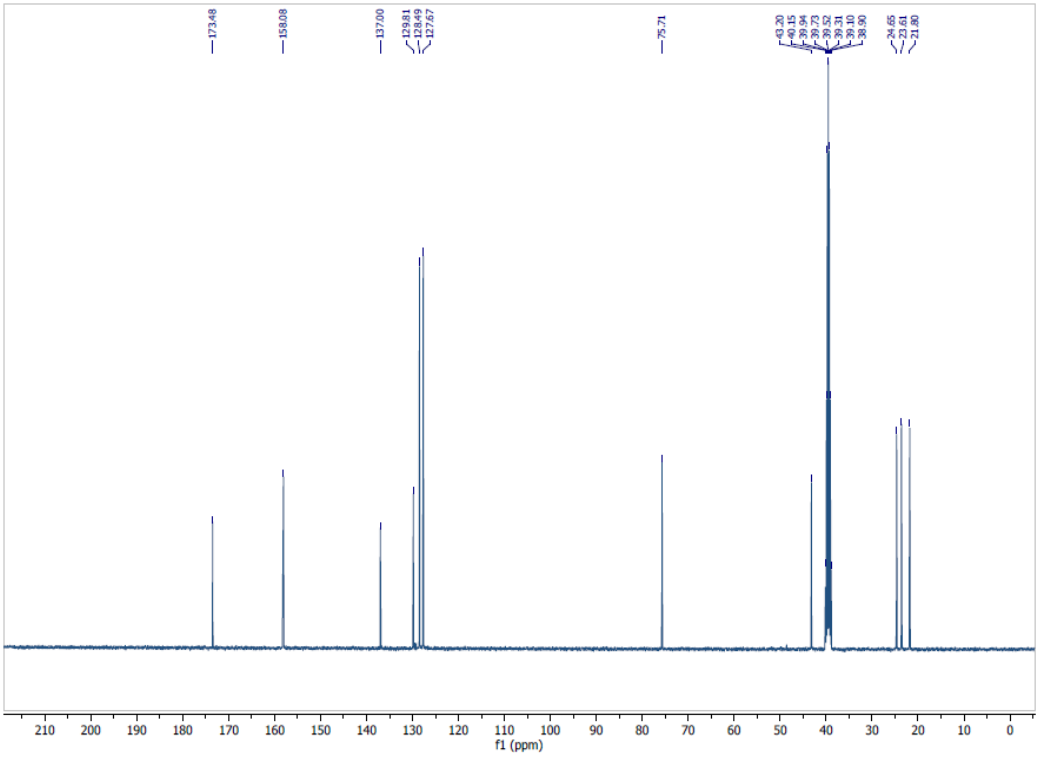
Benzaldehyde w/ Phe:


f1 (ppm)

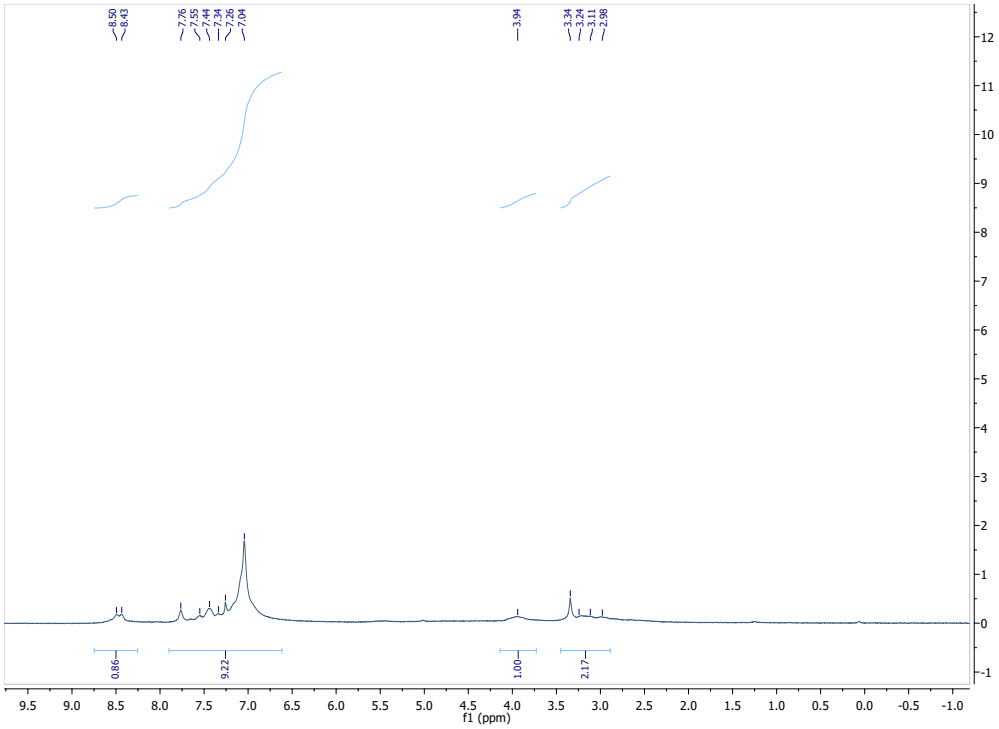

f1 (ppm)

Benzaldehyde w/ Leu:

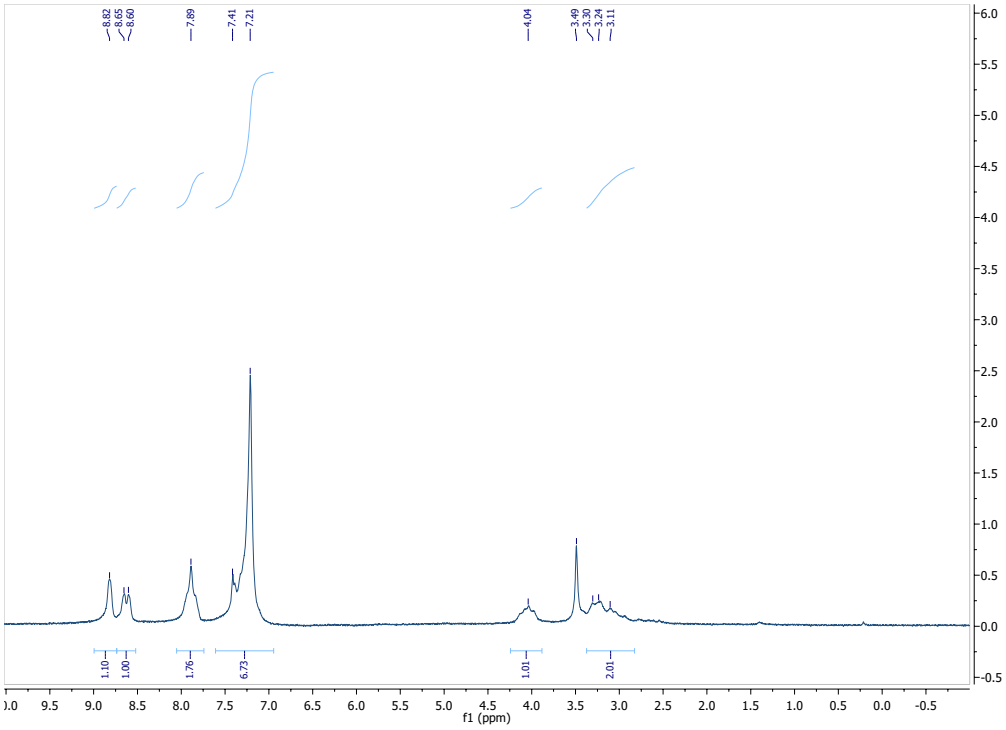




2-Pyridinecarboxaldehyde w/ Phe:



3-Pyridinecarboxaldehyde w/ Phe:



2-Phenylbenzaldehyde w/ Phe: