Supplementary Materials: Design of Iridium N-Heterocyclic Carbene Amino Acid Catalysts for Asymmetric Transfer Hydrogenation of Aryl Ketones

Chad M. Bernier and Joseph S. Merola*

1. X-Ray Crystallographic Structure of $Ir(IMe)_2(Gly)(H)(I)$

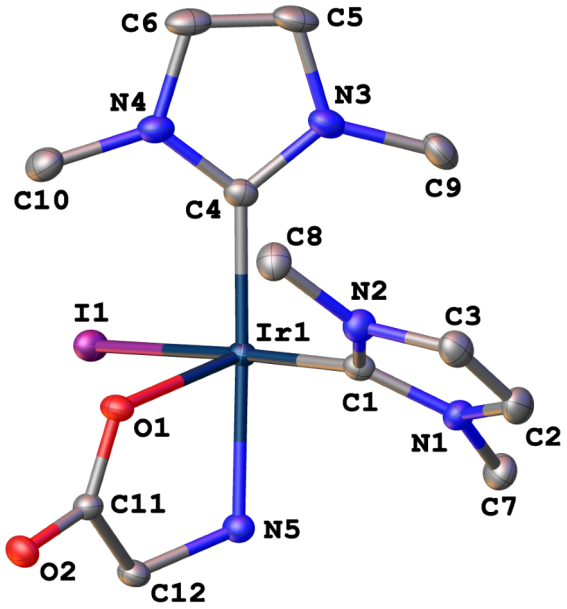

Figure S1. Displacement ellipsoid plot (50% probability) of $Ir(IMe)_2(Gly)(H)(I)$ (CSD 2062242). Hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths and angles from the structure of $Ir(IMe)_2(Gly)(H)(I)$ obtained by single-crystal X-ray diffraction.

Atoms	Bond lengths (Å)
Ir1–C1	1.986
Ir1–C4	2.004
Ir1–O1	2.231
Ir1–N5	2.157
Ir1–I1	2.738
Atoms	**Bond angles (°)**
C1–Ir1–C4	89.39
C1–Ir1–O1	91.49
C1–Ir1–N5	90.53
C4–Ir1–O1	101.52
C4–Ir1–I1	93.28
O1–Ir1–I1	91.60
N5–Ir1–I1	86.85

2. NMR Spectra of Iridium NHC Amino Acid Complexes

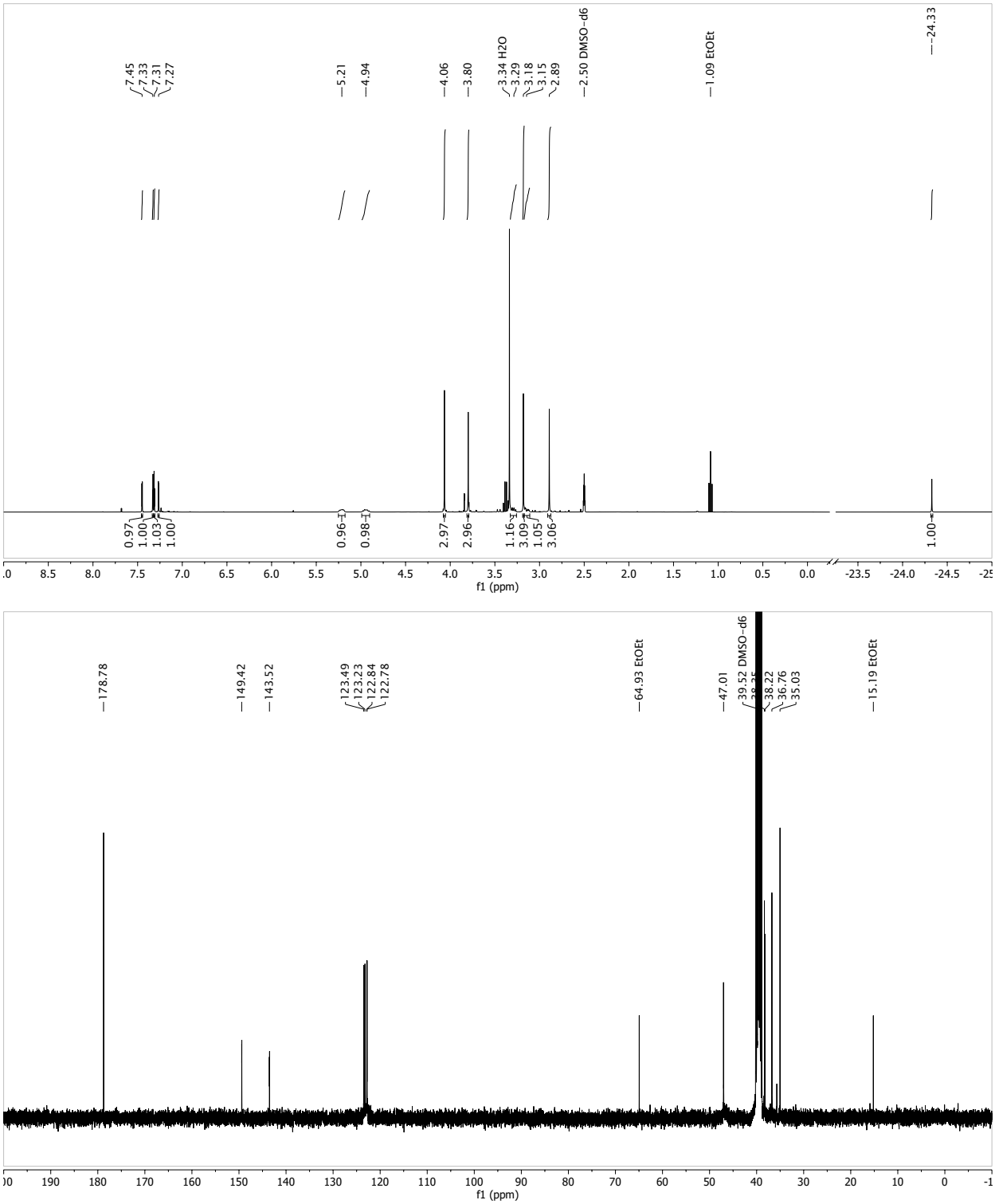

Figure S2. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of Ir(IMe)$_2$(Gly)(H)(I) in DMSO-d_6.

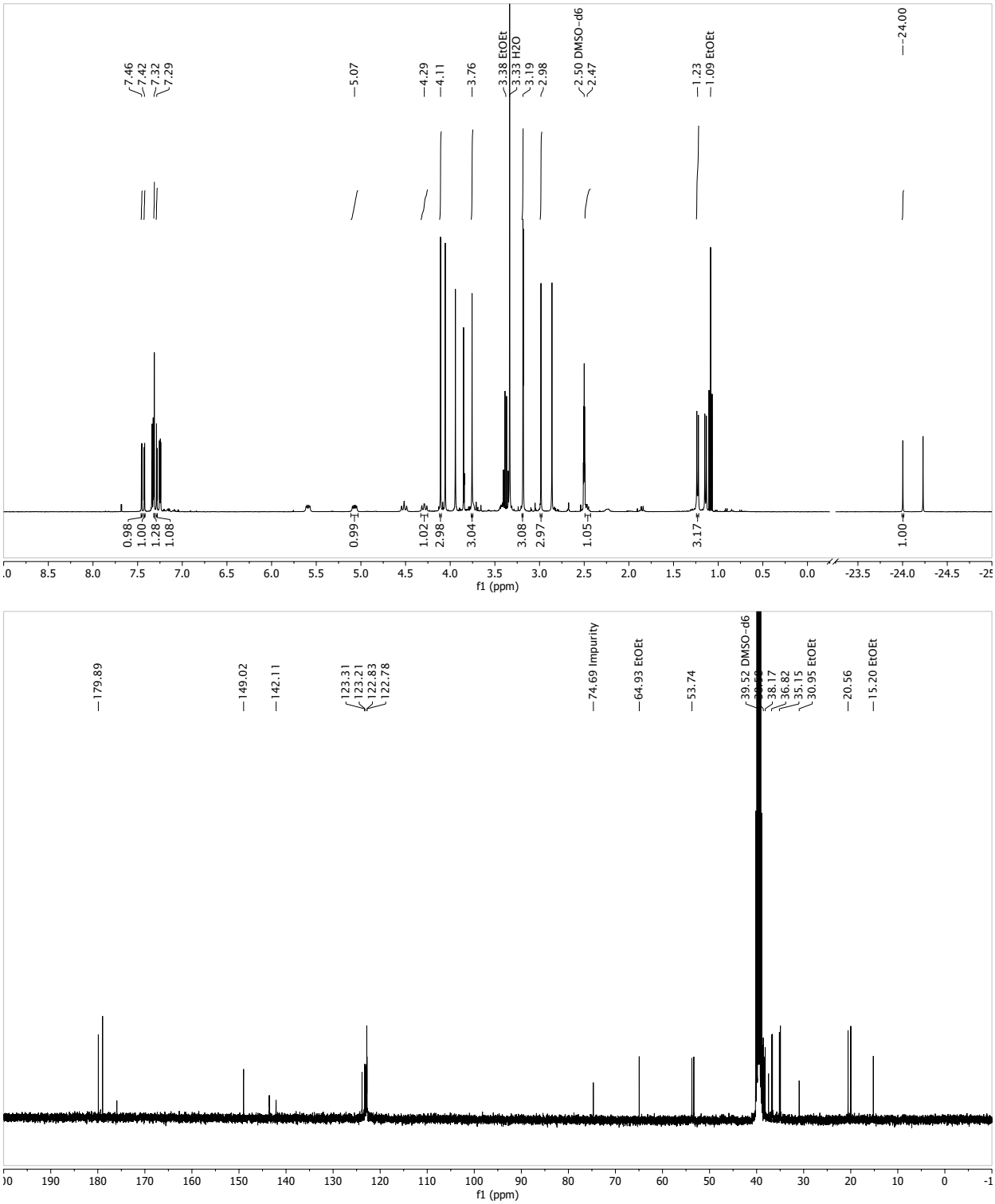

Figure S3. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the major isomer of Ir(IMe)$_2$(L – Ala)(H)(I) in DMSO-d_6.

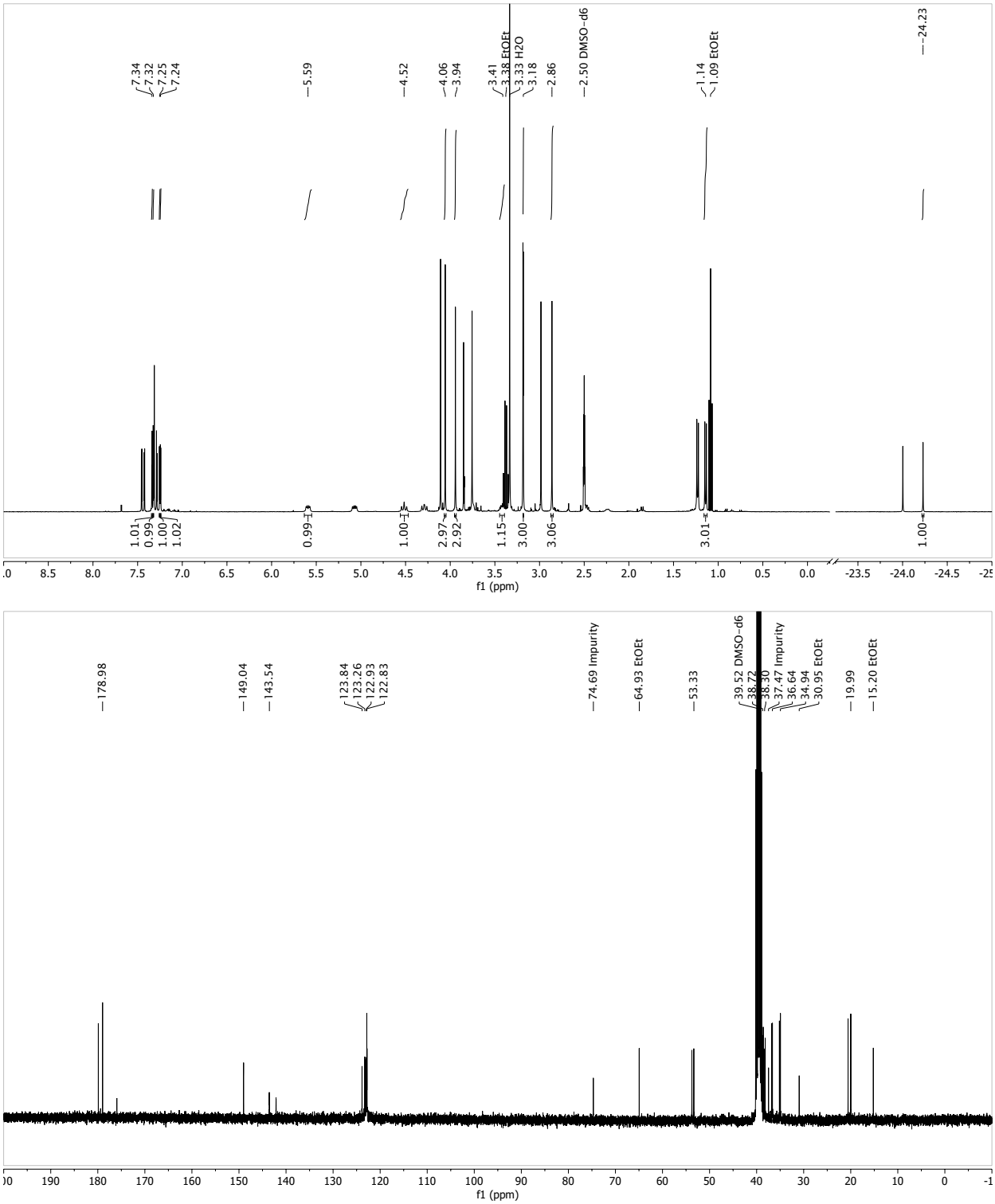

Figure S4. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the minor isomer of Ir(IMe)$_2$(L−Ala)(H)(I) in DMSO-d_6.

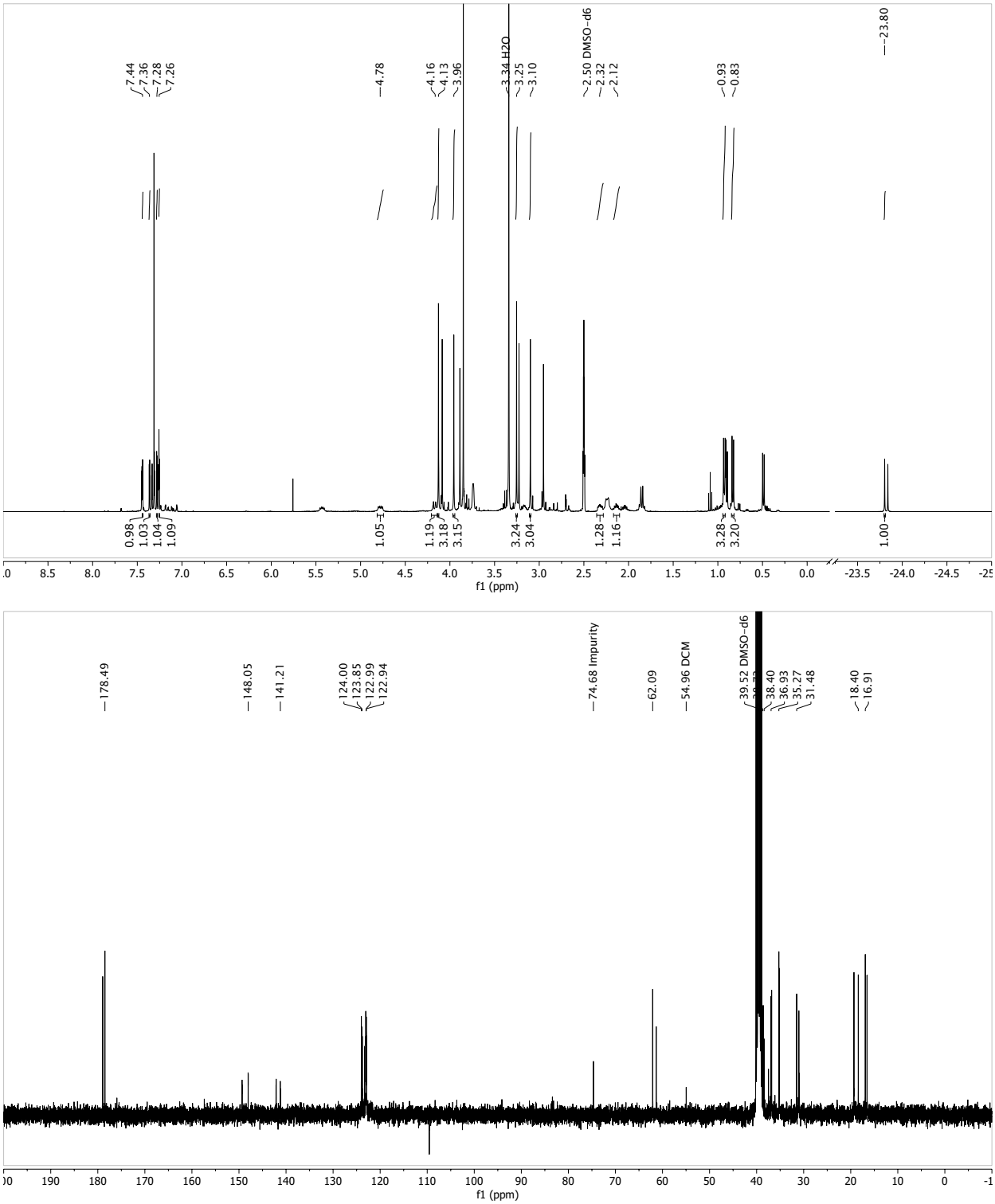

Figure S5. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the major isomer of Ir(IMe)$_2$(L–Val)(H)(I) in DMSO-d_6.

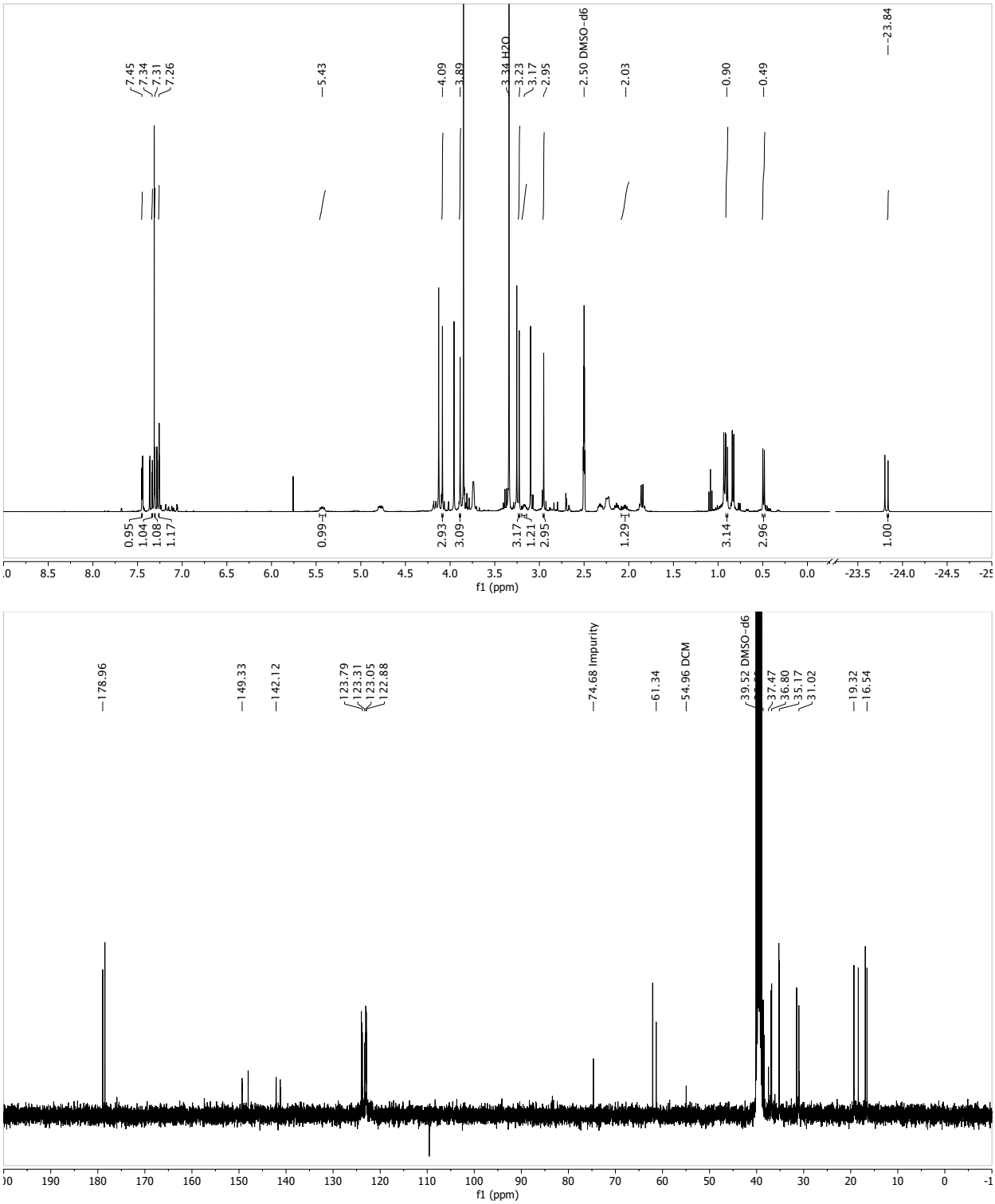

Figure S6. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the minor isomer of Ir(IMe)$_2$(L−Val)(H)(I) in DMSO-d_6.

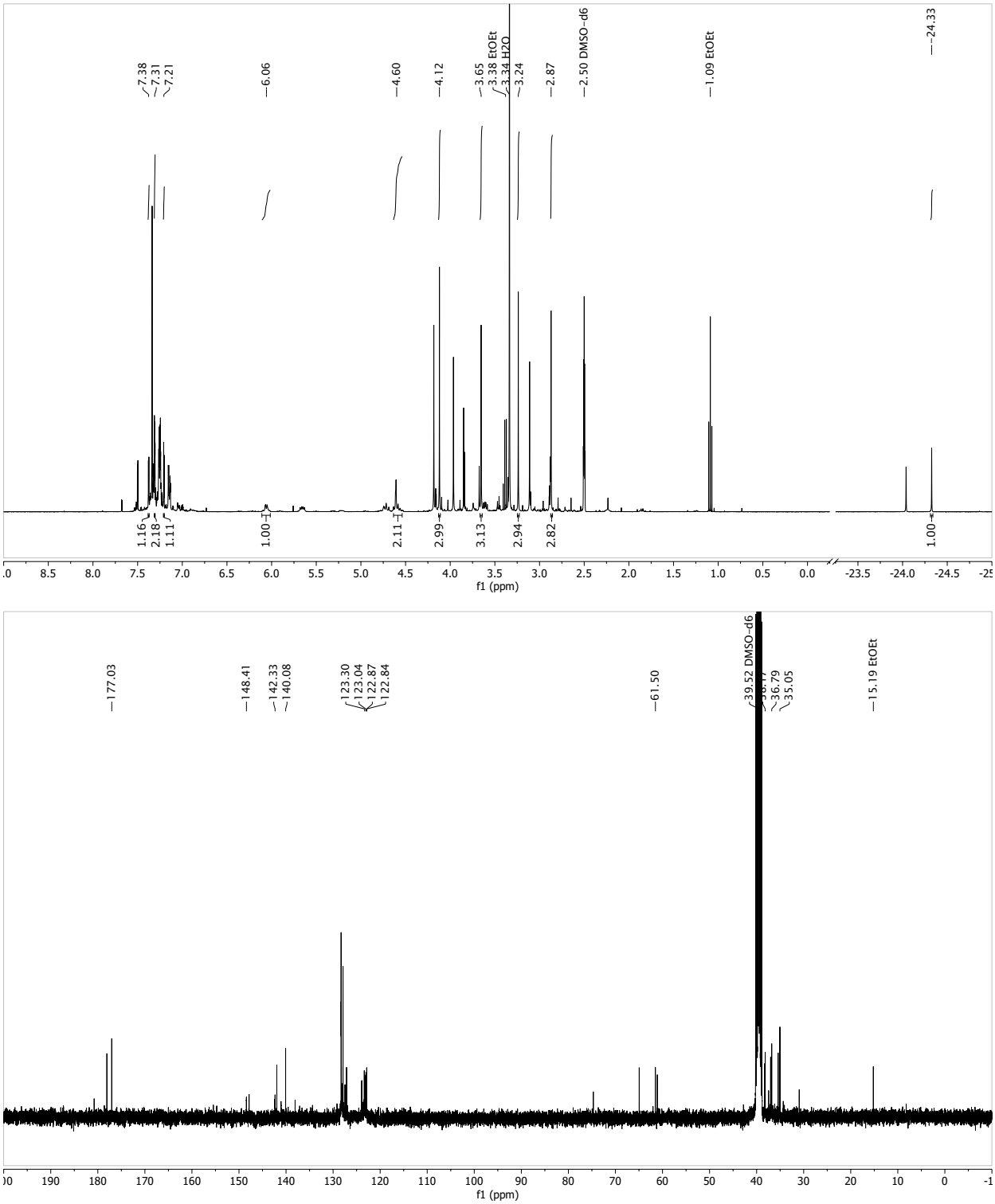

Figure S7. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the major isomer of Ir(IMe)$_2$(L−Phg)(H)(I) in DMSO-d_6.

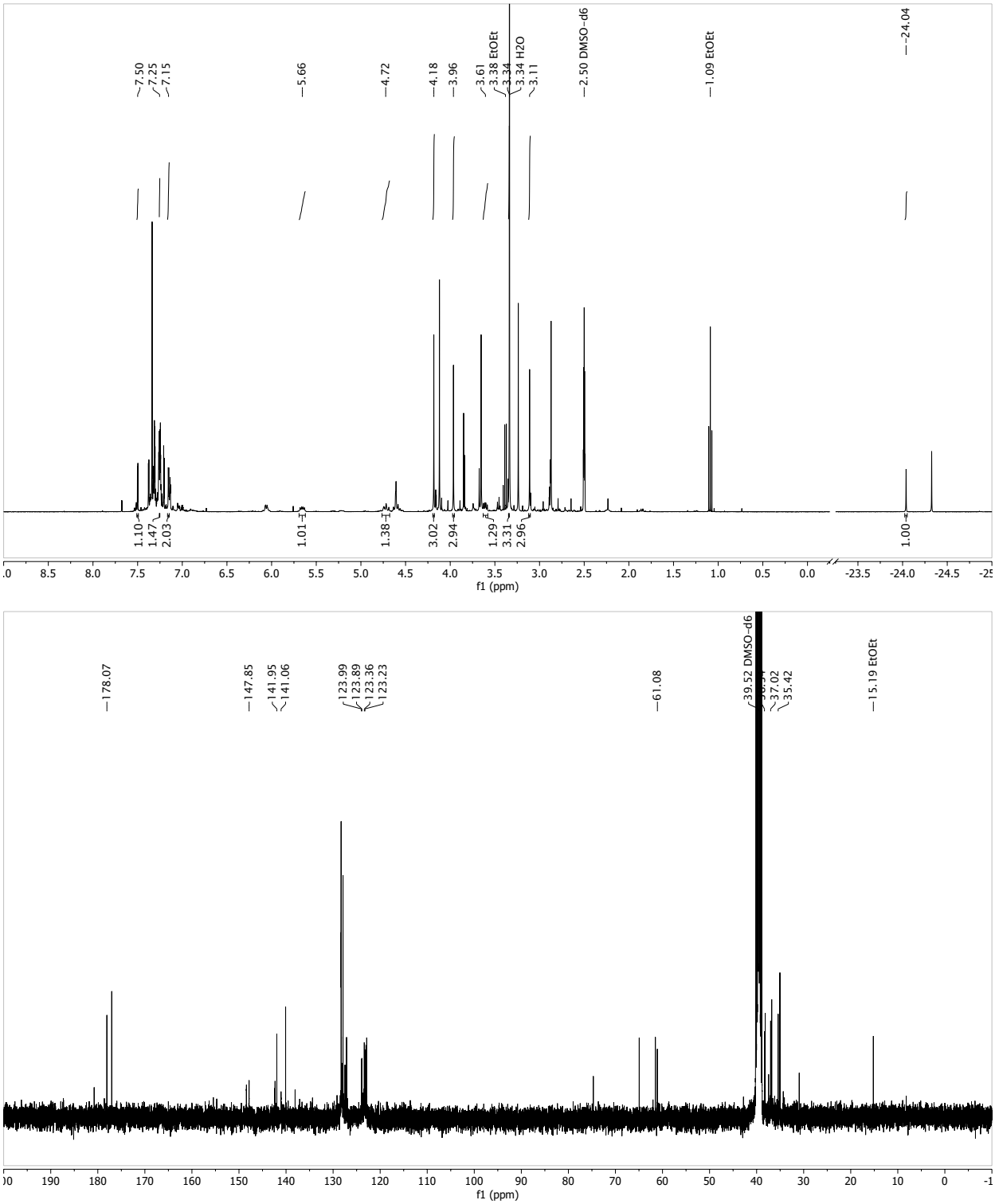

Figure S8. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of the minor isomer of Ir(IMe)$_2$(L−Phg)(H)(I) in DMSO-d_6.

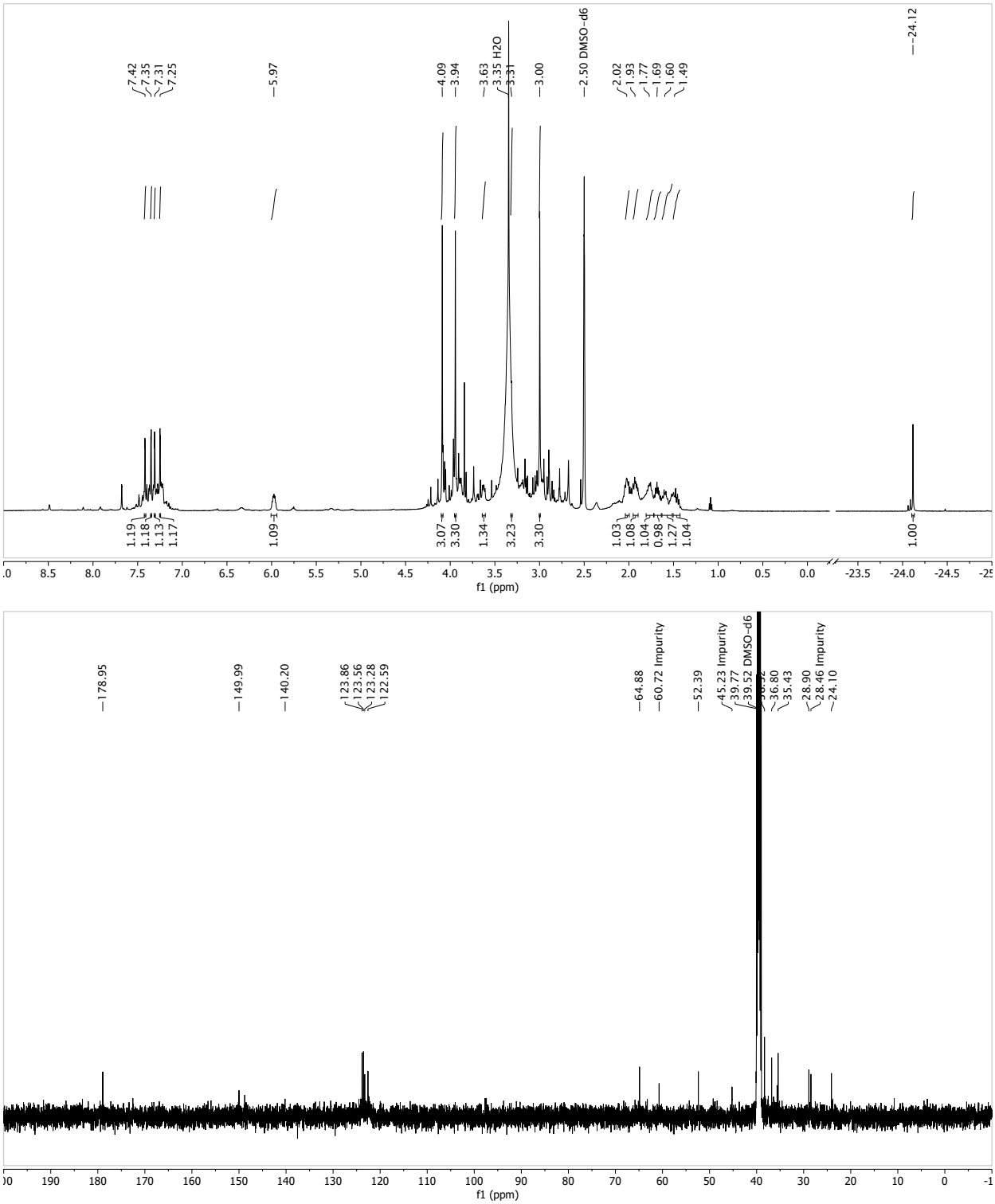

Figure S9. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of Ir(IMe)$_2$(L−Pro)(H)(I) in DMSO-d_6.

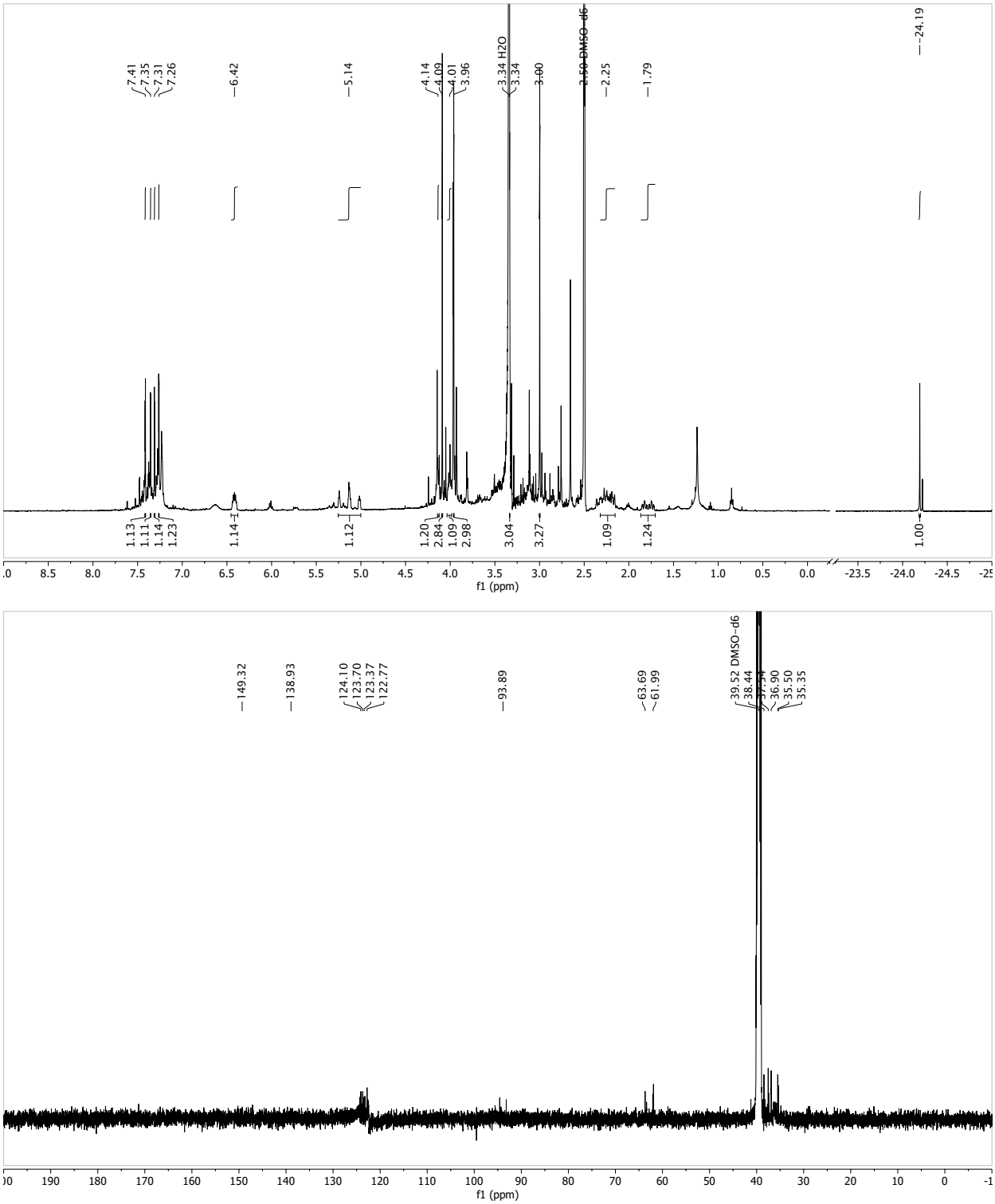

Figure S10. ^{1}H (top, 400 MHz) and ^{13}C (bottom, 101 MHz) NMR spectra of Ir(IMe)$_2$(L–F–Pro)(H)(I) in DMSO-d_6.

3. GC Chromatograms of Alcohol Products from ATH Studies

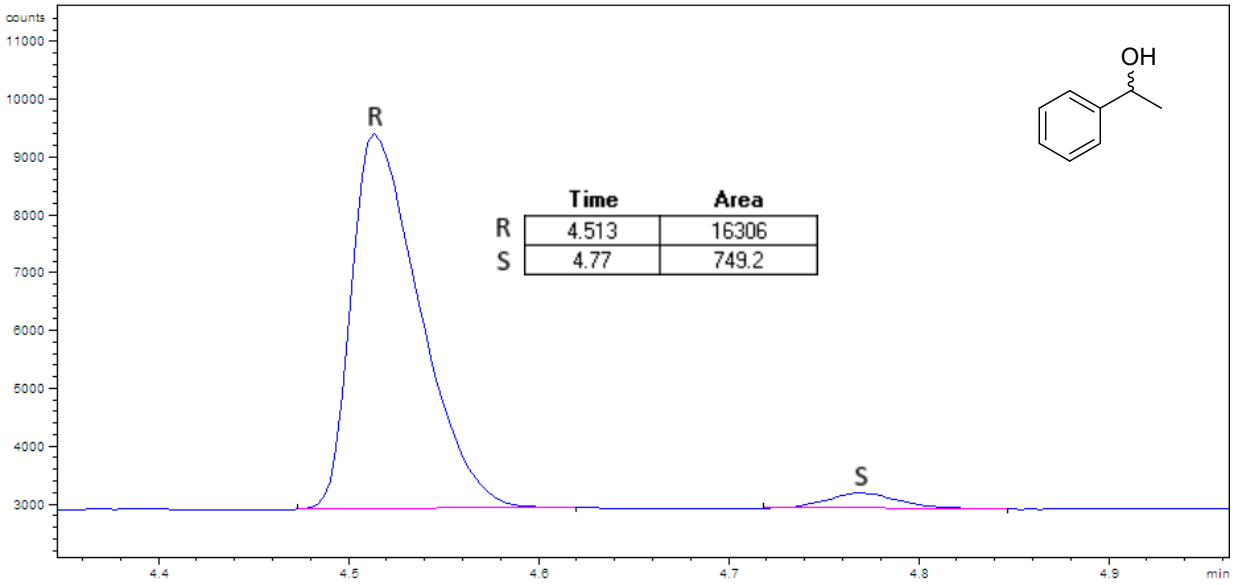

Figure S11. FID trace of 1-phenylethanol (column temp = 130 °C).

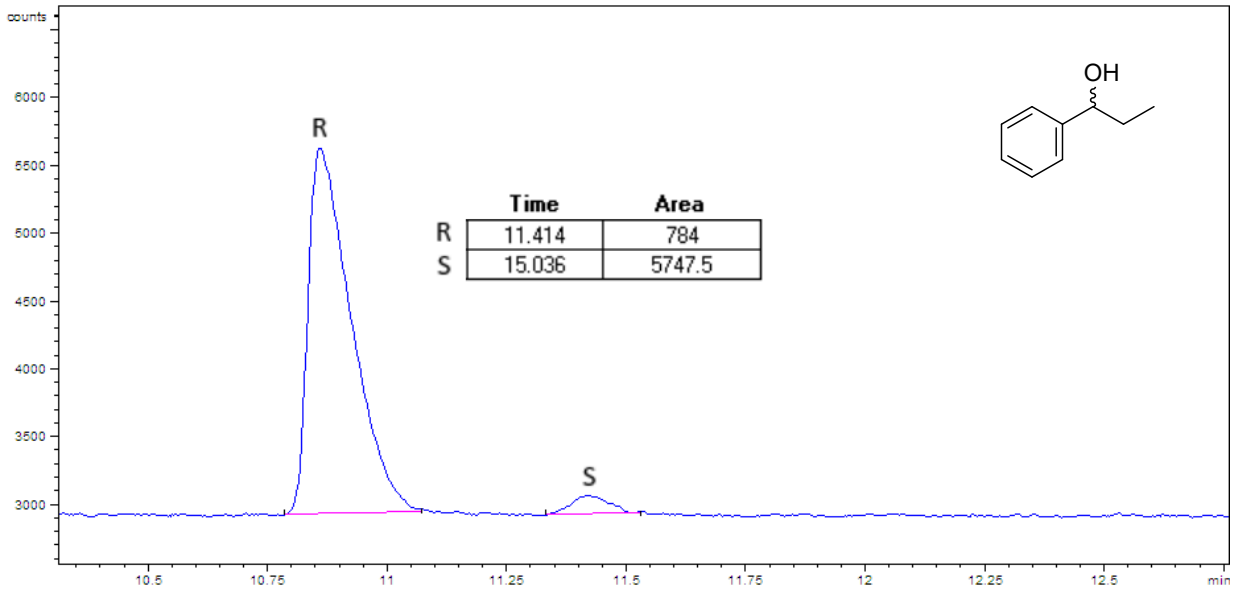

Figure S12. FID trace of 1-phenylpropanol (column temp = 120 °C).

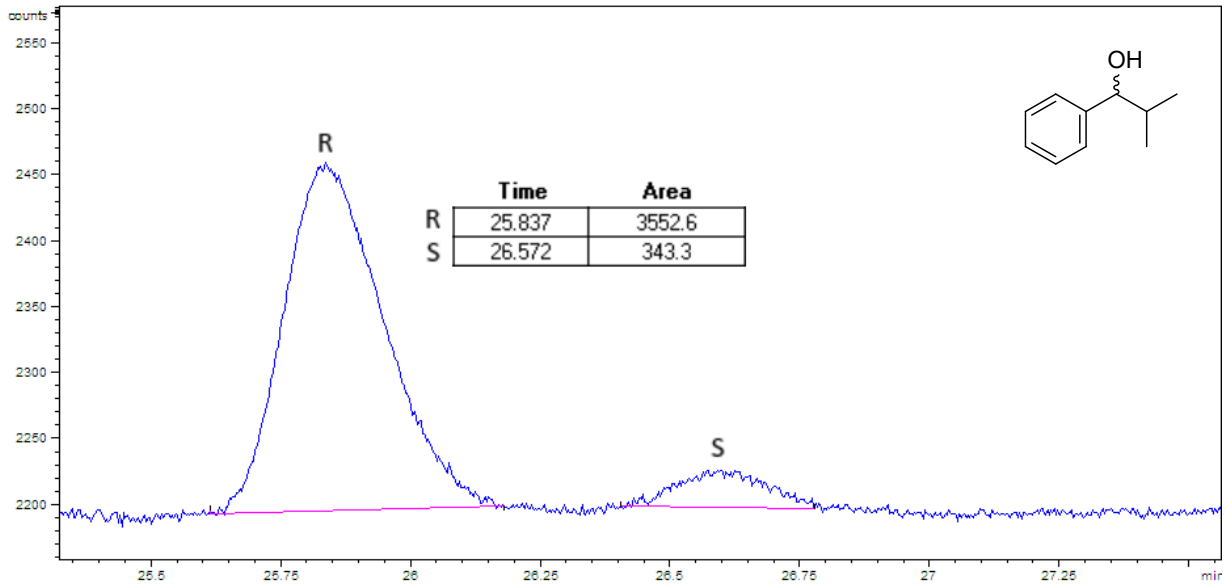

Figure S13. FID trace of 2-methyl-1-phenylpropanol (column temp = 110 °C).

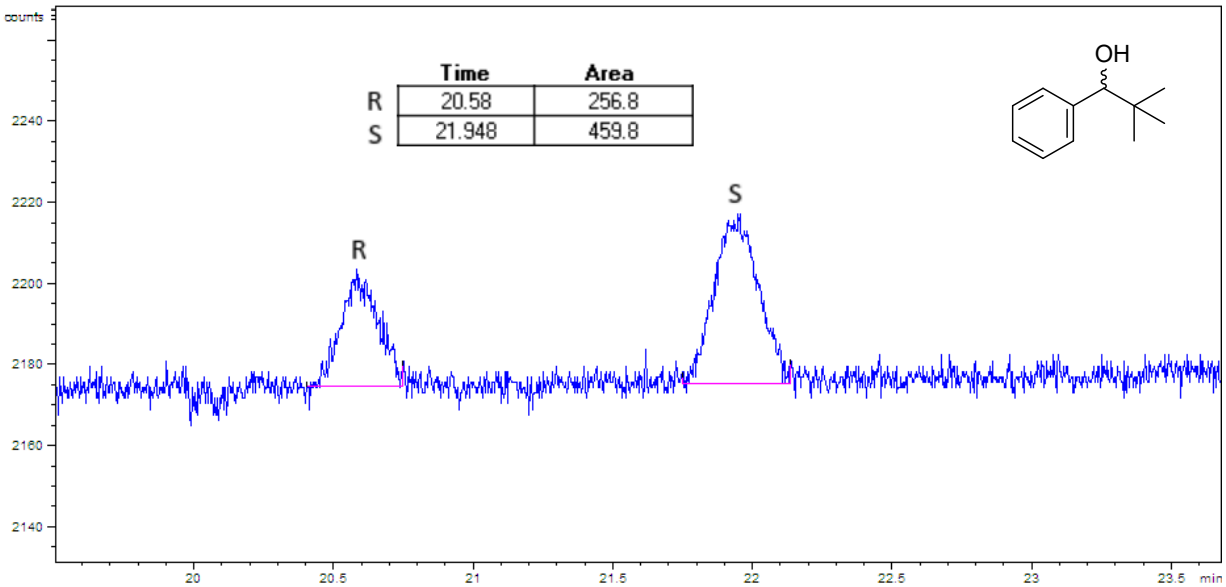

Figure S14. FID trace of 2,2-dimethyl-1-phenylpropanol (column temp = 120 °C).

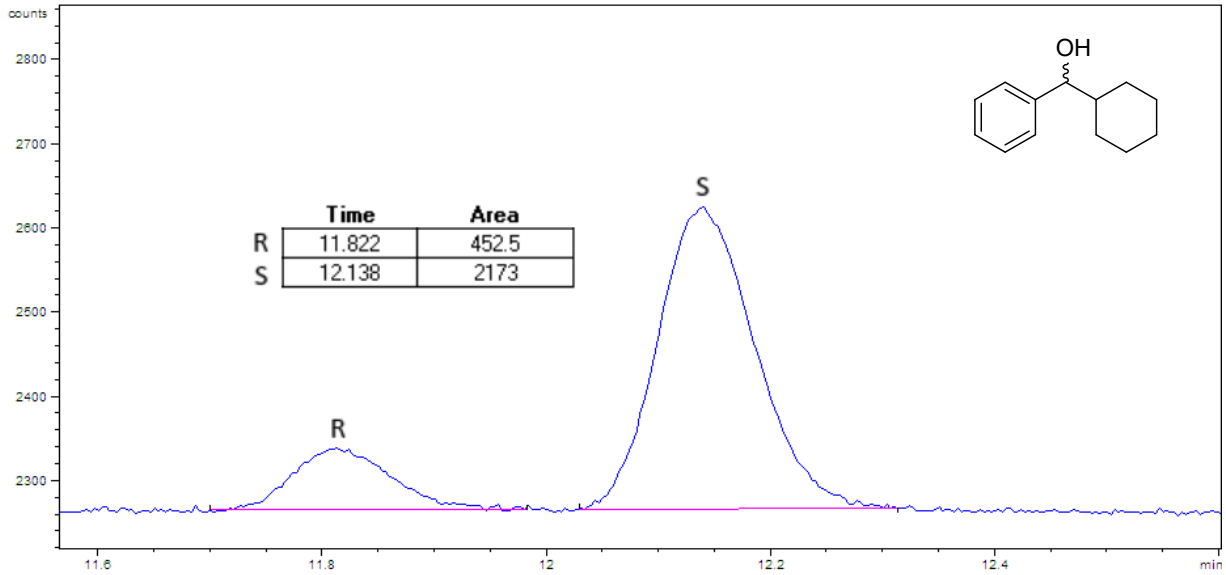

Figure S15. FID trace of cyclohexyl(phenyl)methanol (column temp = 160 °C).

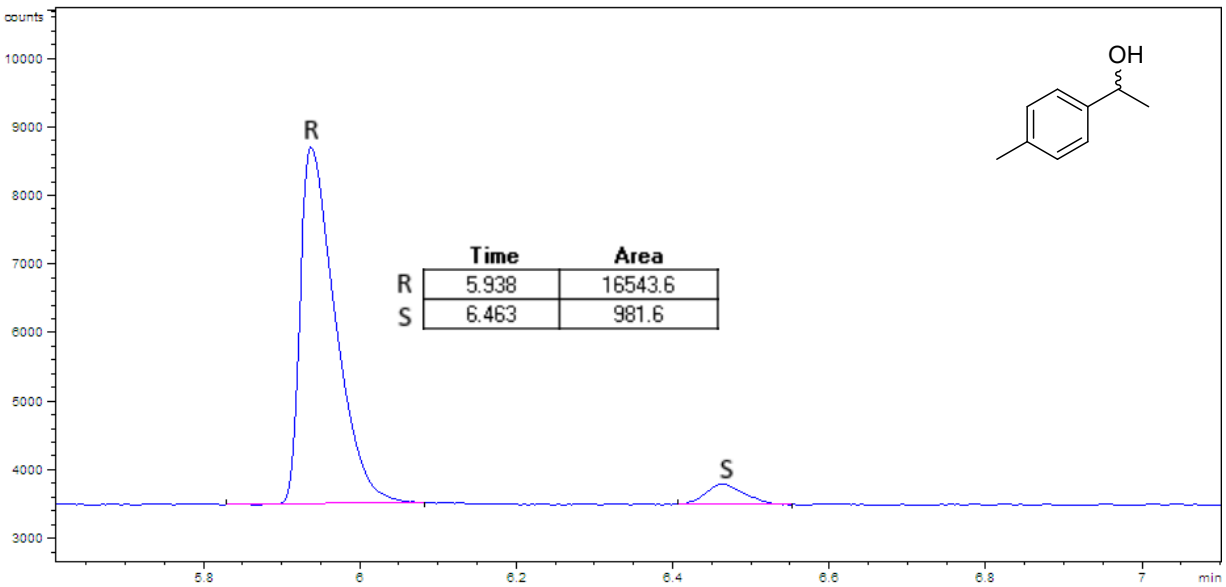

Figure S16. FID trace of 1-(*p*-tolyl)ethanol (column temp = 130 °C).

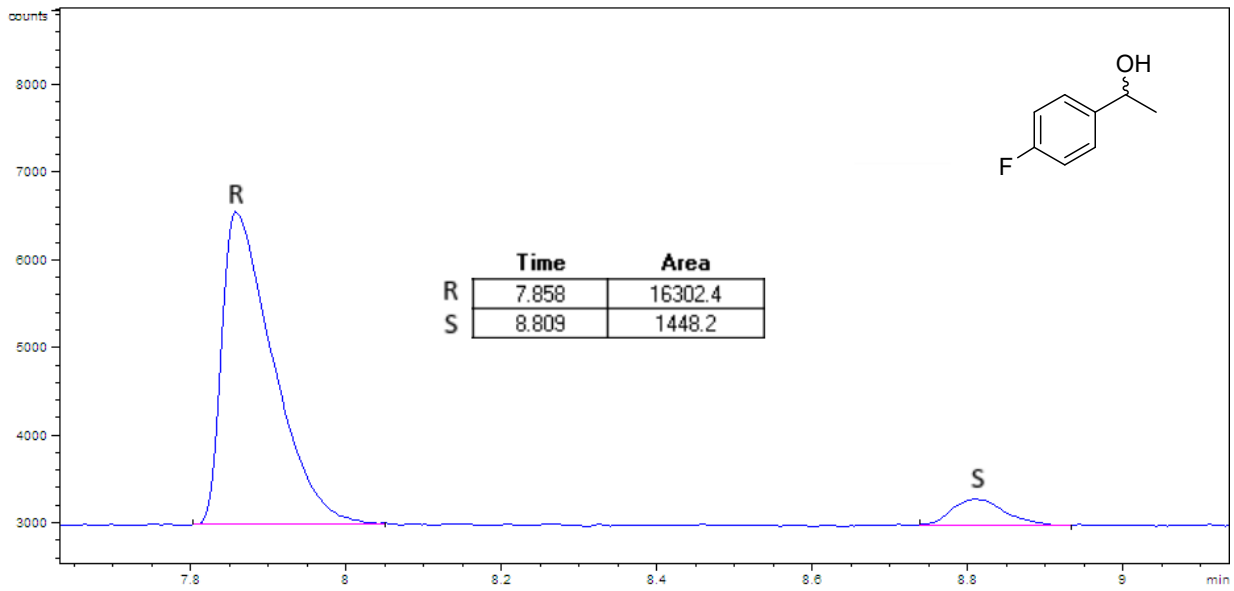

Figure S17. FID trace of 1-(4-fluorophenyl)ethanol (column temp = 120 °C).

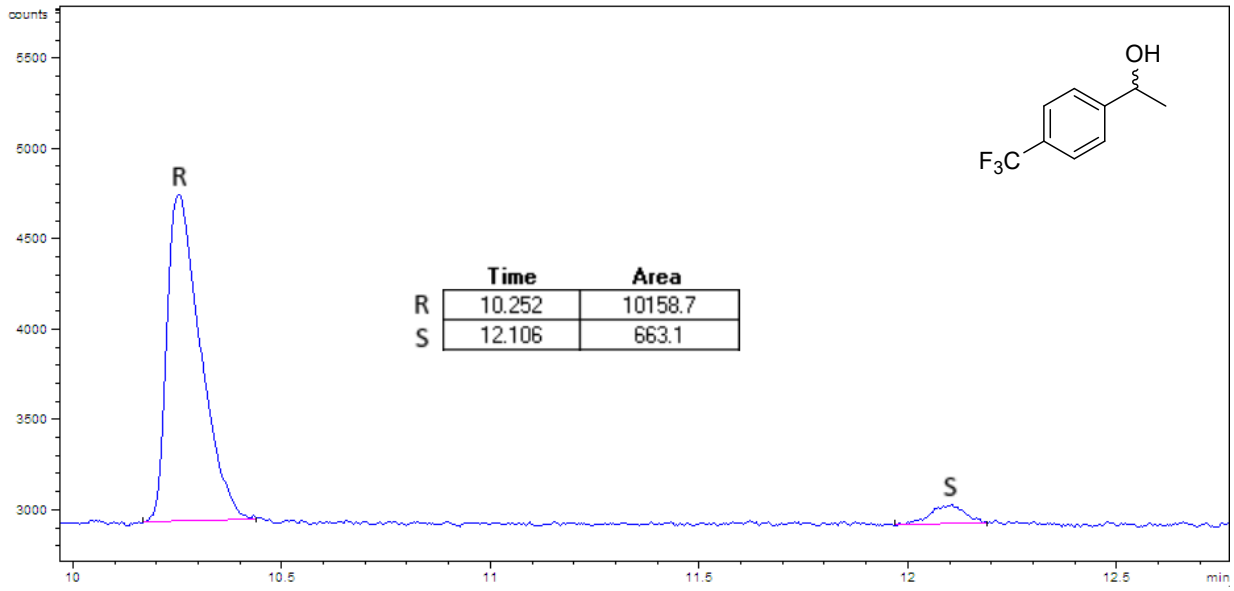

Figure S18. FID trace of 1-(4-(trifluoromethyl)phenyl)ethanol (column temp = 120 °C).

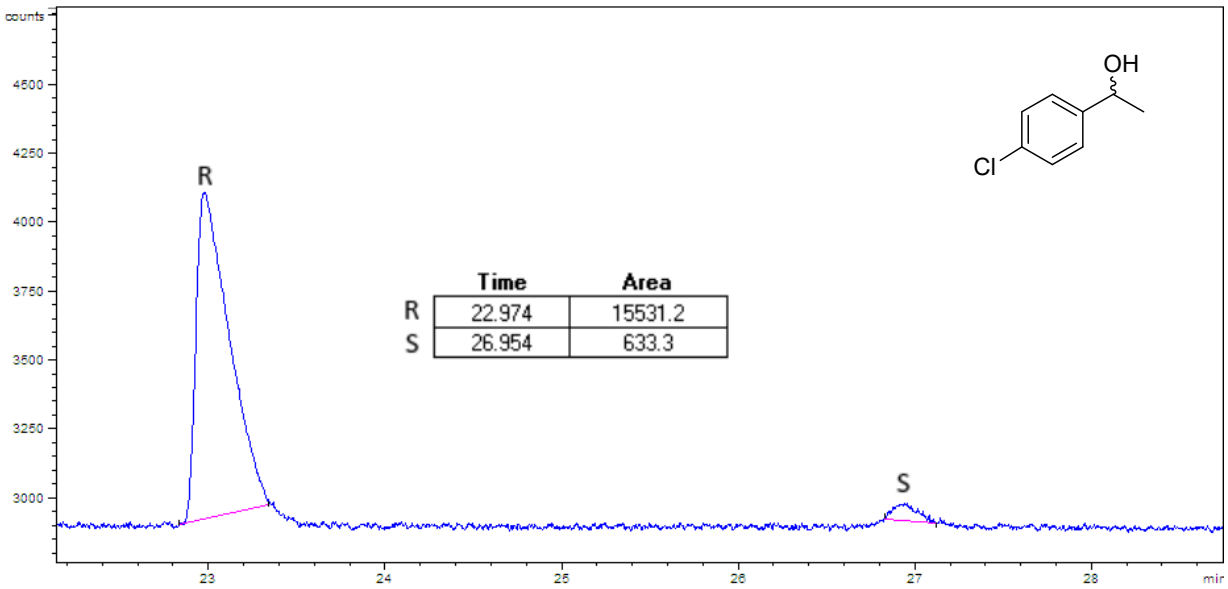

Figure S19. FID trace of 1-(4-chlorophenyl)ethanol (column temp = 120 °C).