Supplementary materials

Ketoprofen-based ionic liquids: synthesis and interactions with bovine serum albumin

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CHARACTERIZATION OF KETOPROFEN AMINO ACID ESTER DERIVATIVES

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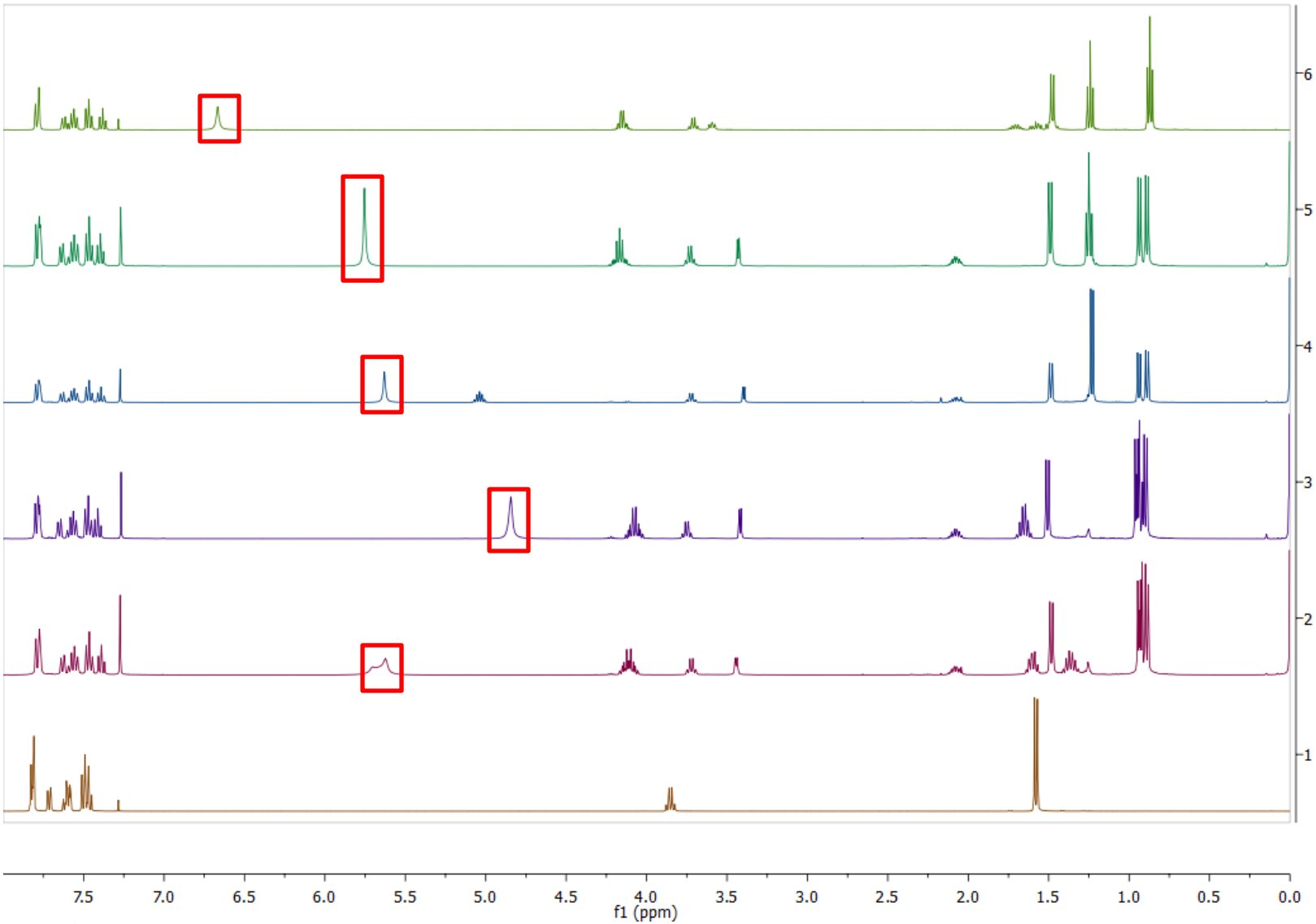


Fig. S1. ^{1}H NMR spectra of ketoprofen and its derivatives (in the red square, the protonated amino group is marked) – from the top: [L-LeuOEt][KETO], [L-ValOEt][KETO], [L-ValOiPr][KETO], [L-ValOPr][KETO], [L-ValOBu][KETO] and [KETO]

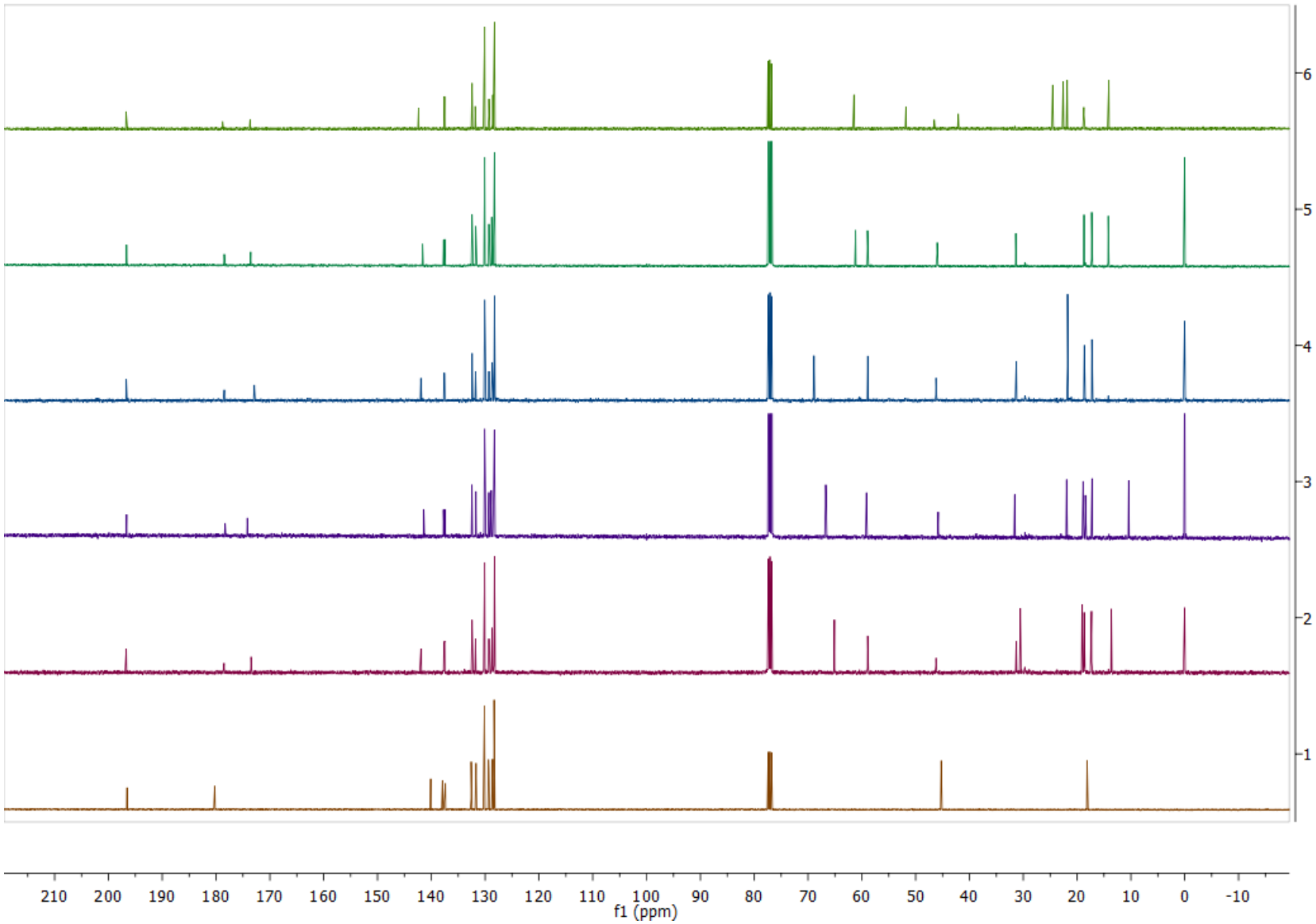


Fig. S2. ^{13C} NMR spectra of ketoprofen and its derivatives – from the top: [L-LeuOEt][KETO], [L-ValOEt][KETO], [L-ValOiPr][KETO], [L-ValOPr][KETO], [L-ValOBu][KETO] and [KETO]

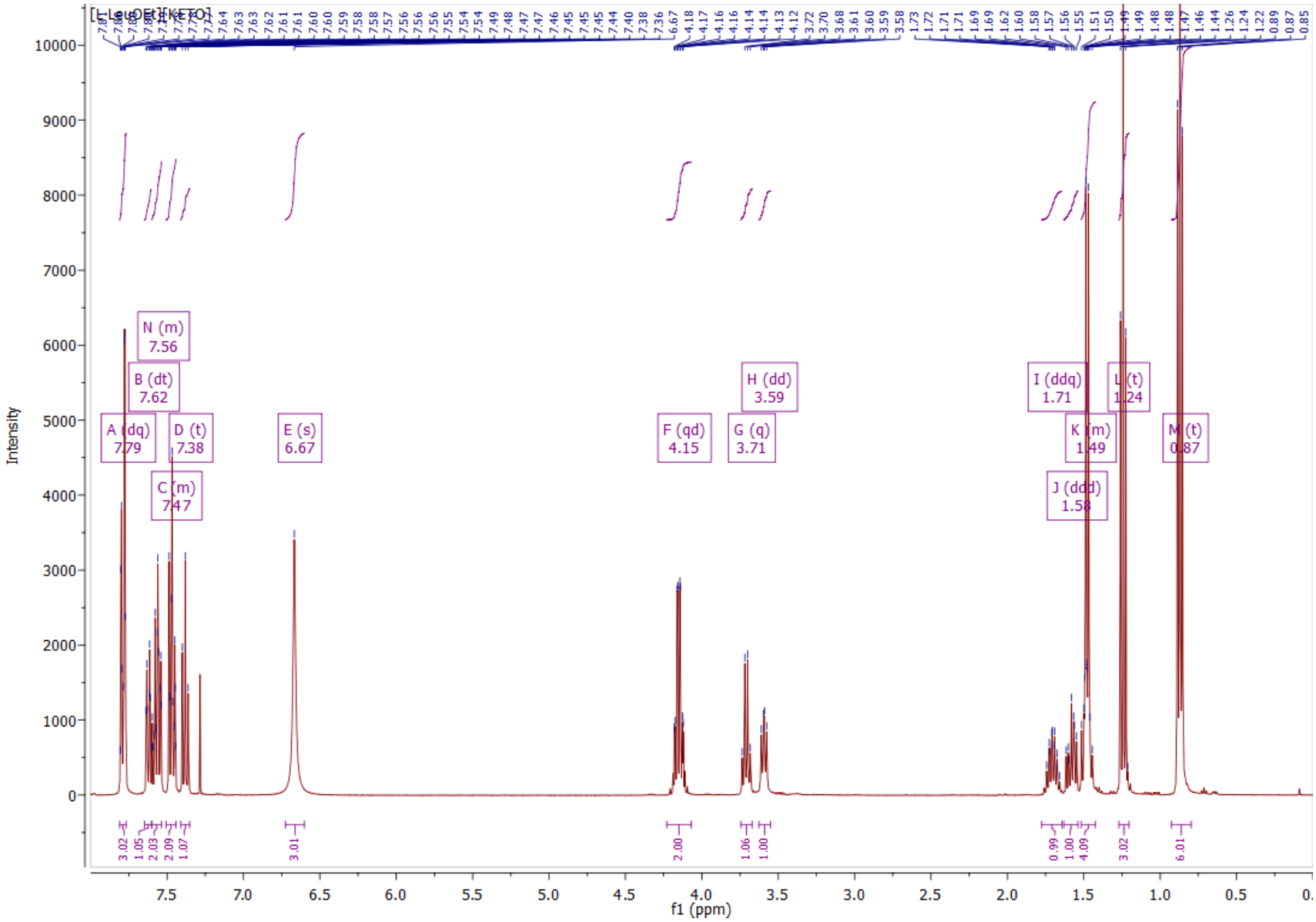


Fig.S3. ^{1}H NMR spectra of L-leucine ethyl ester ketoprofenate

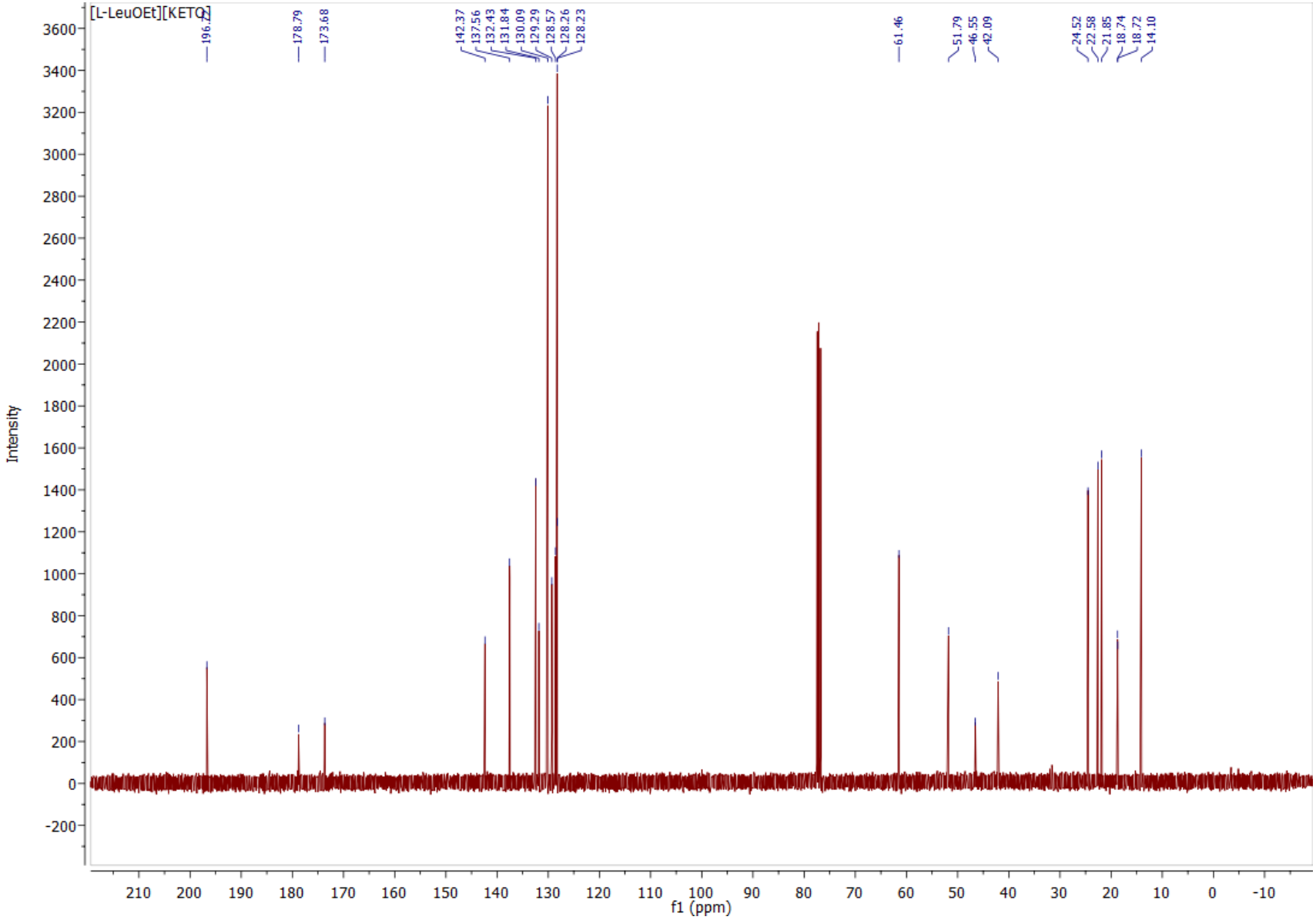


Fig. S4. ^{13}C NMR spectra of L-leucine ethyl ester ketoprofenate.

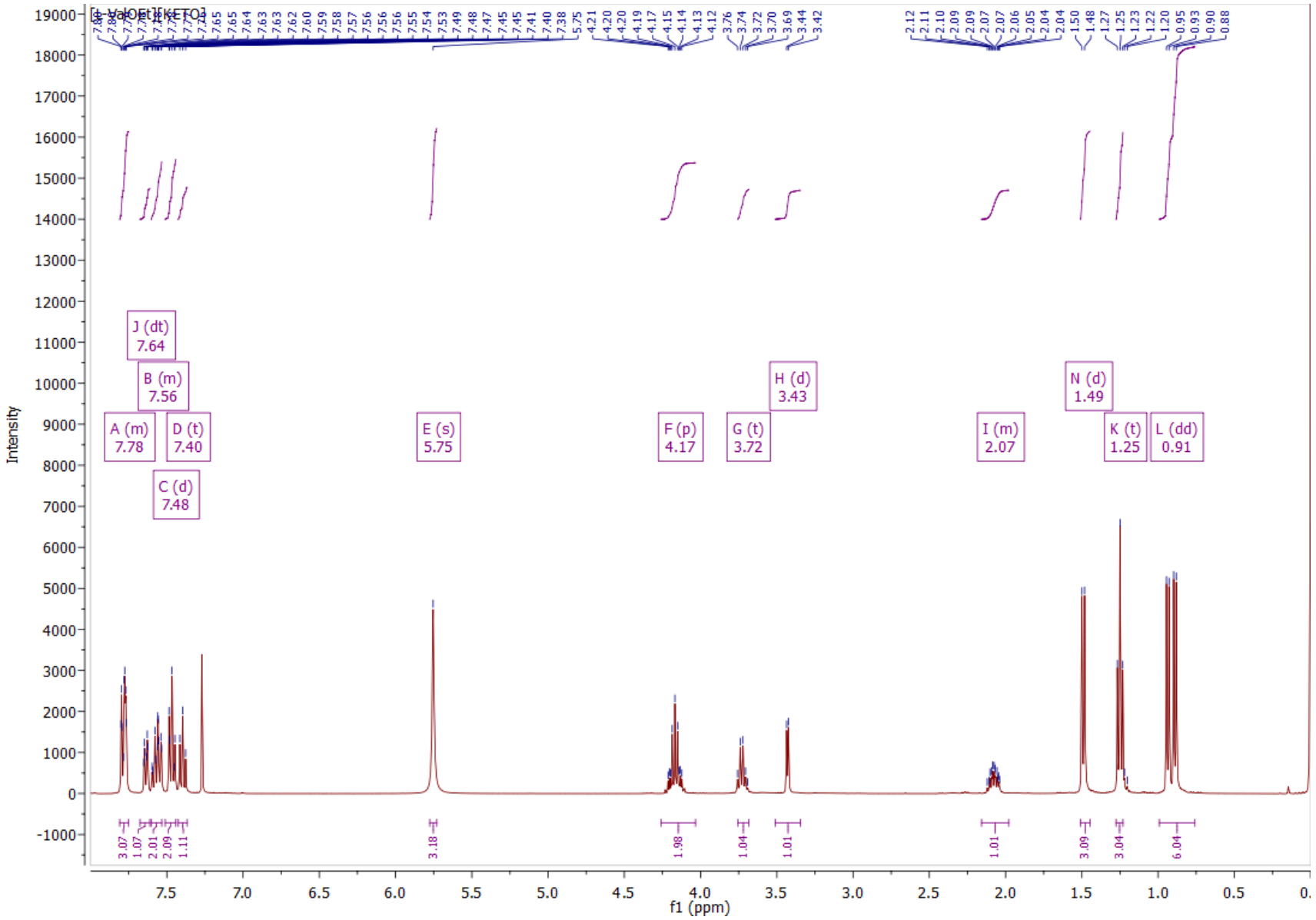


Fig.S5. 1H NMR spectra of L-valine ethyl ester ketoprofenate

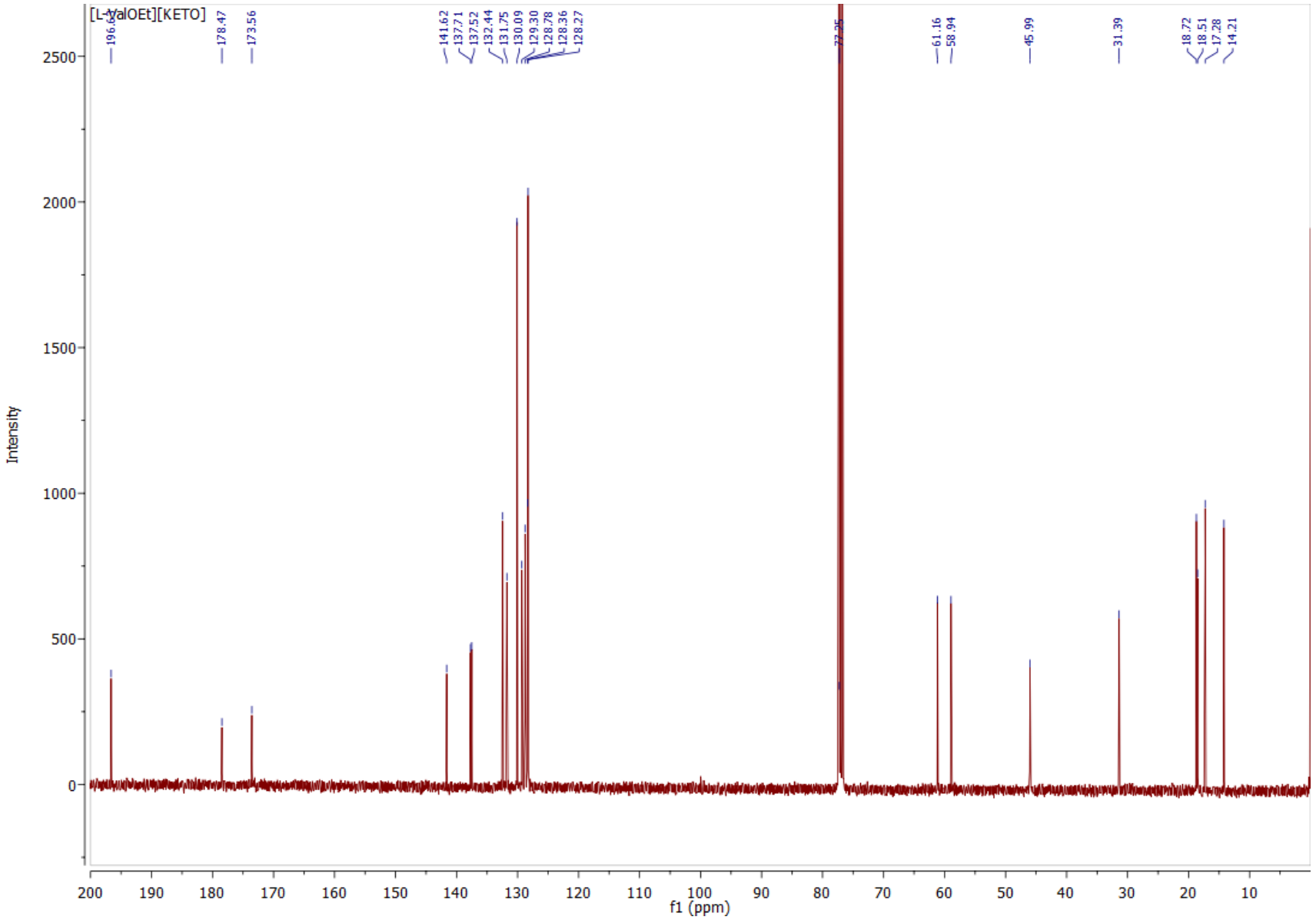


Fig. S6. ^{13}C NMR spectra of L-valine ethyl ester ketoprofenate

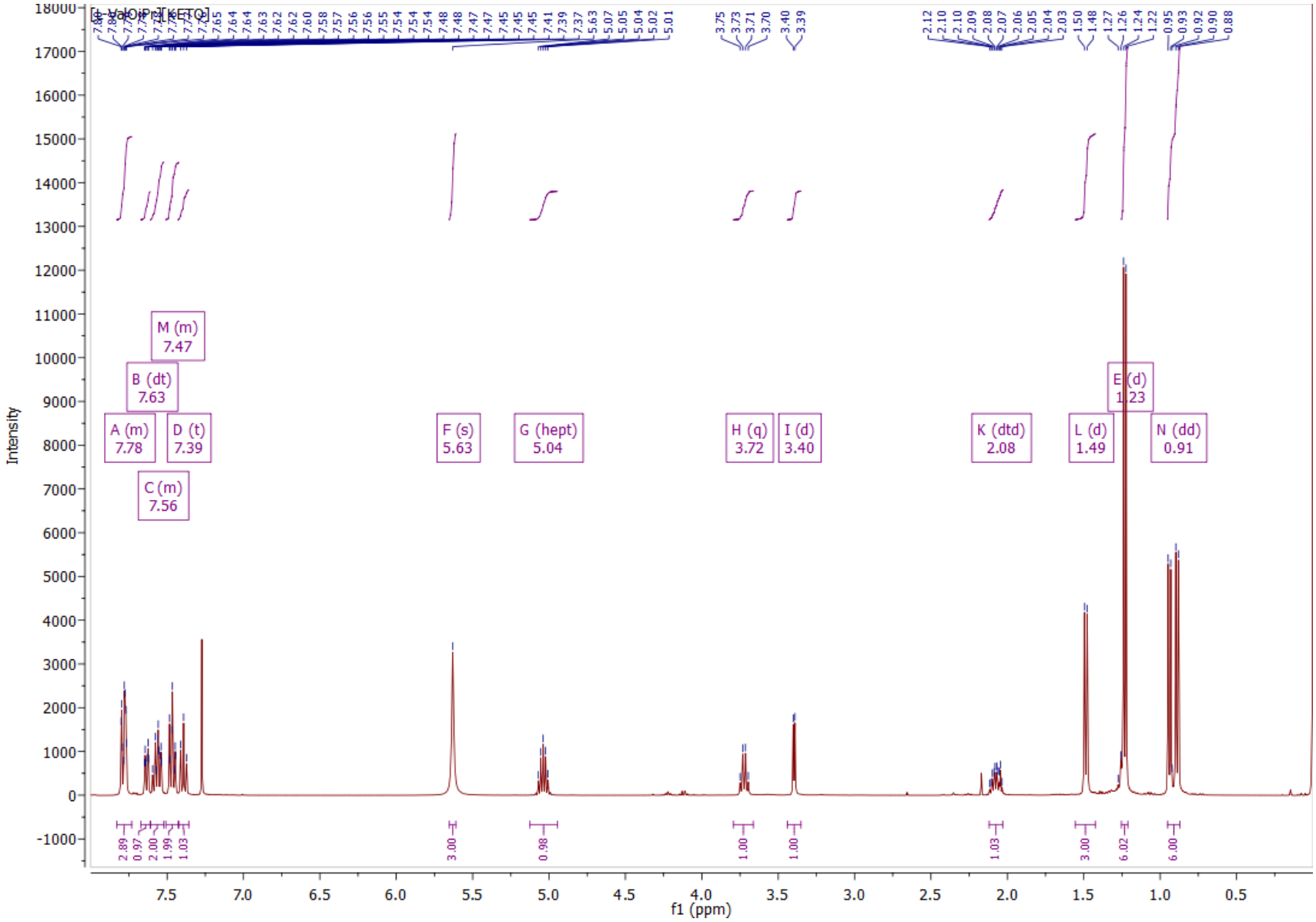


Fig. S7. ^{1}H NMR spectra of L-valine isopropyl ester ketoprofenate

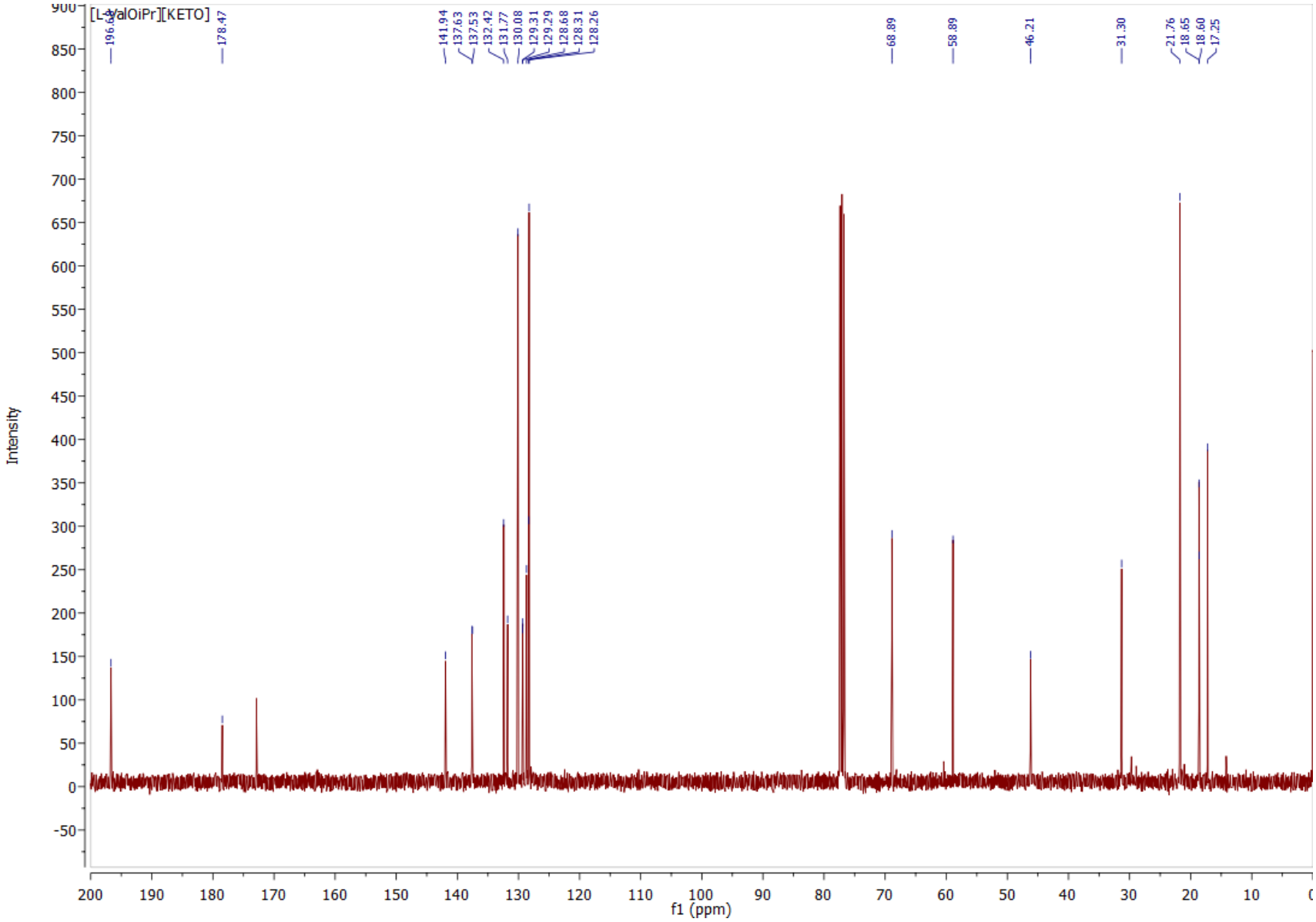


Fig. S8. ^{13}C NMR spectra of L-valine isopropyl ester ketoprofenate

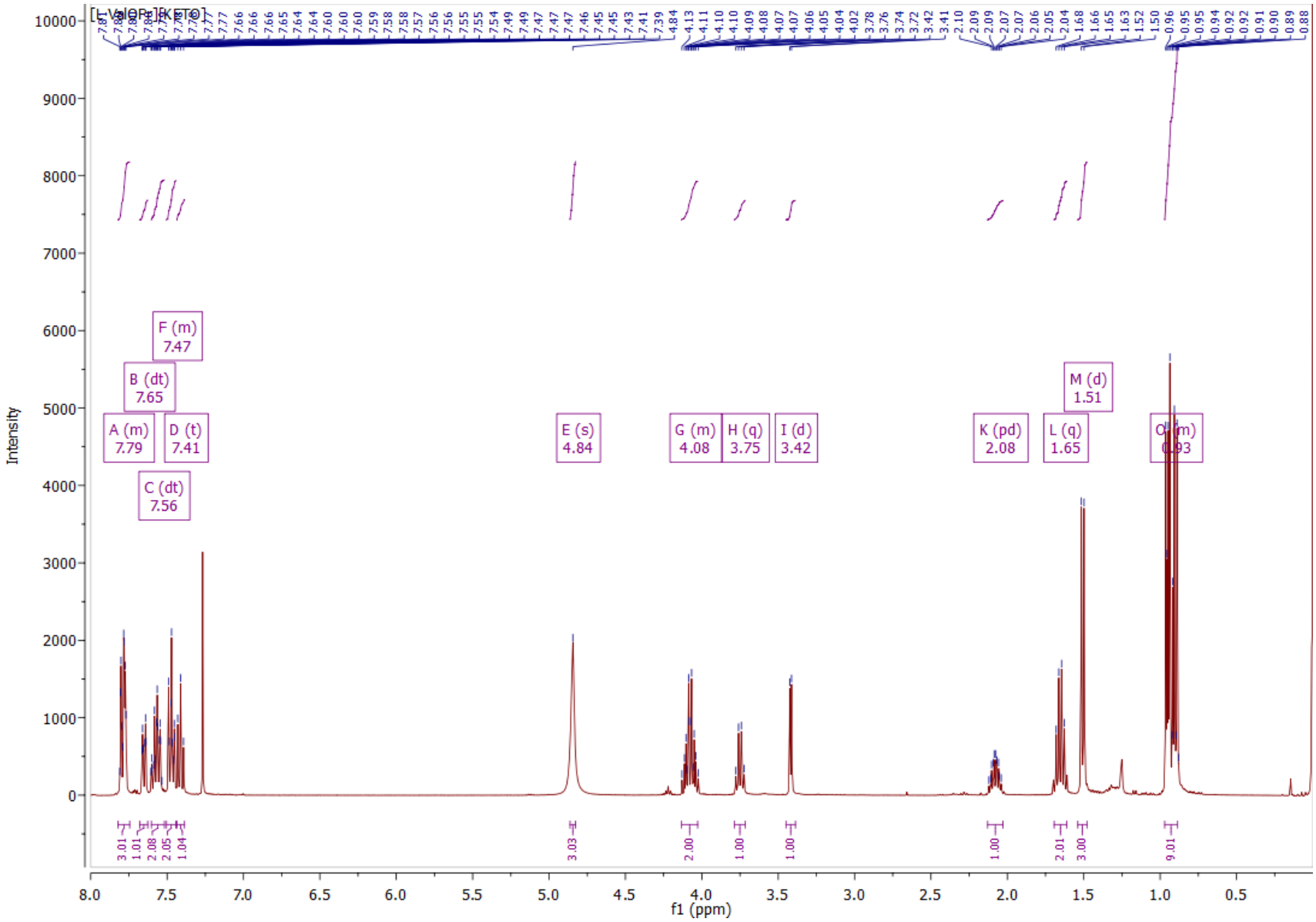


Fig. S9. 1H NMR spectra of L-valine propyl ester ketoprofenate

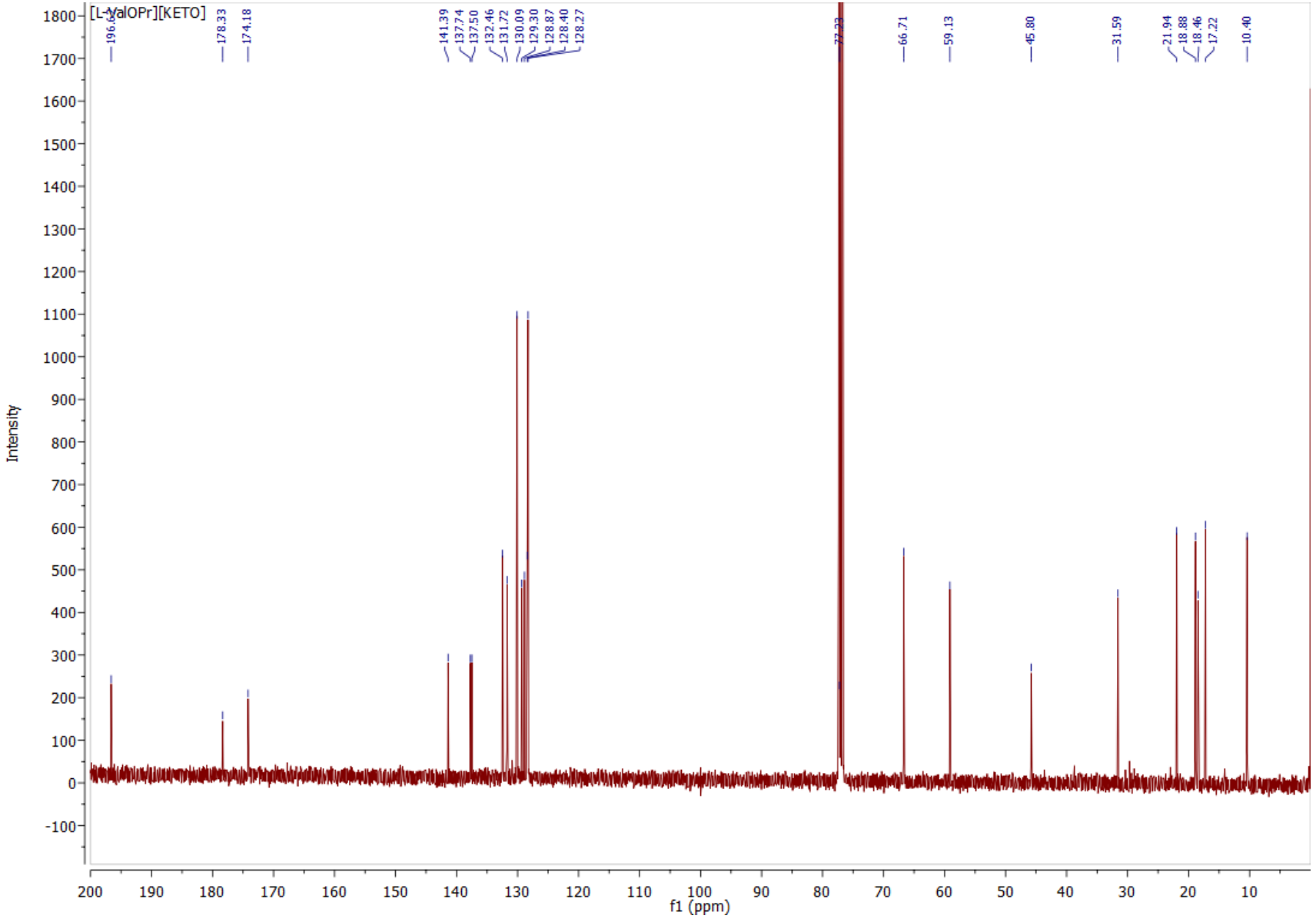


Fig. S10. ^{13}C NMR spectra of L-valine propyl ester ketoprofenate

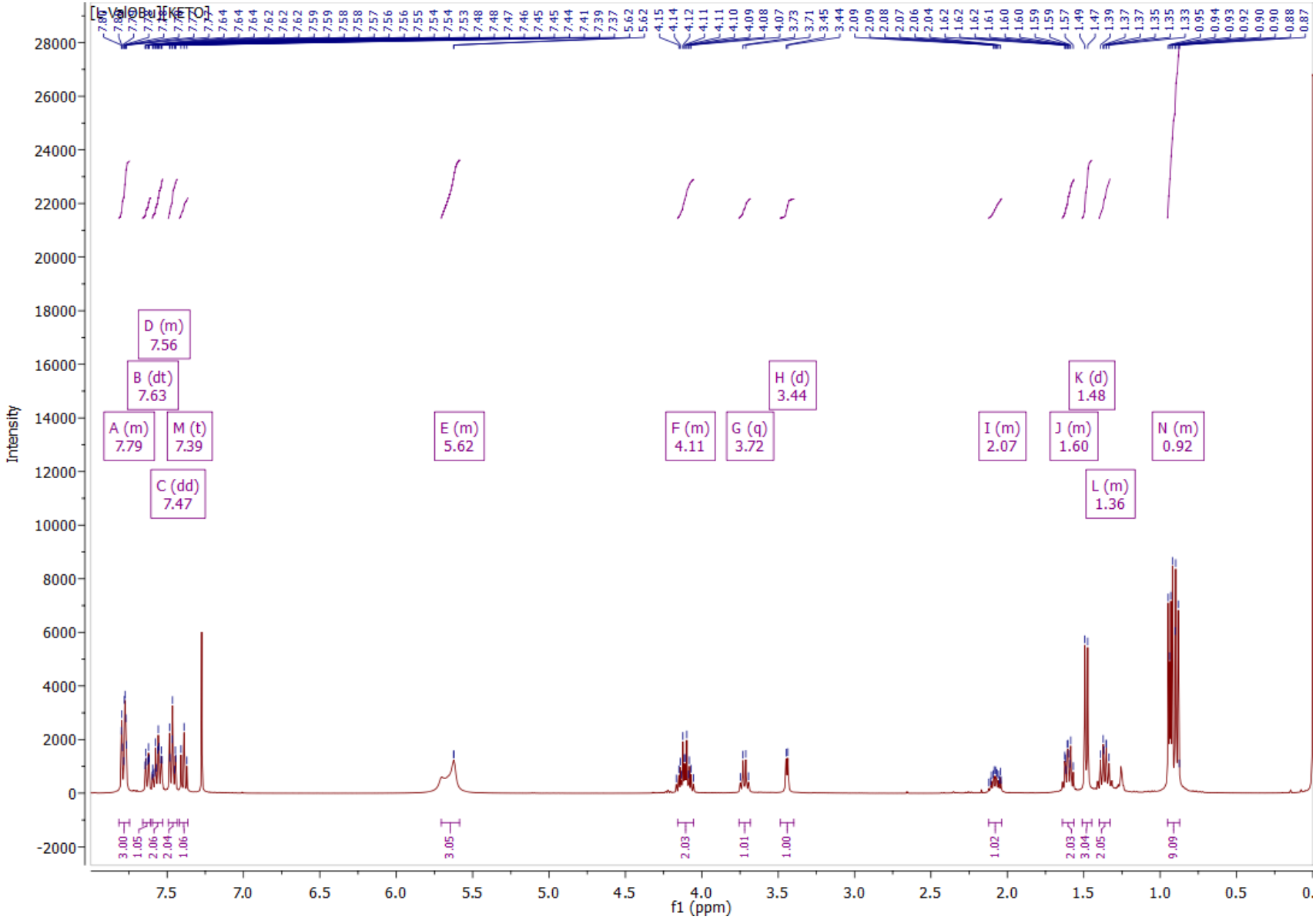


Fig. S11. [1]H NMR spectra of L-valine butyl ester ketoprofenate

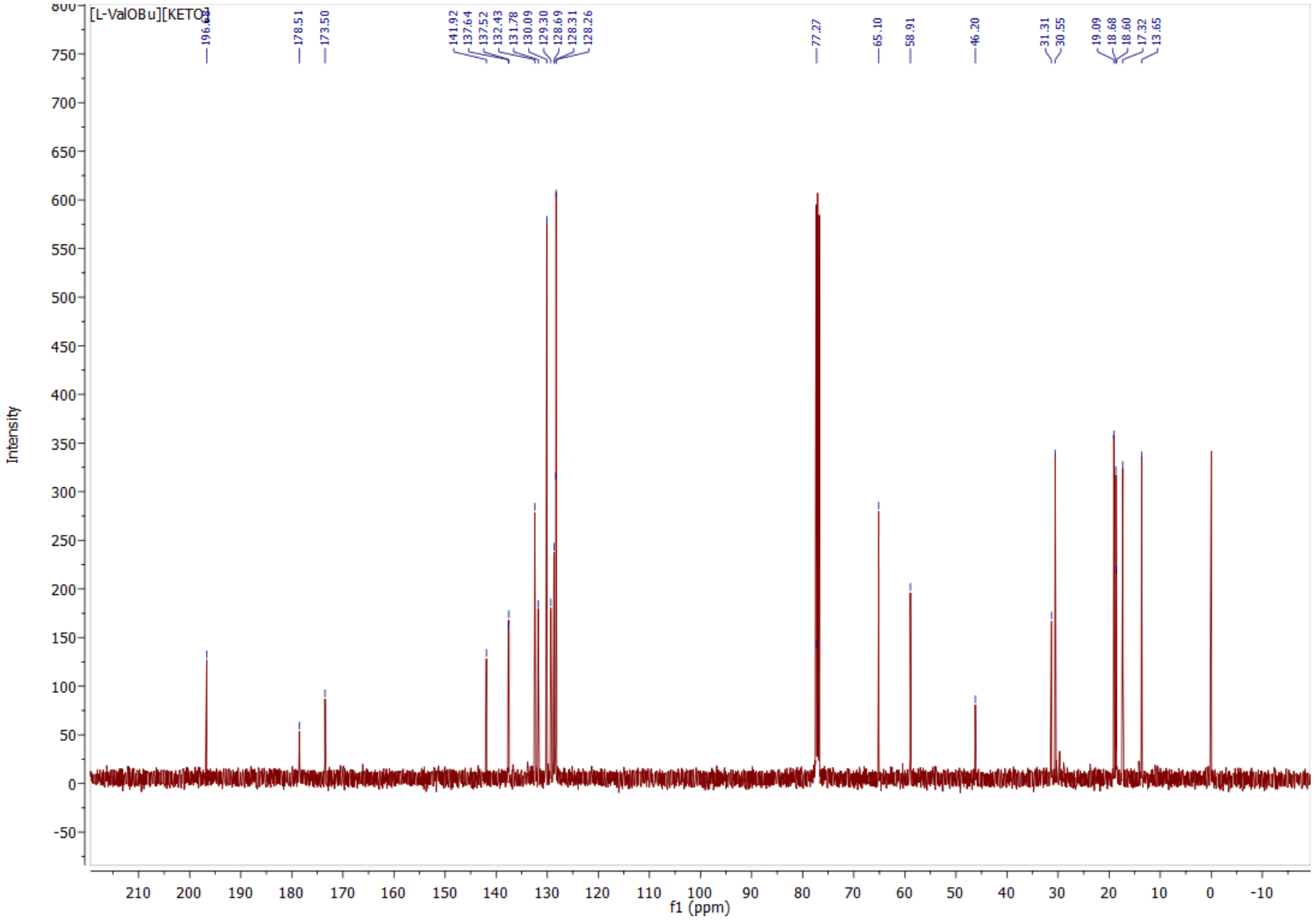


Fig. 12. ^{13}C NMR spectra of L-valine butyl ester ketoprofenate

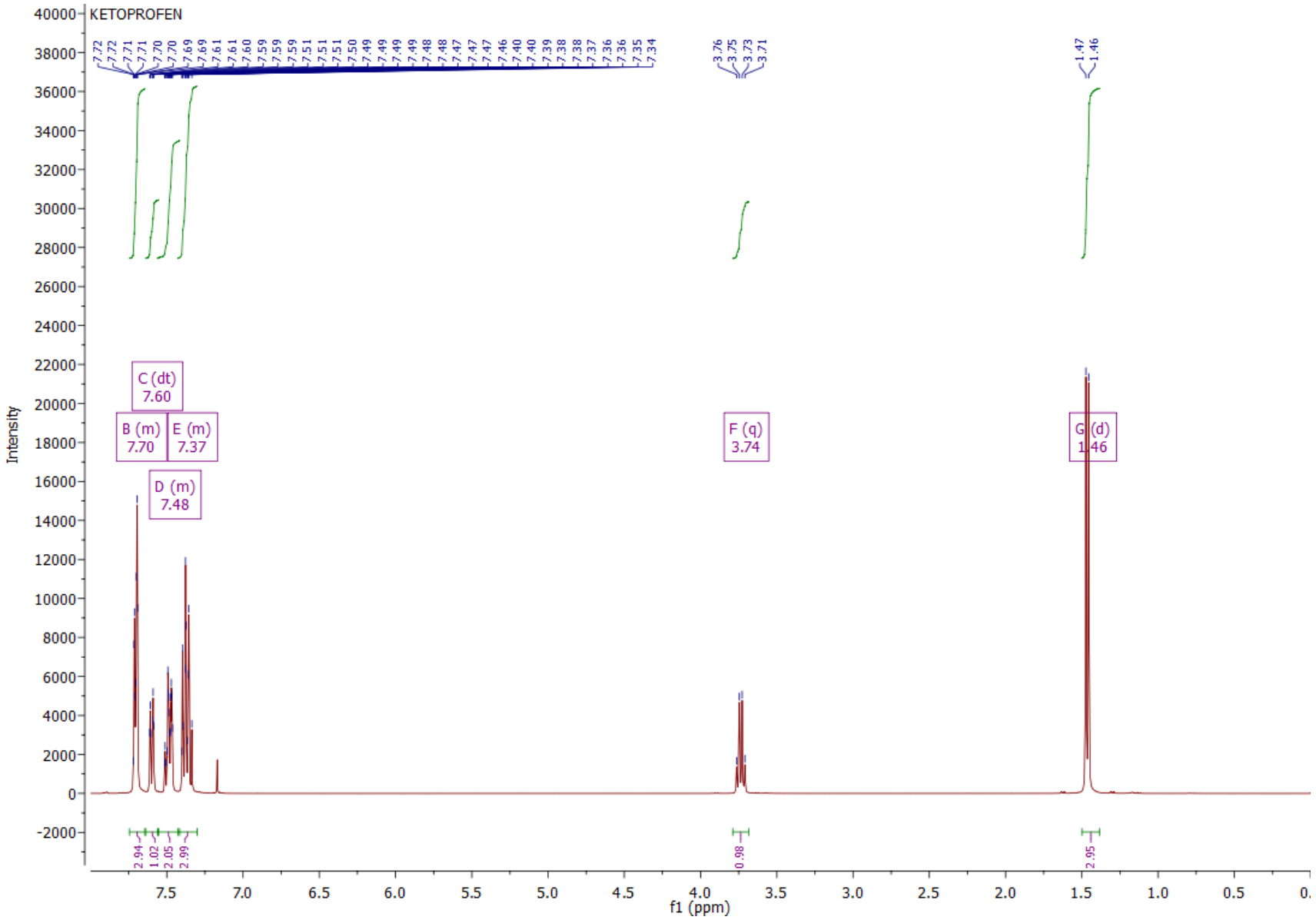


Fig.S13. ^{1}H NMR spectra of ketoprofen

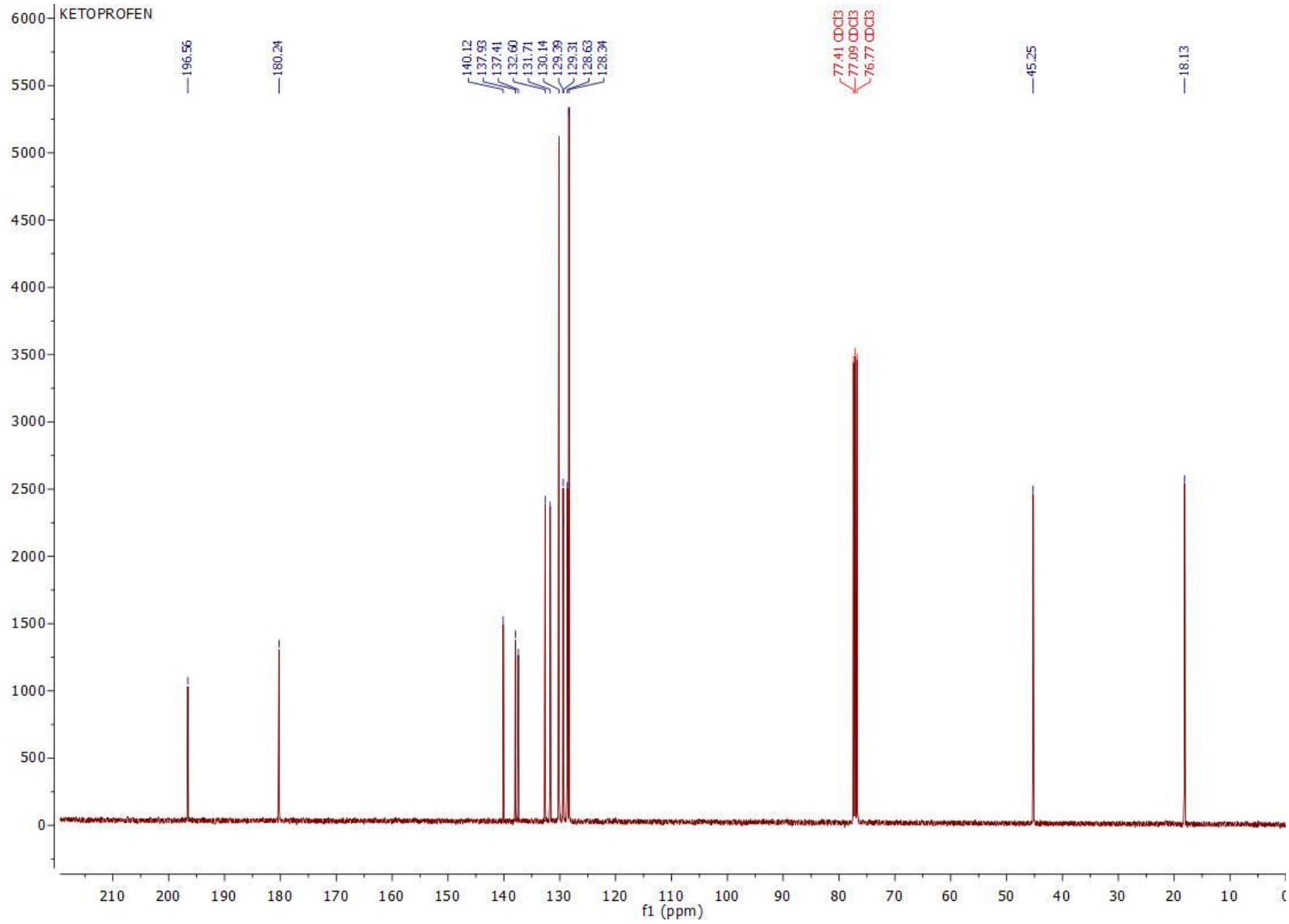


Fig. S14. ^{13}C NMR spectra of ketoprofen

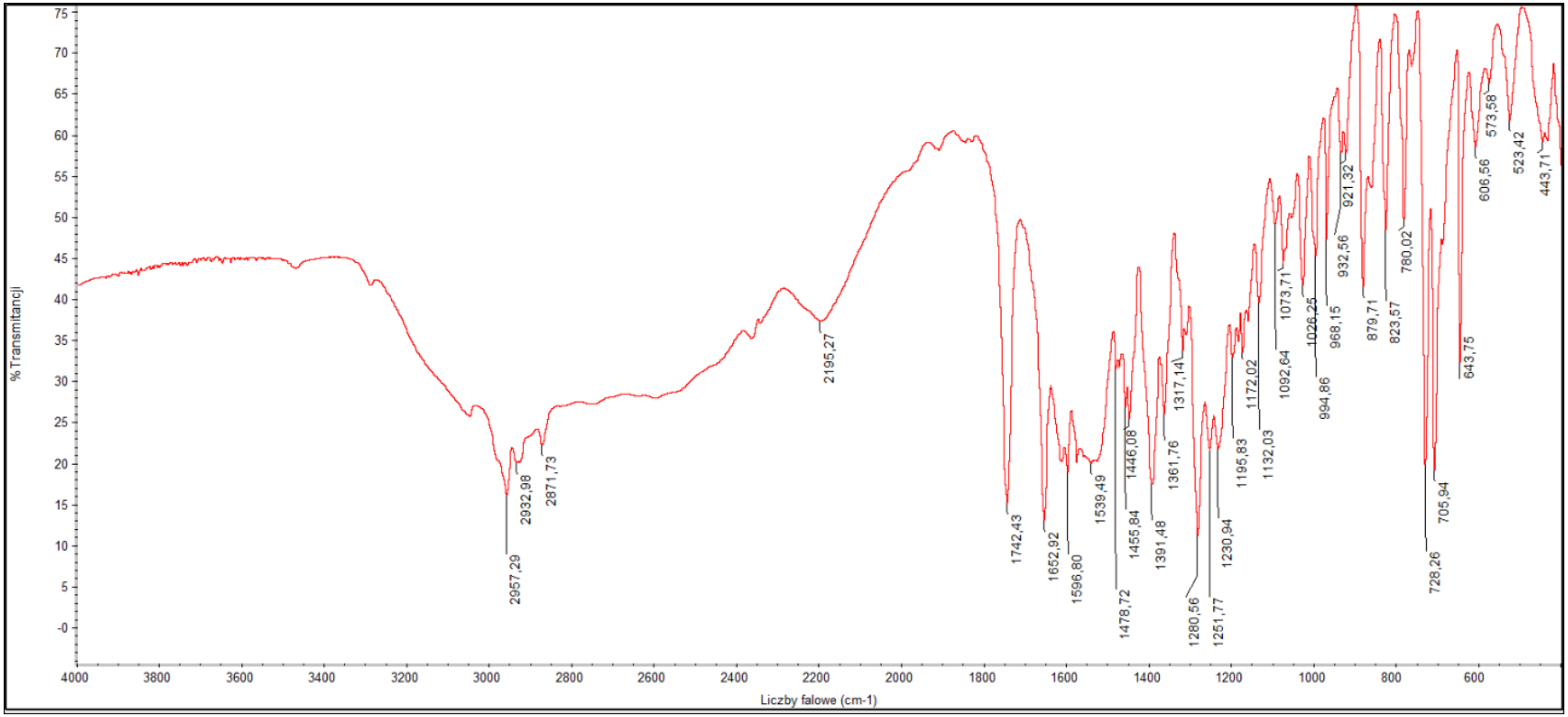


Fig. S15. FT-IR spectra of [L-LeuOEt][KETO]

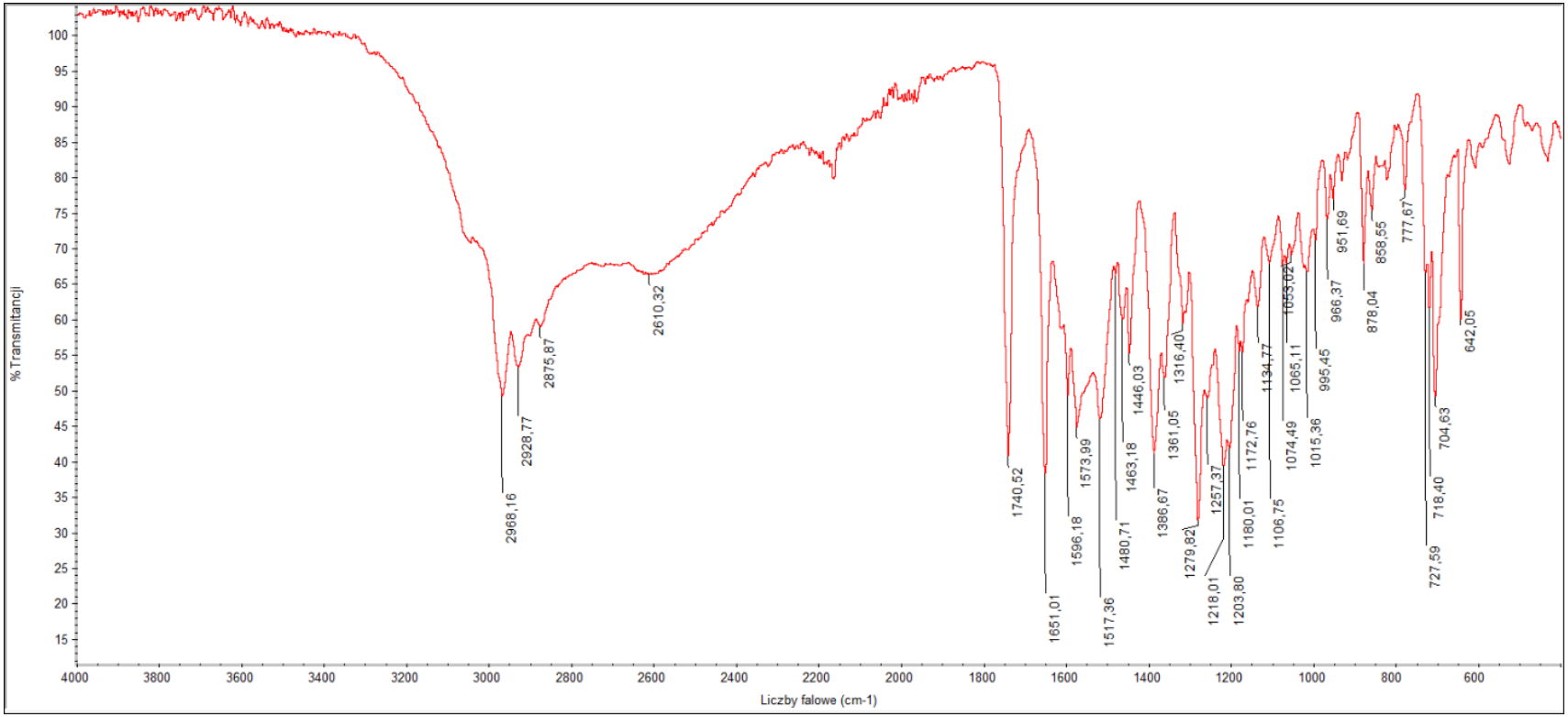


Fig. S16. FT-IR spectra of [L-ValOEt][KETO]

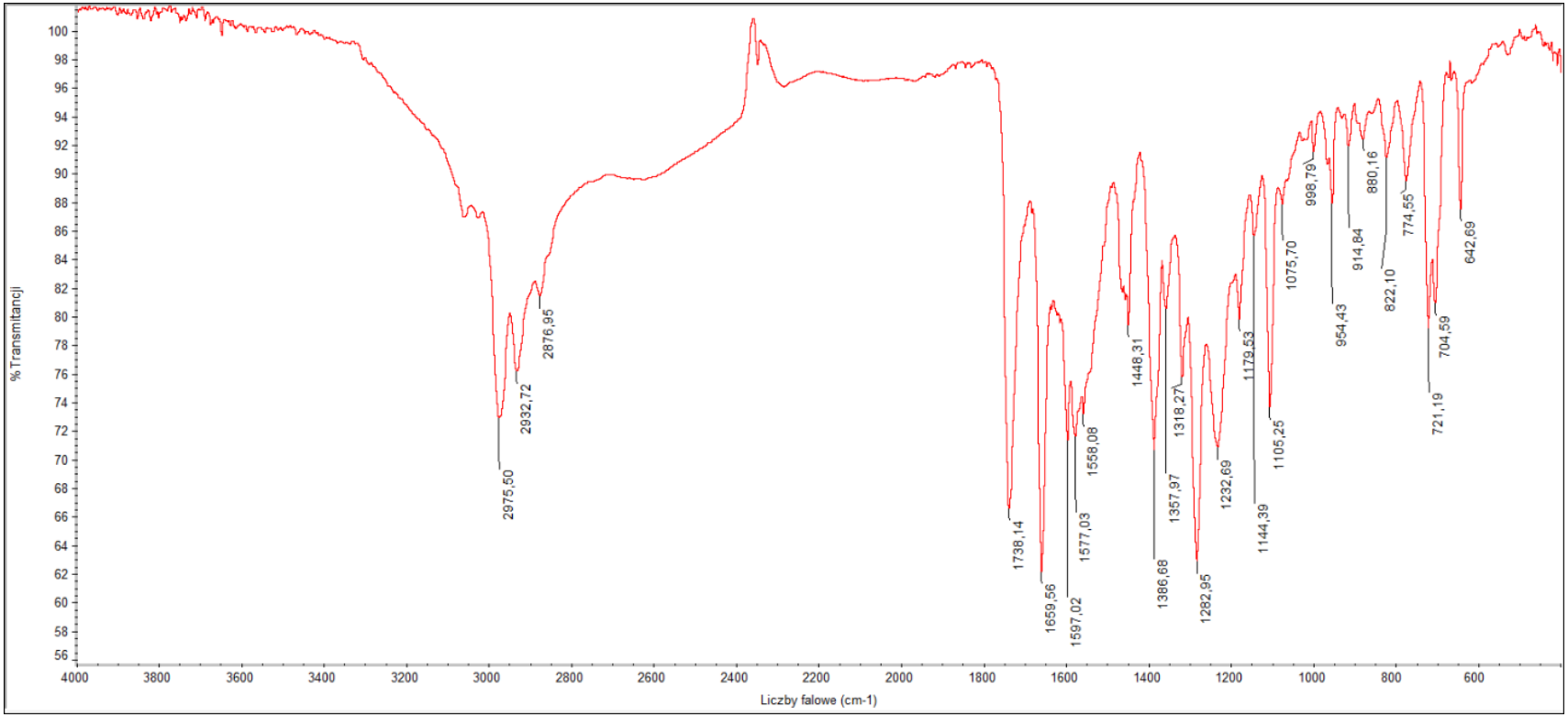


Fig. S17. FT-IR spectra of [L-ValOiPr][KETO]

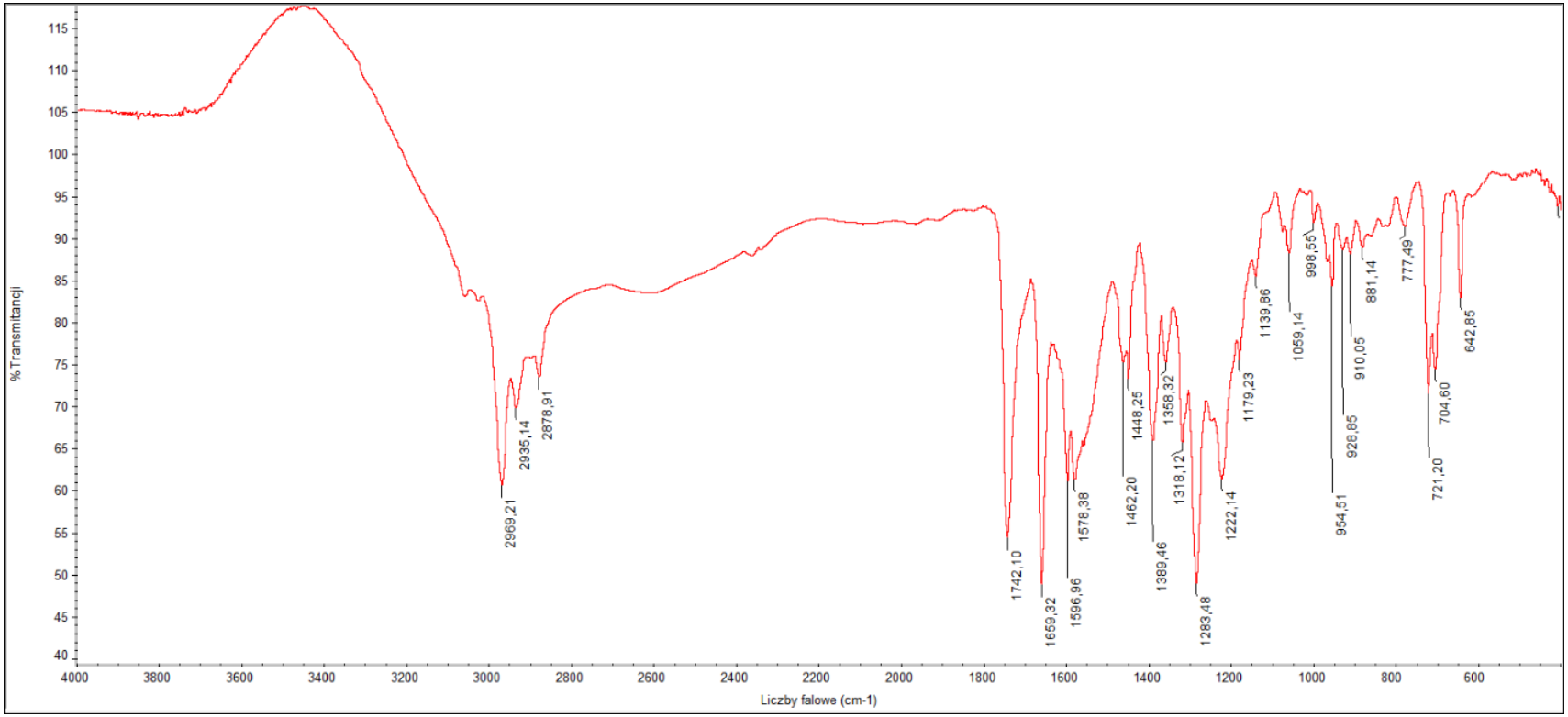


Fig. S18. FT-IR spectra of [L-ValOPr][KETO]

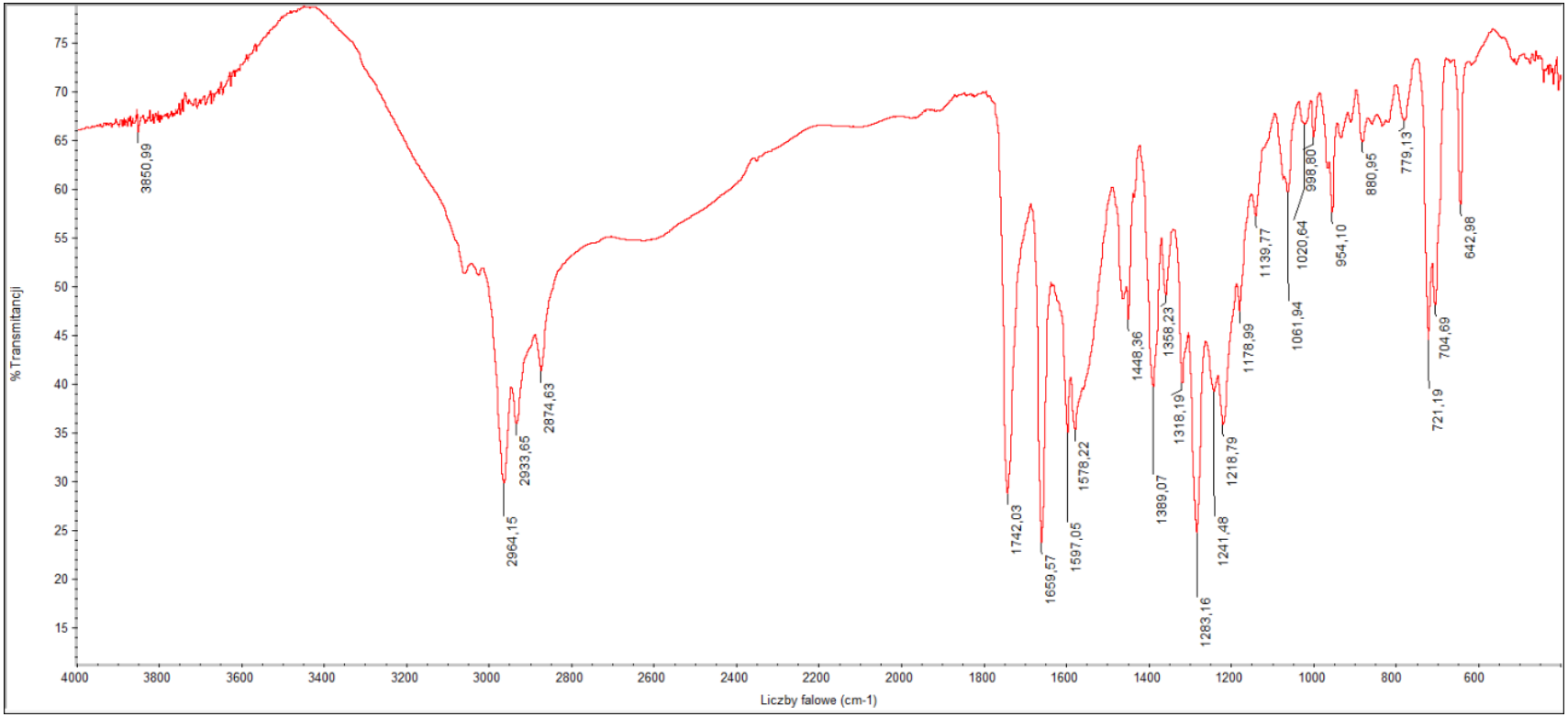


Fig. S19. FT-IR spectra of [L-ValOBu][KETO]

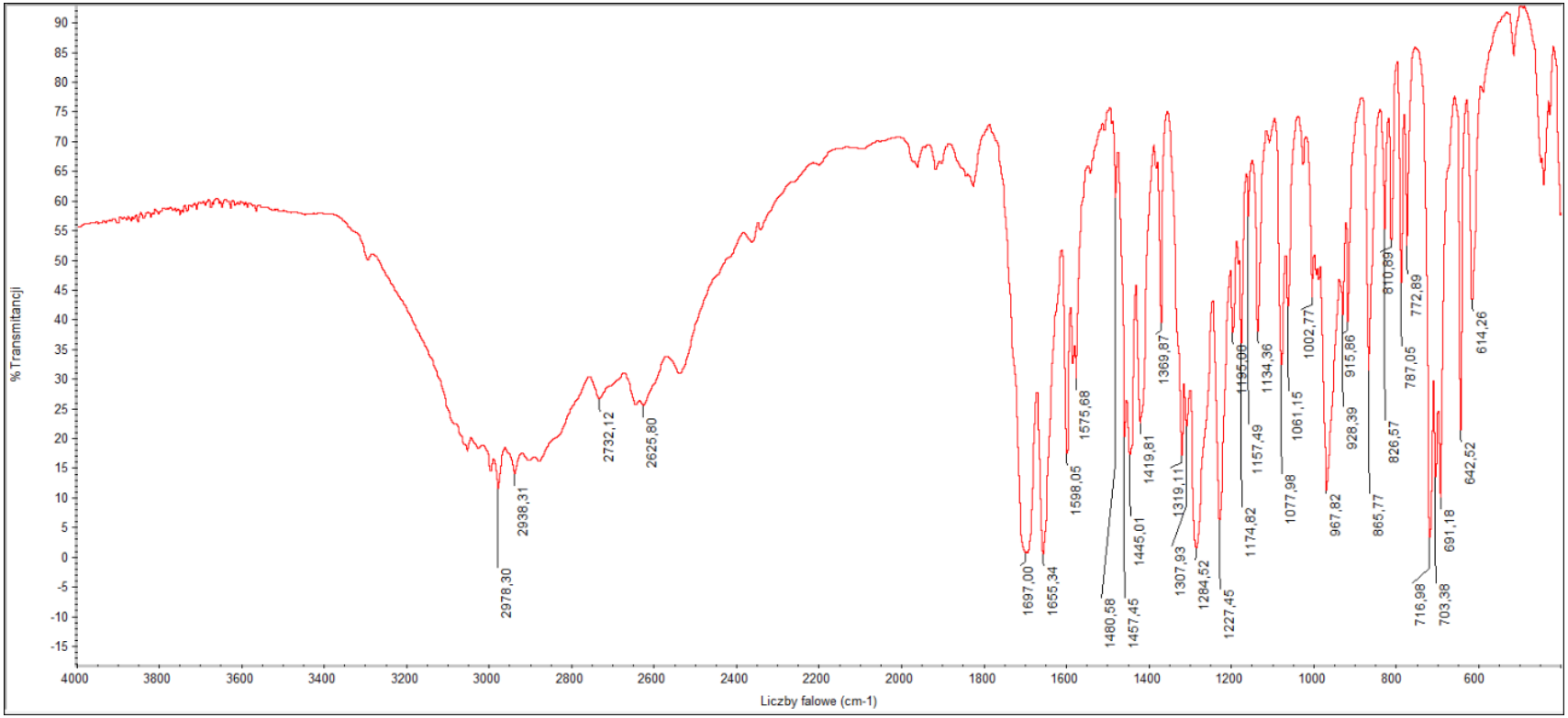


Fig. S20. FT-IR spectra of [KETO]

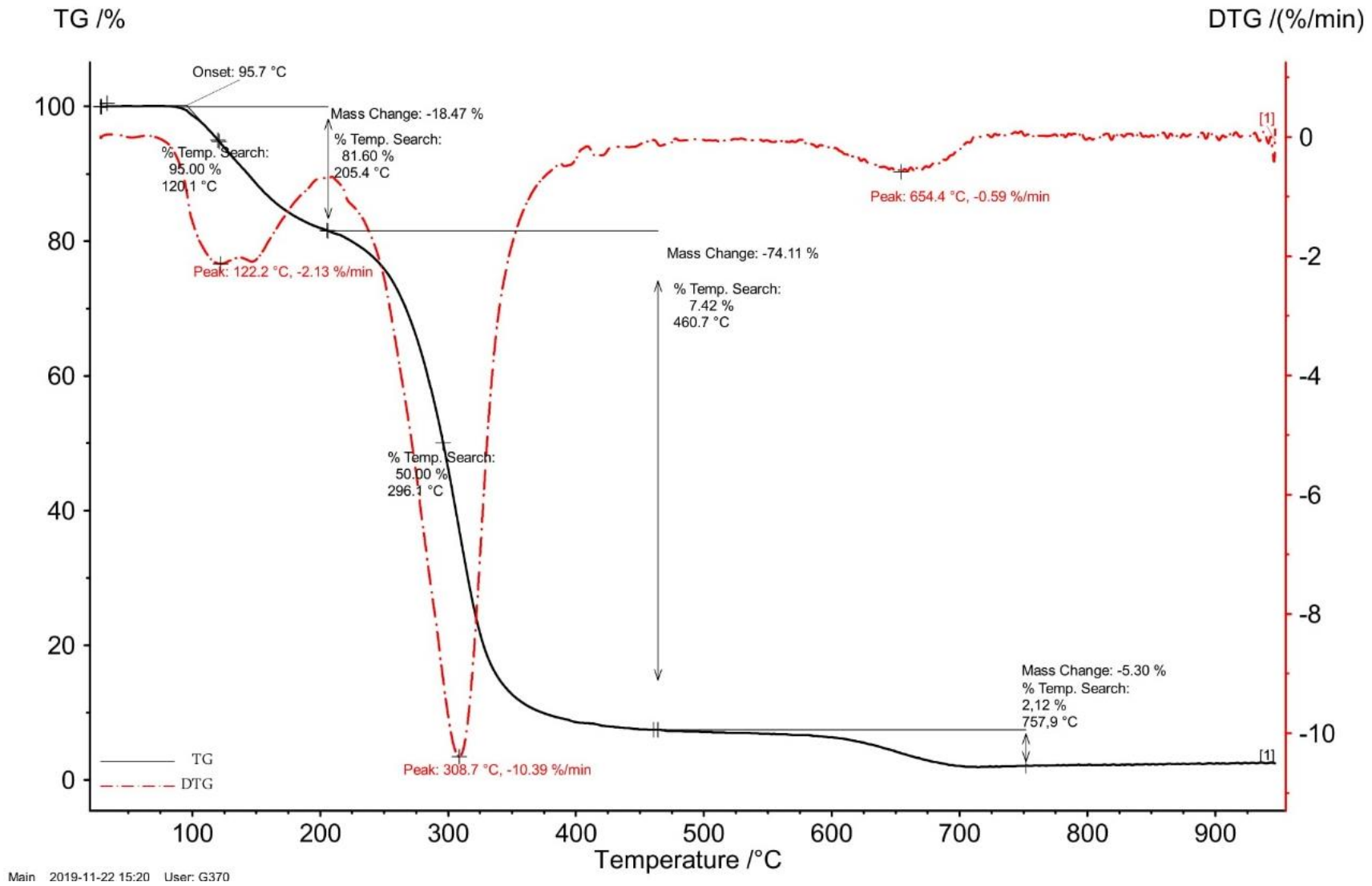


Fig. S21. The TG and DTG curves of [L-LeuOEt][KETO]

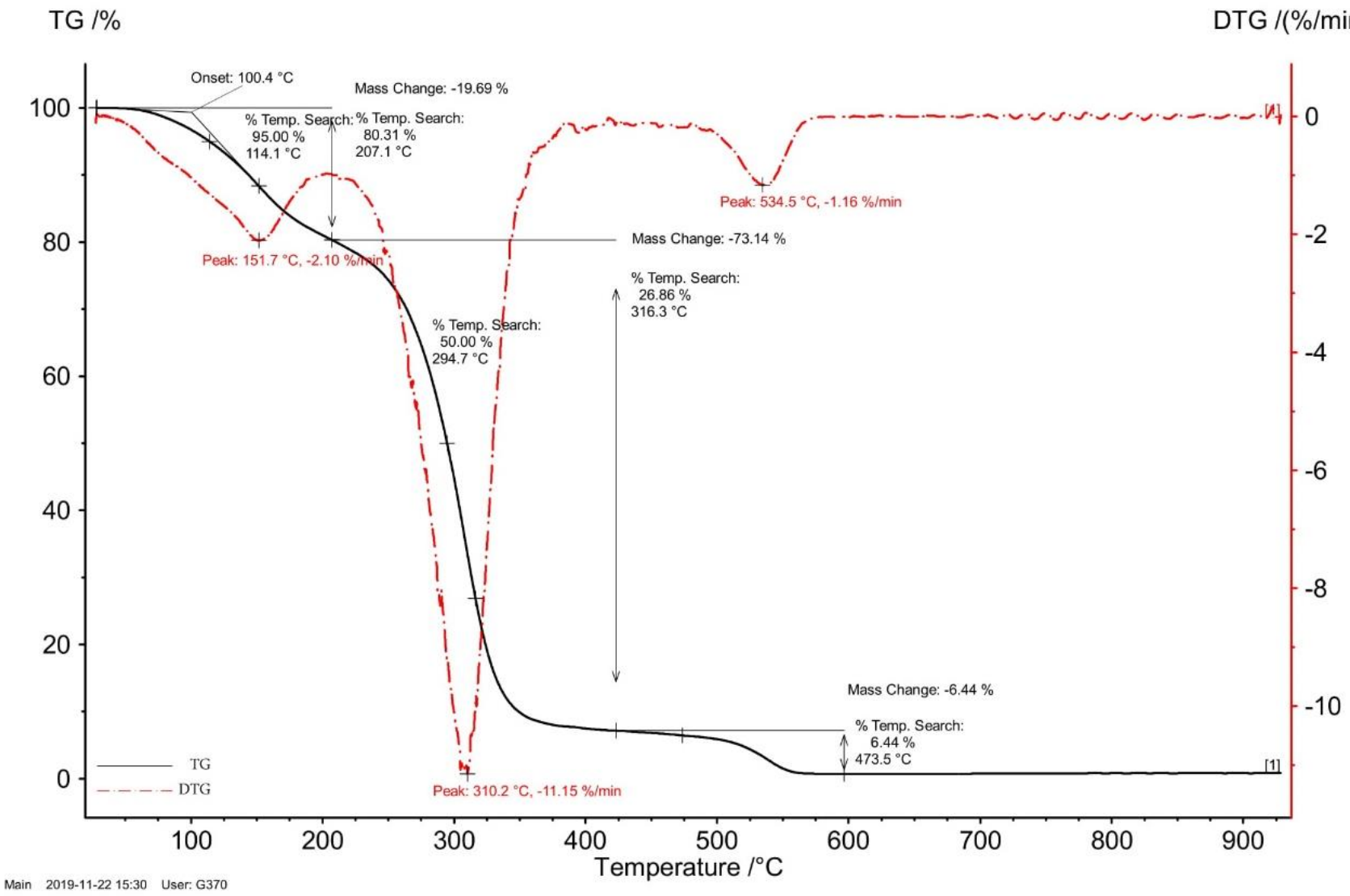


Fig. S22. The TG and DTG curves of [L-ValOEt][KETO]

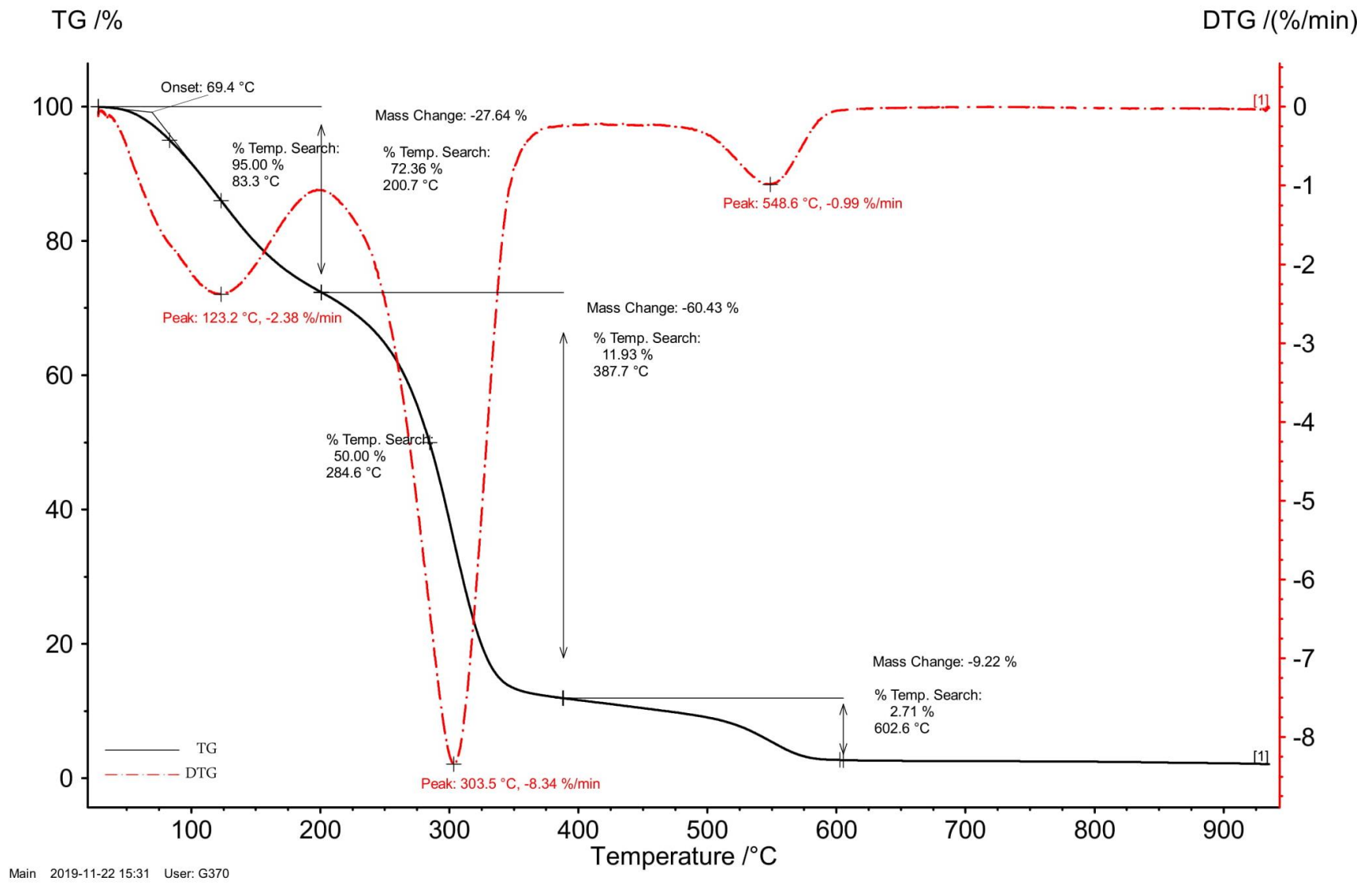


Fig. S23. The TG and DTG curves of [L-ValOiPr][KETO]

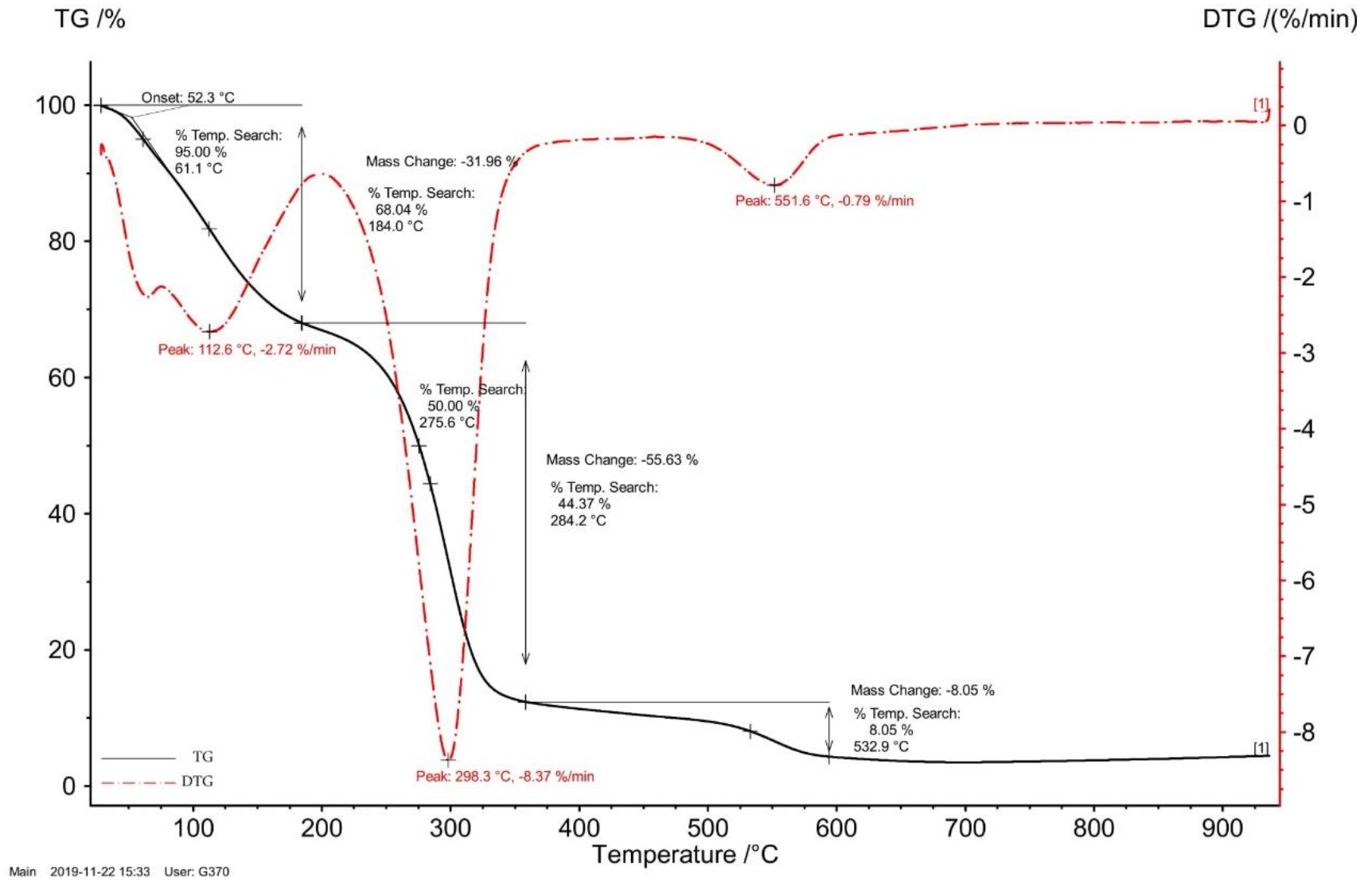


Fig. S24. The TG and DTG curves of [L-ValOPr][KETO]

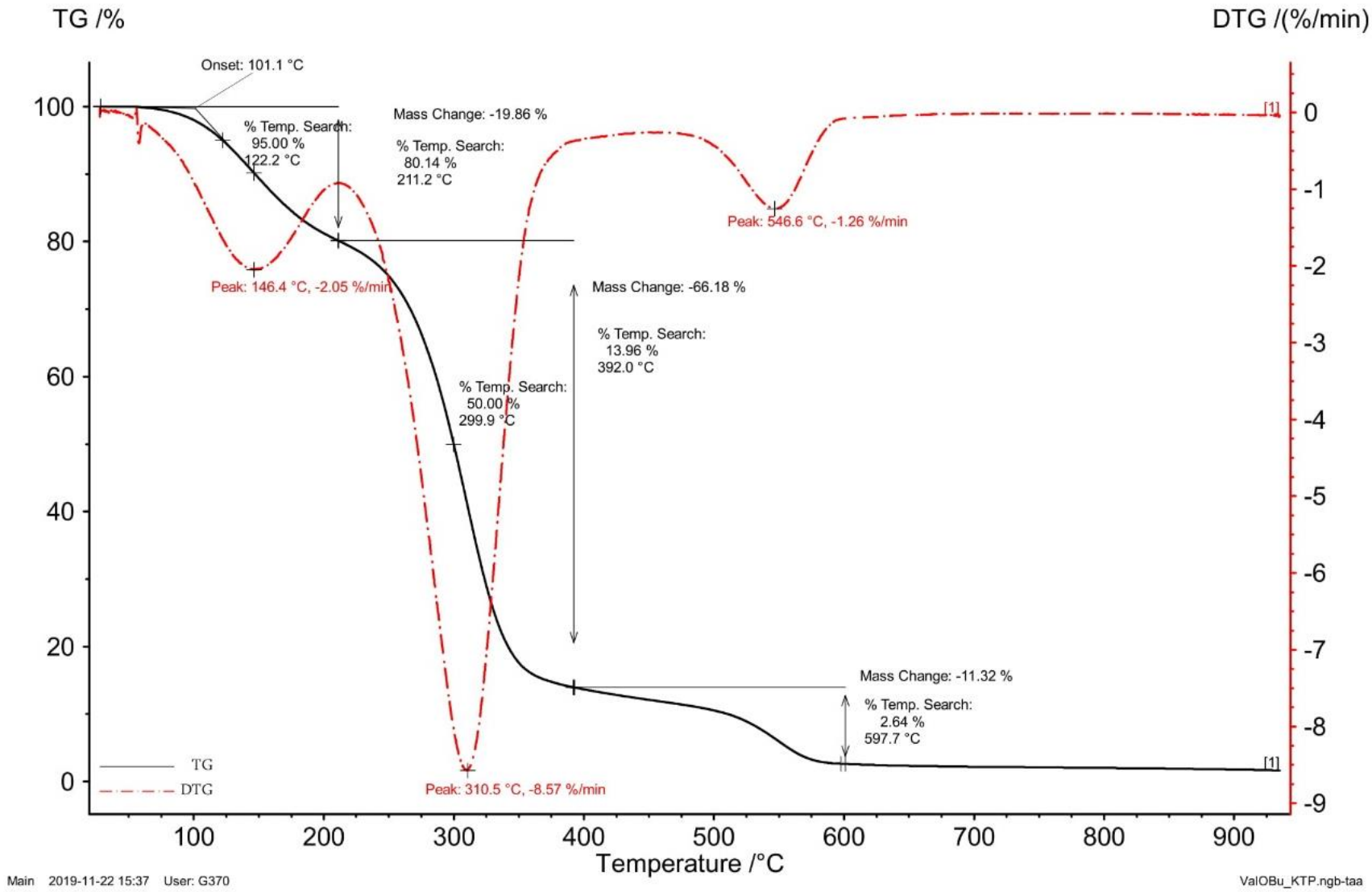


Fig. S25. The TG and DTG and curves of [L-ValOBu][KETO]

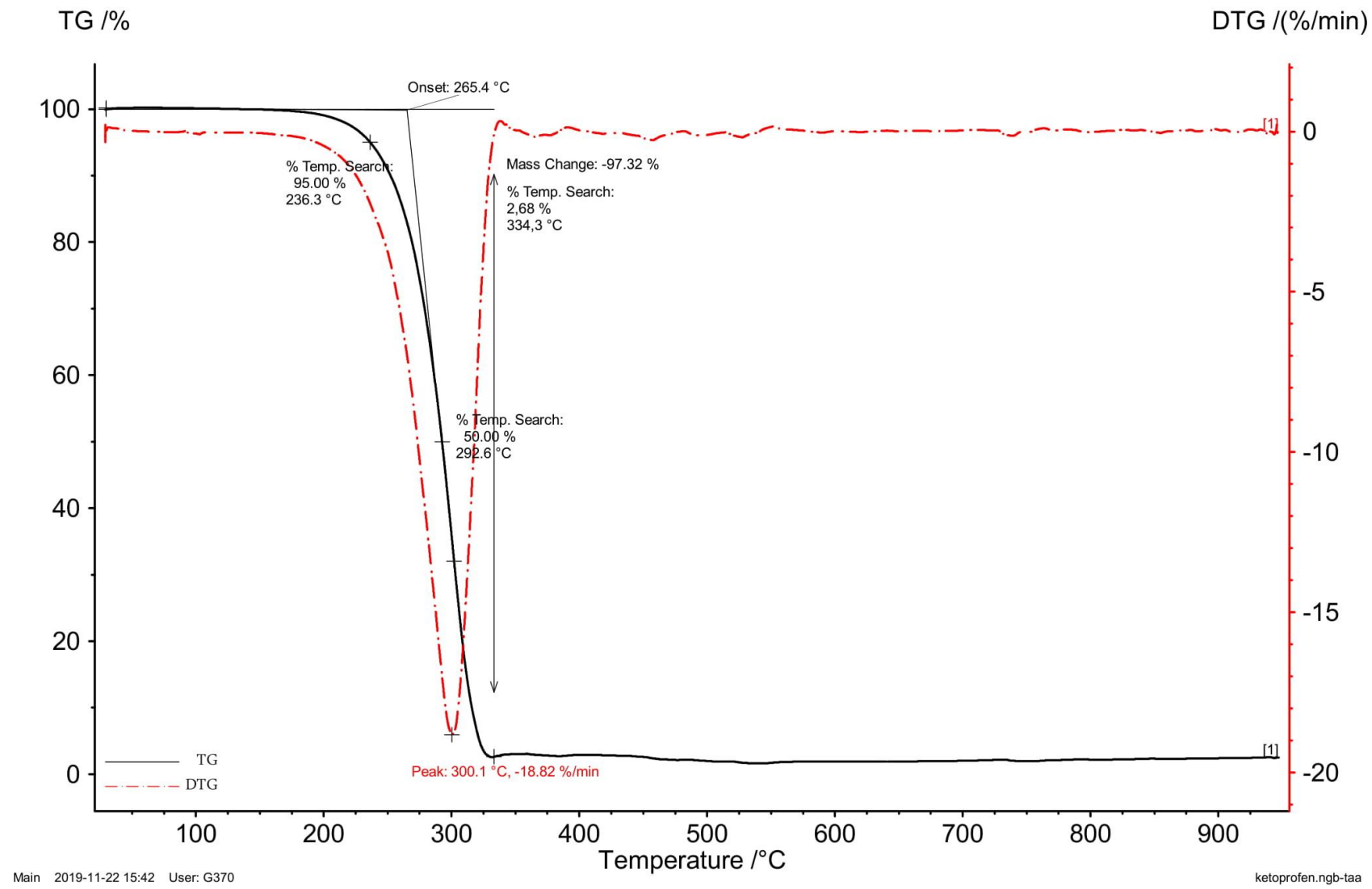


Fig. S26. The TG and DTG curves of [KETO]

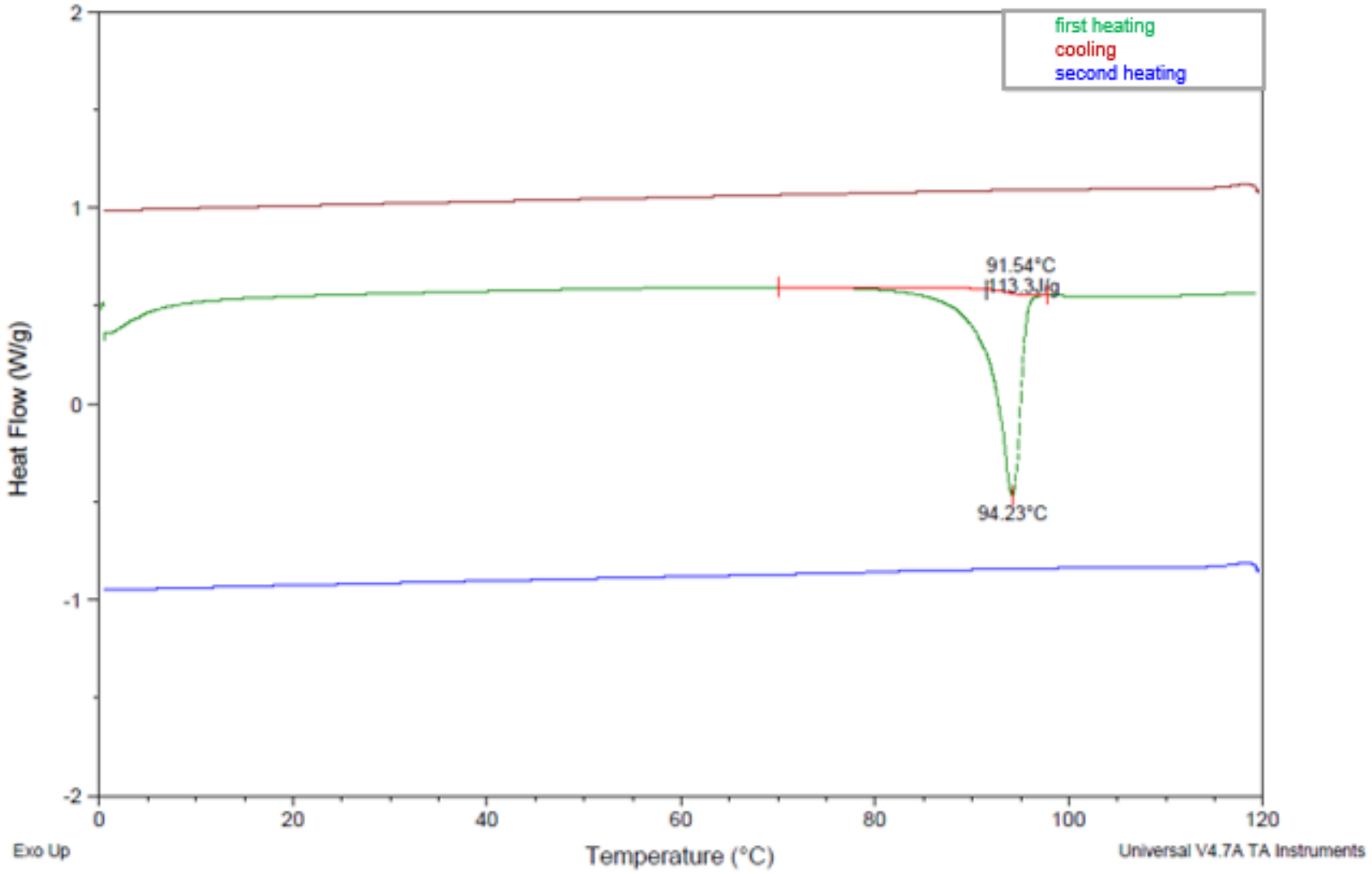


Figure S27. The DSC curves of [L-LeuOEt][KETO]

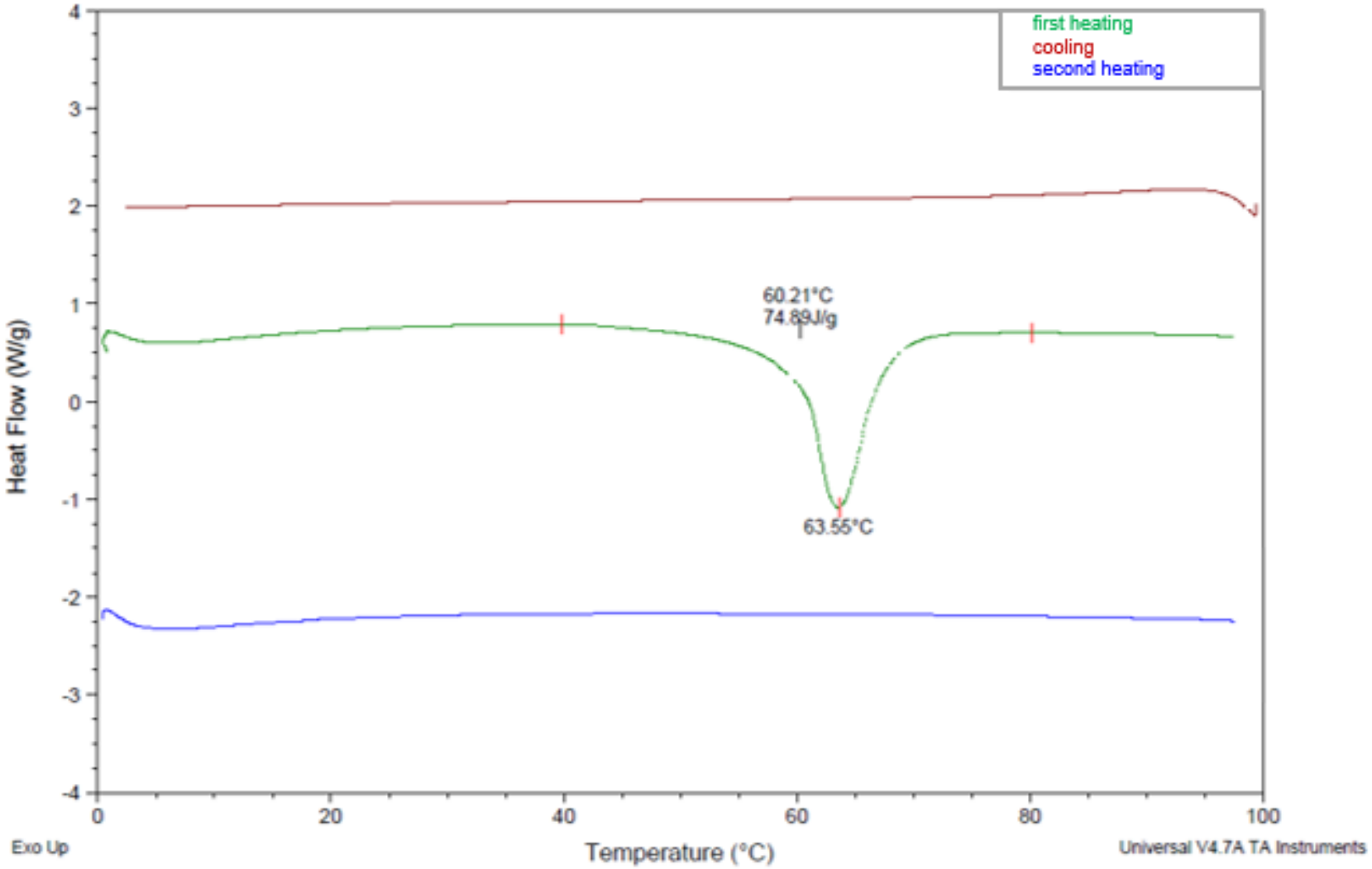


Figure S28. The DSC curves of [L-ValOEt][KETO]

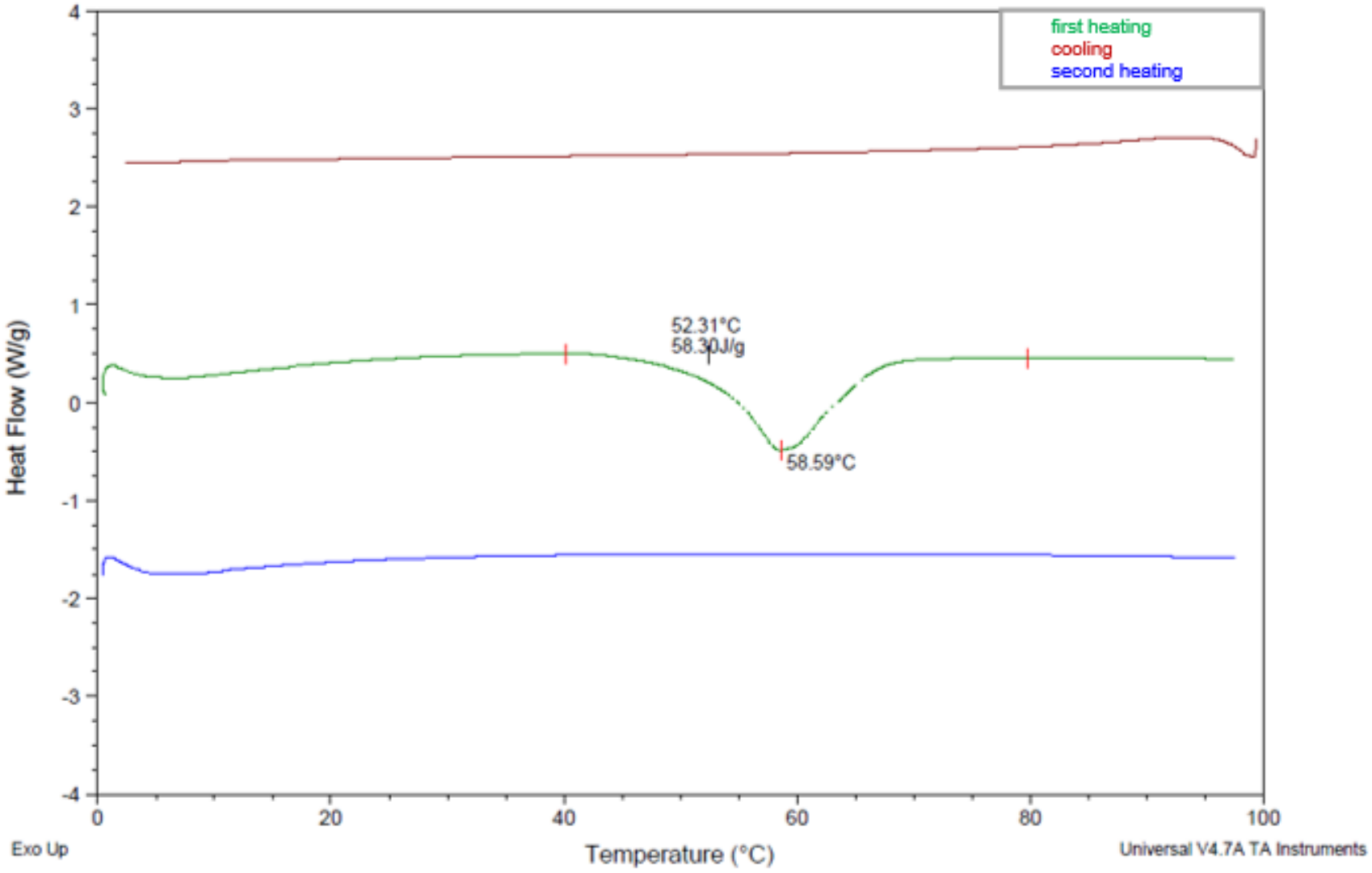


Figure S29. The DSC curves of [L-ValOiPr][KETO]

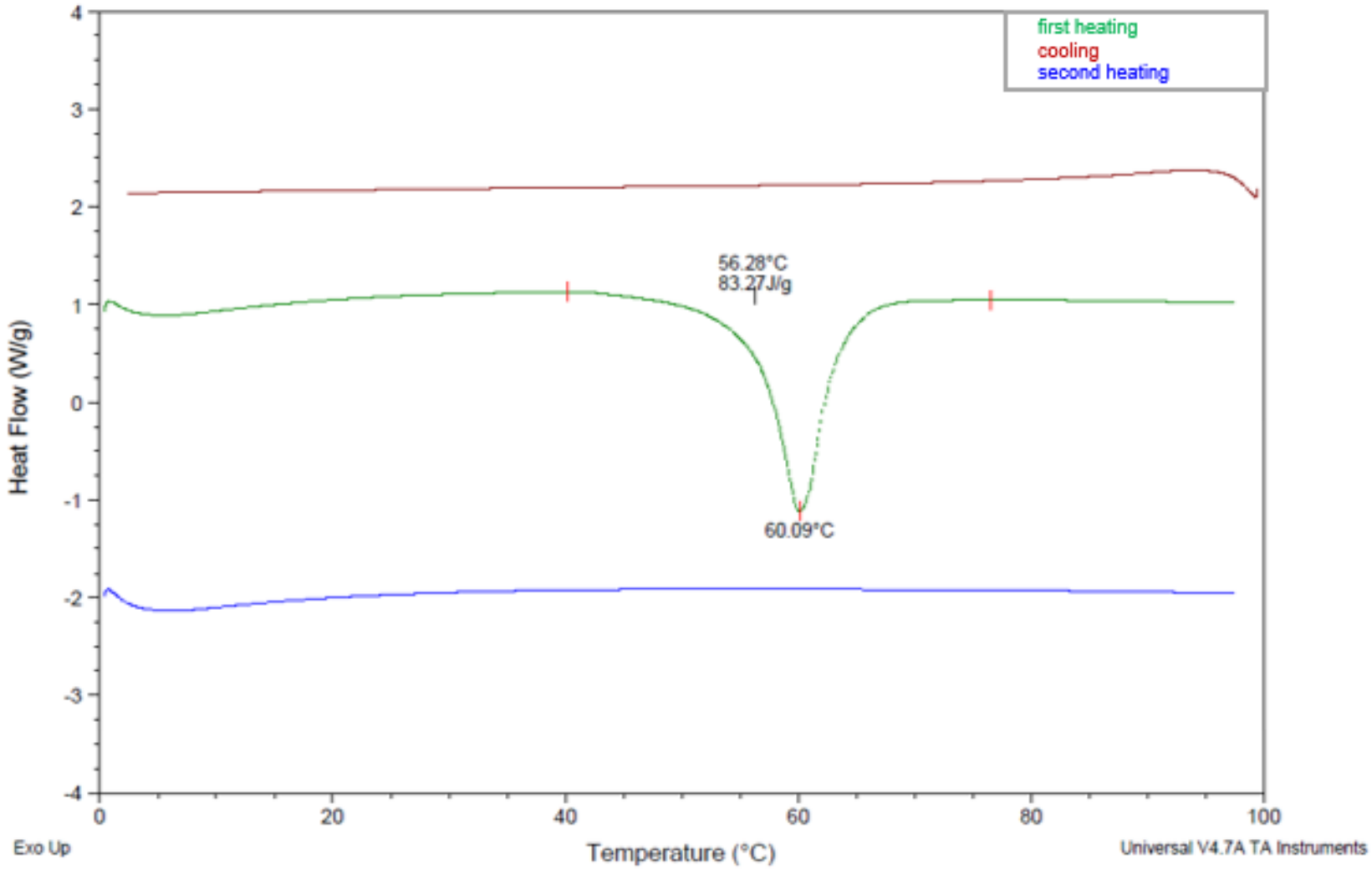


Figure S30. The DSC curves of [L-ValOPr][KETO]

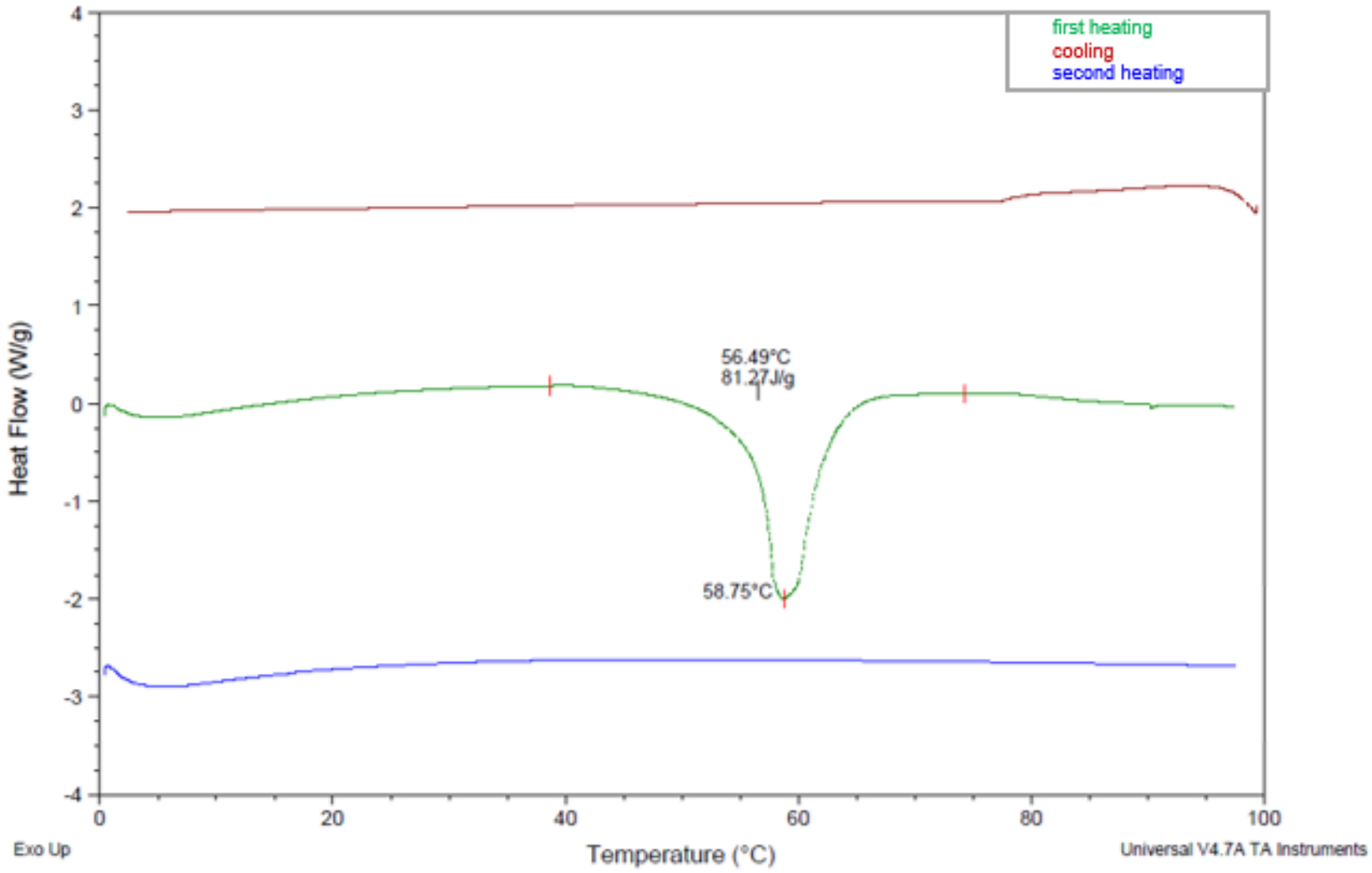


Figure S31. The DSC curves of [L-ValOBu][KETO]

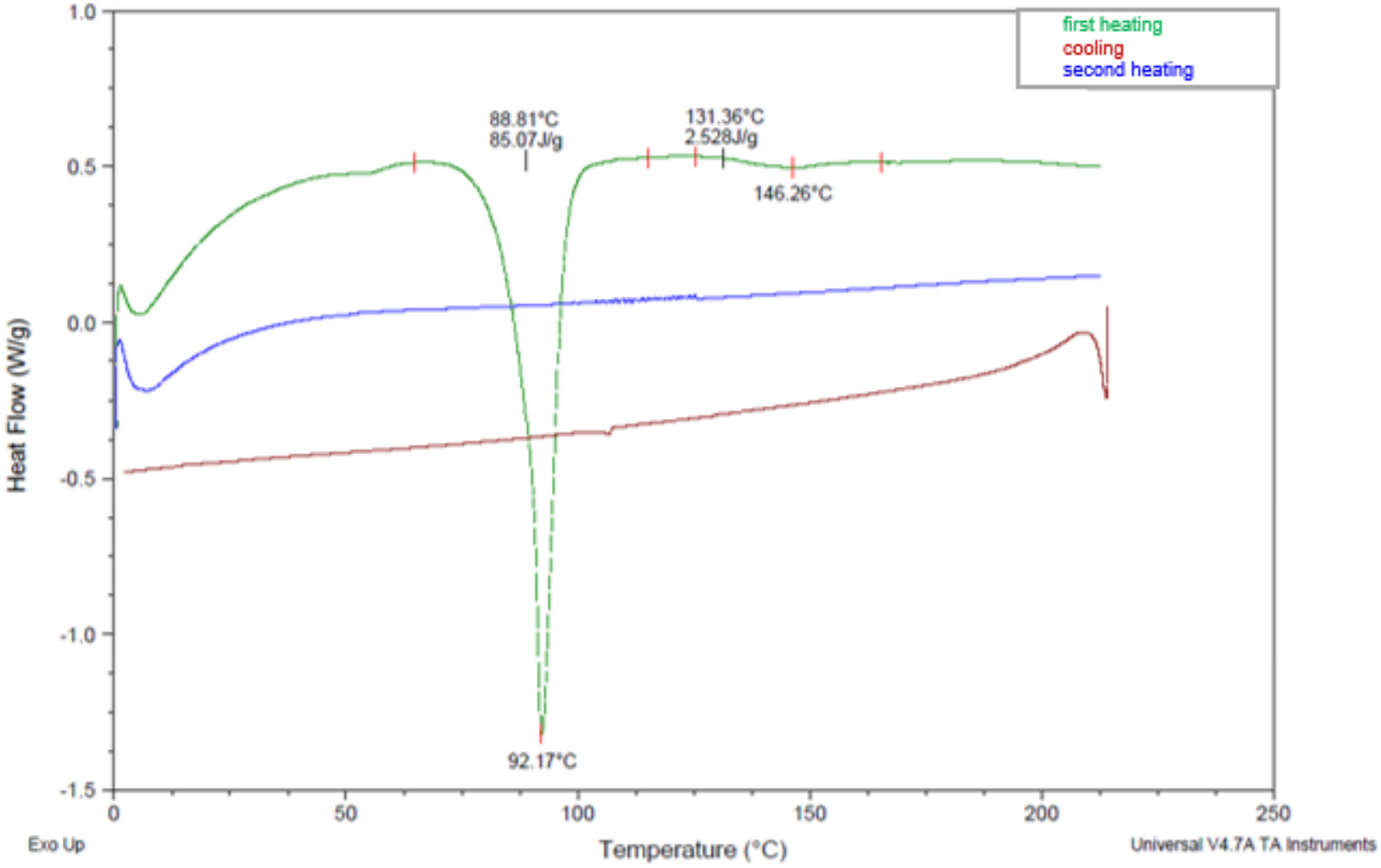
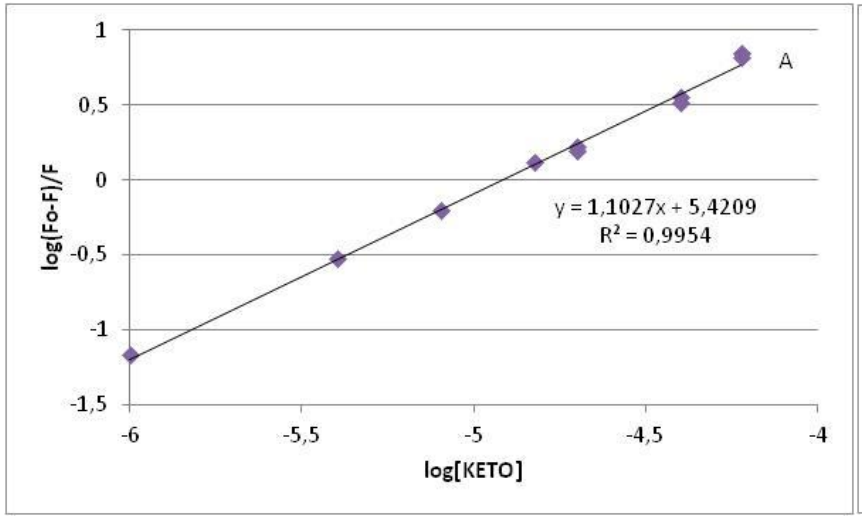
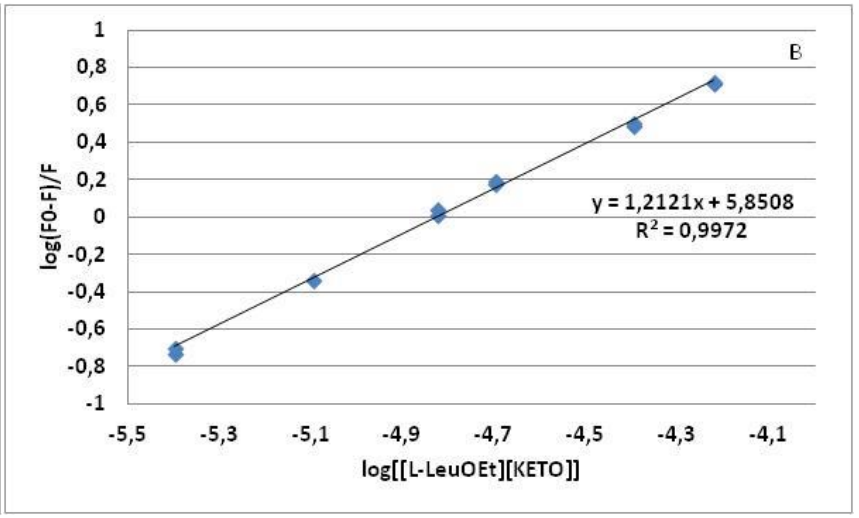
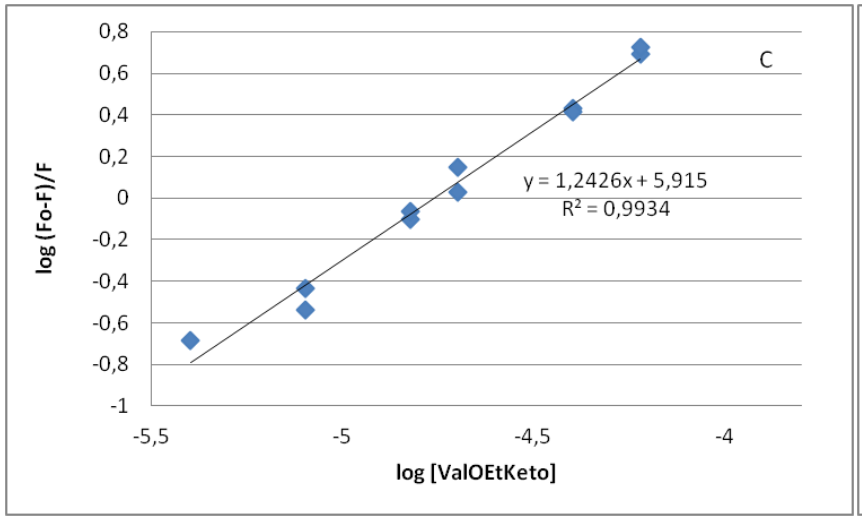
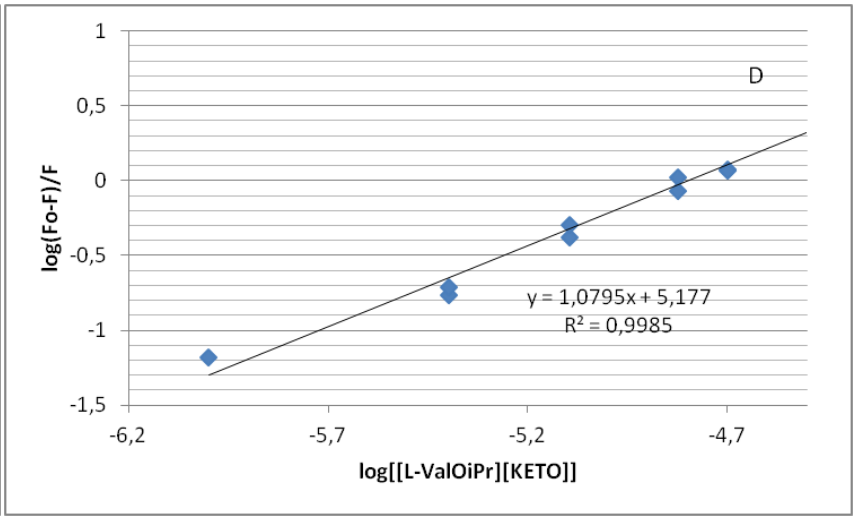


Figure S32. The DSC curves of [KETO]


A
log(Fo-F)/F
log[KETO]
y = 1,1027x + 5,4209
R² = 0,9954
1
0,5
0
-0,5
-1
-1,5
-6
-5,5
-5
-4,5
-4


B
log(FO-F)/F
log[[L-LeuOEt][KETO]]
y = 1,2121x + 5,8508
R² = 0,9972
1
0,8
0,6
0,4
0,2
0
-0,2
-0,4
-0,6
-0,8
-1
-5,5
-5,3
-5,1
-4,9
-4,7
-4,5
-4,3
-4,1


C
log (Fo-F)/F
log [ValOEtKeto]
y = 1,2426x + 5,915
R² = 0,9934
0,8
0,6
0,4
0,2
0
-0,2
-0,4
-0,6
-0,8
-1
-5,5
-5
-4,5
-4


D
log(Fo-F)/F
log[[L-ValOiPr][KETO]]
y = 1,0795x + 5,177
R² = 0,9985
1
0,5
0
-0,5
-1
-1,5
-6,2
-5,7
-5,2
-4,7

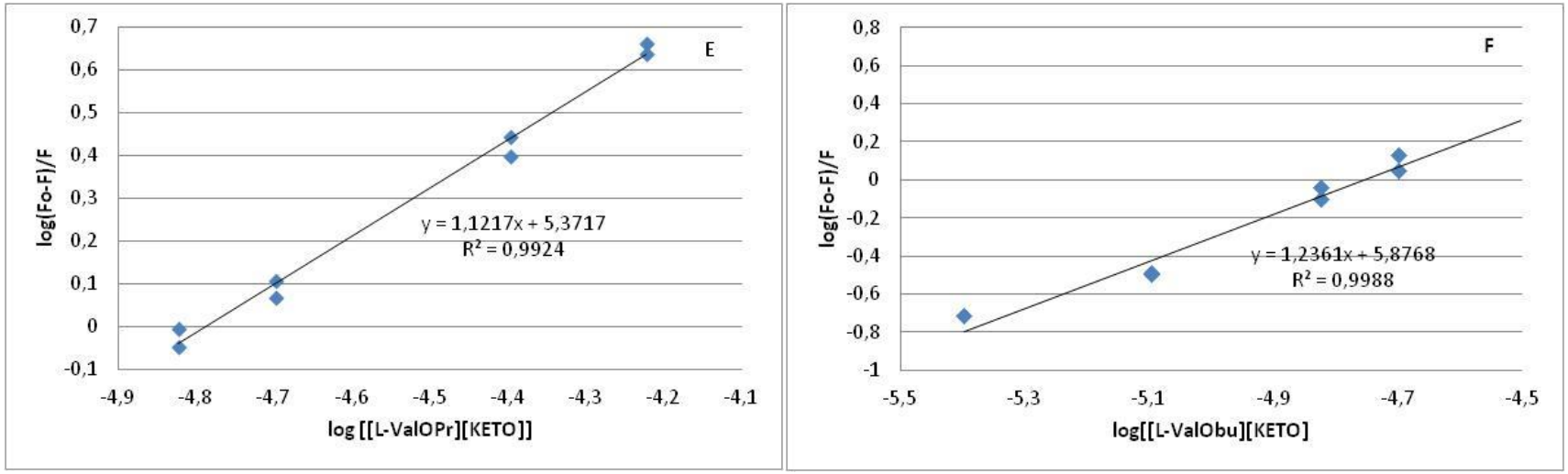


Fig. S33. The plot of log (Fo-F)/F vs log. [Q] at 25ºC, where Q is ketoprofen (A); [L-LeuOEt][KETO] (B); [L-ValOEt][KETO] (C); [L-ValOiPr][KETO] (D) [L-ValOPr][KETO] (E) and [L-ValOBu][KETO] (F).

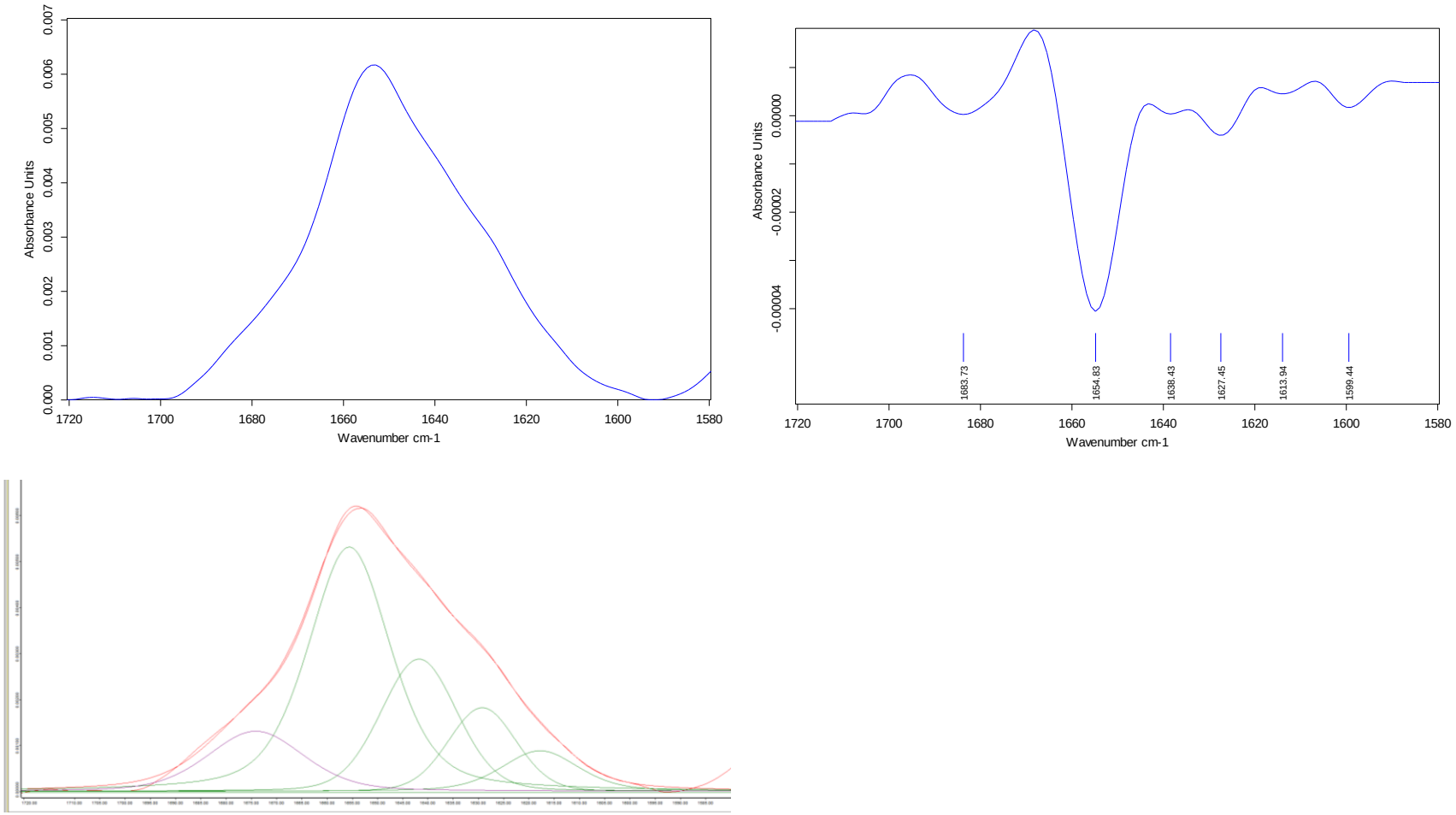


Fig. S34. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I region of native BSA in PBS buffer (pH 7.4, 50 mM) at concentration of 20 mg/mL.

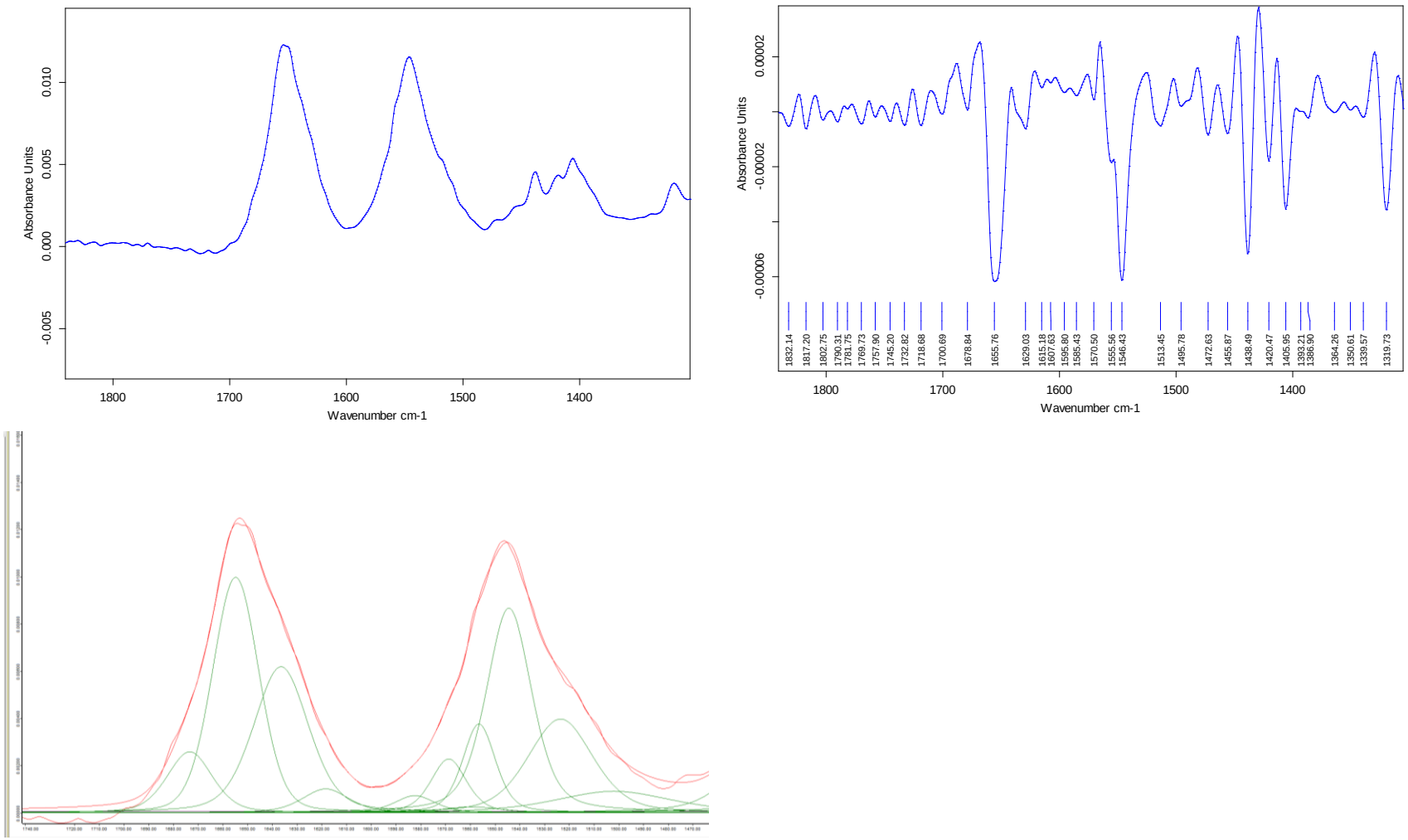


Fig. S35. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-ketoprofen (1:1) in PBS buffer (pH 7.4, 50 mM).

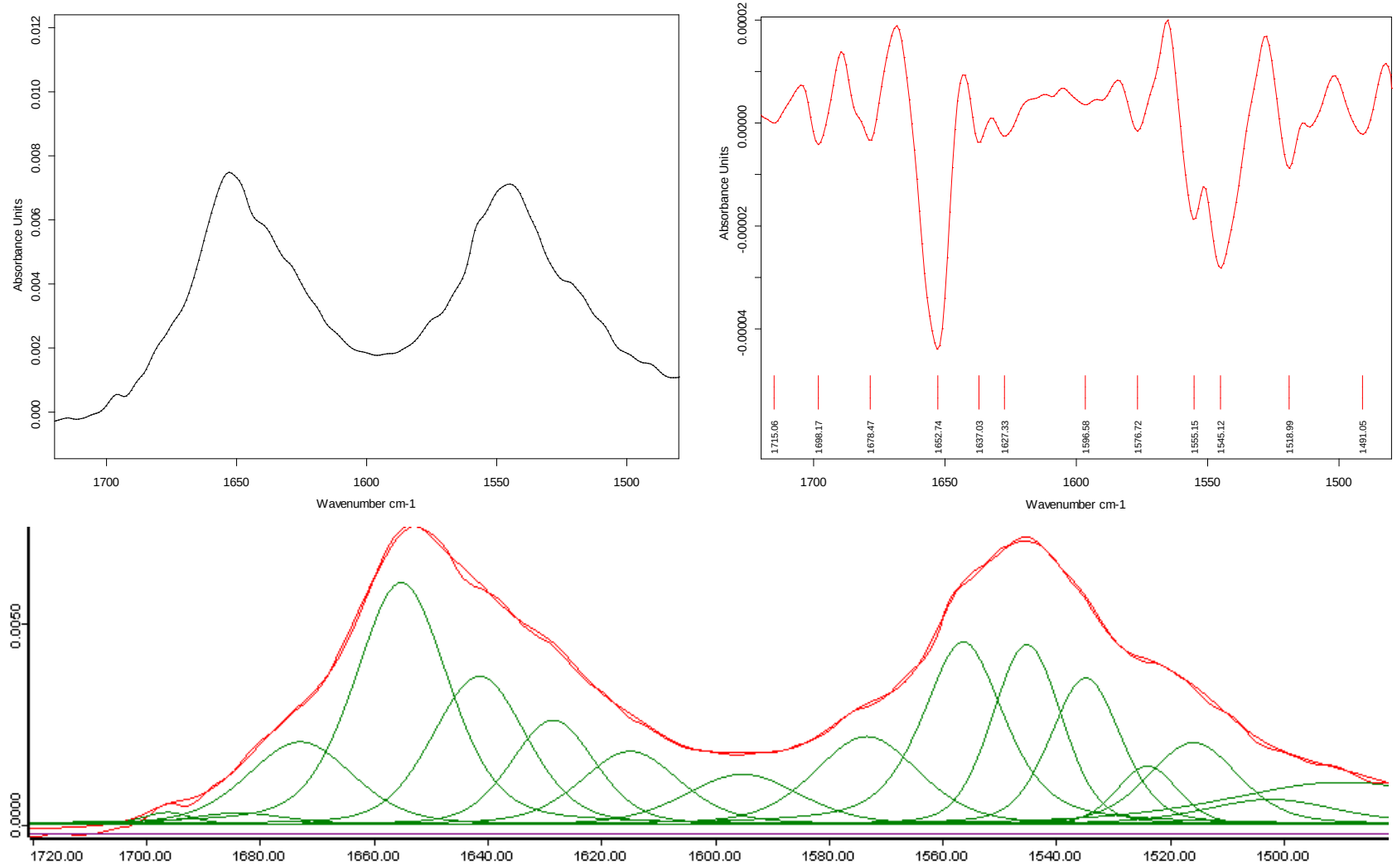


Fig. S36. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-[L-LeuOEt][KETO] (1:1) in PBS buffer (pH 7.4, 50 mM).

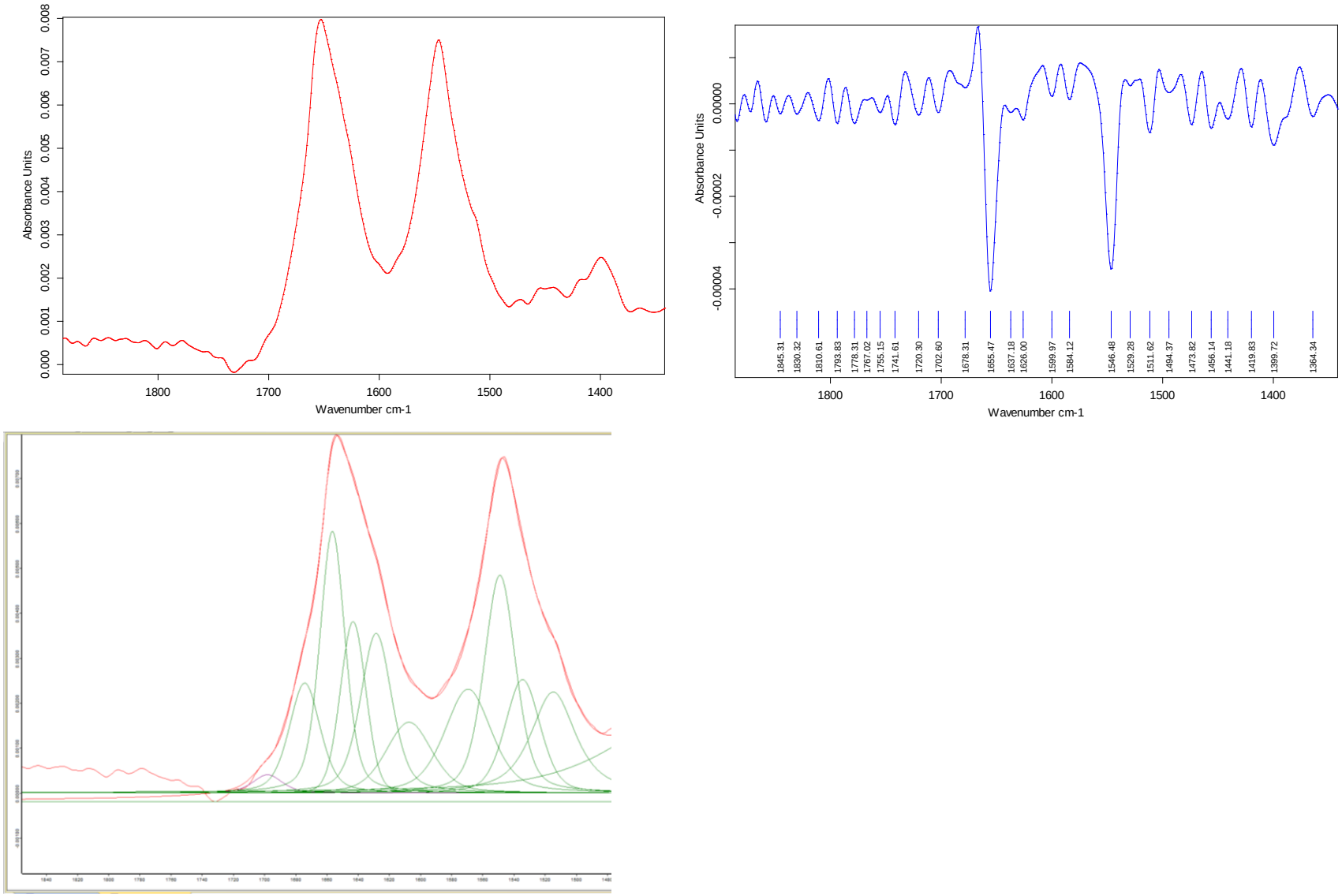


Fig. S37. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-[L-ValOEt][KETO] (1:1) in PBS buffer (pH 7.4, 50 mM).

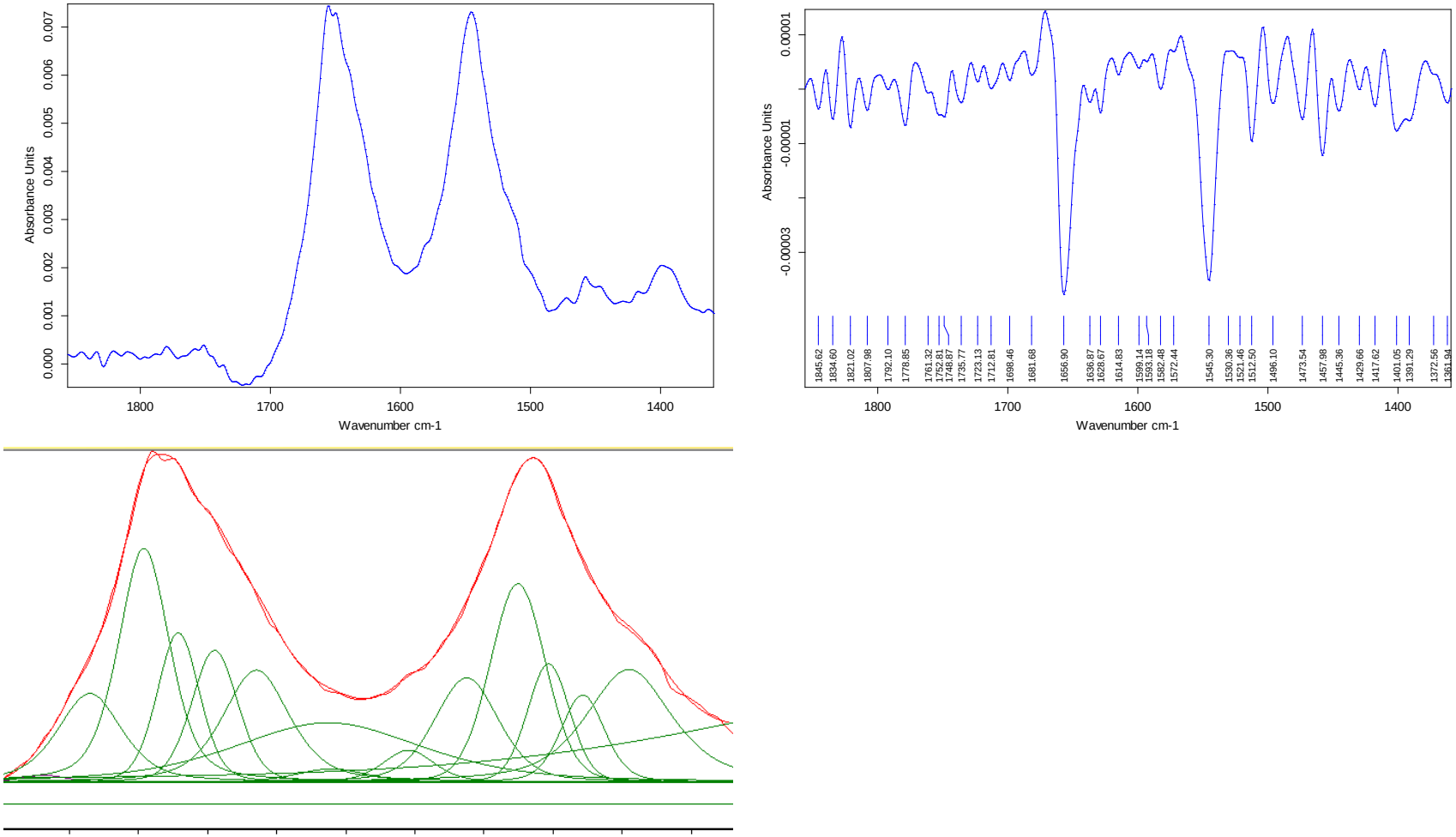


Fig. S38. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-[L-ValOiPr][KETO] (1:1) in PBS buffer (pH 7.4, 50 mM).

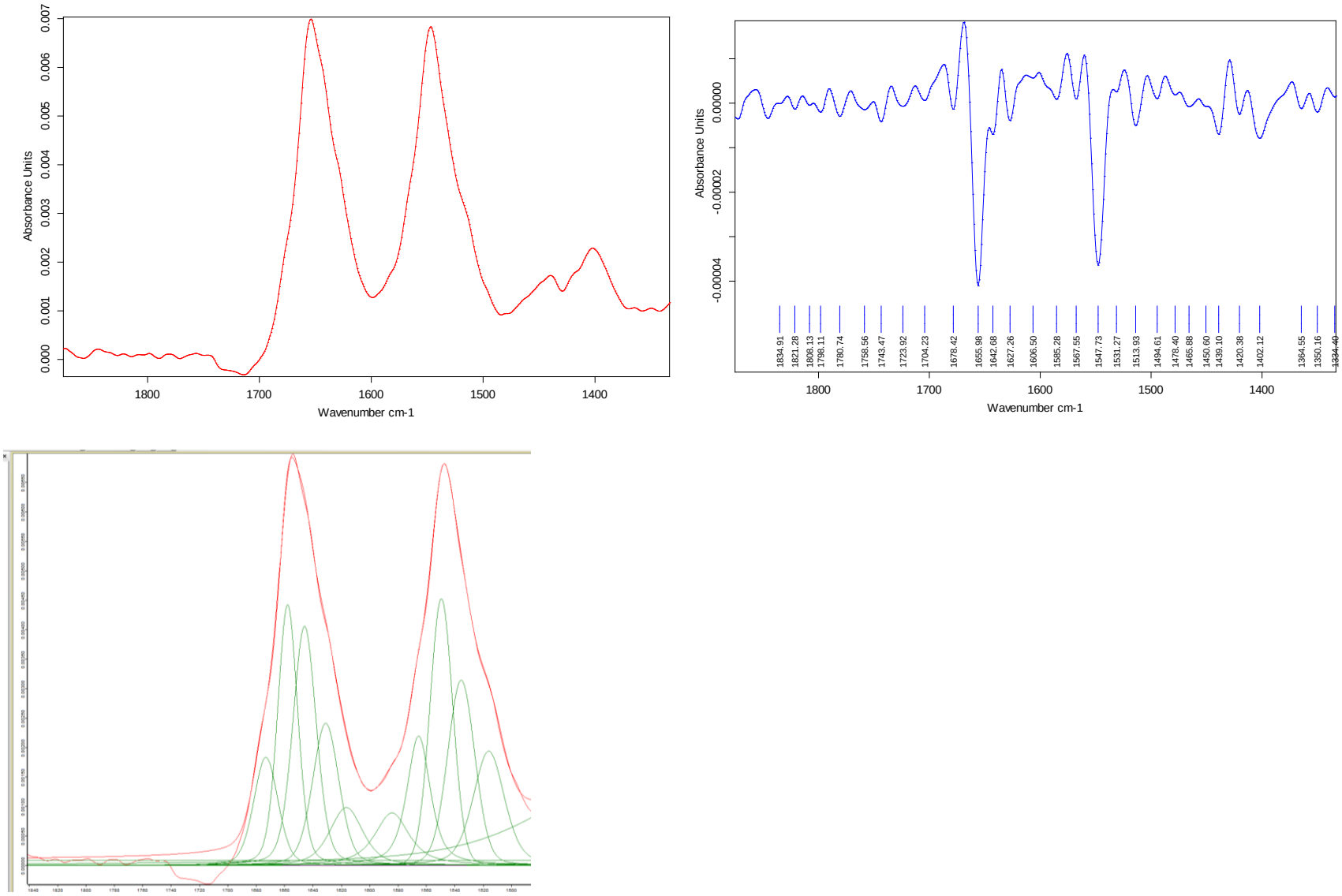


Fig. S39. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-[L-ValOPr][KETO] (1:1) in PBS buffer (pH 7.4, 50 mM).

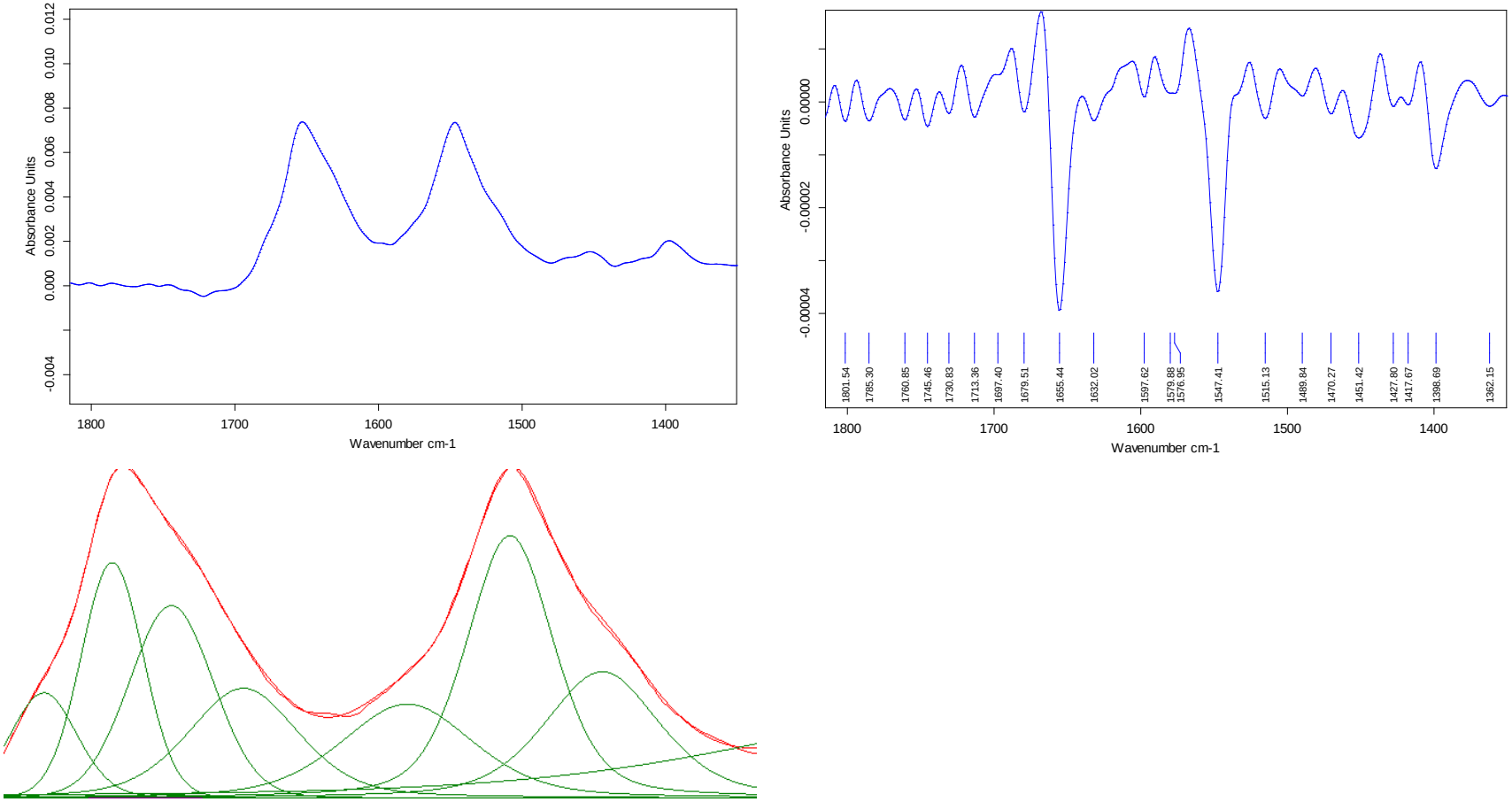


Fig. S40. The original (a), second derivative and deconvoluted ATR-FTIR spectra in Amide I and Amide II region of native BSA-[L-ValOBu][KETO] (1:1) in PBS buffer (pH 7.4, 50 mM).