

Support Information

α -alkylidene δ -lactones inhibit quorum sensing phenotypes in *Chromobacterium* strain CV026 showing interaction within the CviR receptor

Fernanda Favero^{1,2}, Terezinha A. Tolentino¹, Vinicius Fernandes³, Werner Treptow^{3æ}, Alex L. Pereira^{2§}, Angelo H.L. Machado^{1*}.

1: Instituto de Química, Universidade de Brasília, Campus Universitário Darcy Ribeiro, Asa Norte, Brasília, DF, 70910-900, Brazil

2: Campus of Ceilândia, University of Brasília, Centro Metropolitano, Conjunto A, Ceilândia Sul, Brasília, DF, 72220-275, Brazil

3: Laboratório de Biologia Teórica e Computacional, Departamento de Biologia Celular, Universidade de Brasília, Campus Universitário Darcy Ribeiro, Asa Norte, Brasília, DF, 70910-900, Brazil

Corresponding authors. *Angelo H. L. Machado - E-mail: nagelo@unb.br

§ Alex L. Pereira - E-mail: alexpereira@unb.br

æ Werner Treptow - E-mail: treptow@unb.br

Content:

1. Schemes and figures: Page 5–19

Schemes S1. Synthesis of chlorolactone (20).
Scheme S2. Violacein quantification assay.
Figure S1. Violacein quantification assay for 10E .
Figure S2. Violacein quantification assay for 10Z .
Figure S3. Violacein quantification assay for 11E .
Figure S4. Violacein quantification assay for 11Z .
Figure S5. Violacein quantification assay for 12E .
Figure S6. Violacein quantification assay for 12Z .
Figure S7. Violacein quantification assay for 13E .
Figure S8. Violacein quantification assay for 13Z .
Figure S9. Violacein quantification assay for 14E .
Figure S10. Violacein quantification assay for 15E .
Figure S11. Violacein quantification assay for 16E .
Figure S12. Violacein quantification assay for 17E .
Figure S13. Violacein quantification assay for 18E .
Figure S14. Violacein quantification assay for 19E .
Figure S15. Violacein quantification assay for 20 .
Figure S16. Ligand binding domain for 2/CviR .
Figure S17. Ligand binding domain for 20/CviR .
Figure S18. Overlap of 2 with 10E , and ligand binding domain for 10E/CviR , respectively.
Figure S19. Overlap of 2 with 10Z , and ligand binding domain for 10Z/CviR , respectively.
Figure S20. Overlap of 2 with 11E , and ligand binding domain for 11E/CviR , respectively.
Figure S21. Overlap of 2 with 11Z , and ligand binding domain for 11Z/CviR , respectively.
Figure S22. Overlap of 2 with 12E , and ligand binding domain for 12E/CviR , respectively.
Figure S23. Overlap of 2 with 12E , and ligand binding domain for 12E/CviR , respectively.
Figure S24. Overlap of 2 with 13E , and ligand binding domain for 13E/CviR , respectively.
Figure S25. Overlap of 2 with 13Z , and ligand binding domain for 13E/CviR , respectively.
Figure S26. Overlap of 2 with 14E , and ligand binding domain for 14E/CviR , respectively.
Figure S27. Overlap of 2 with 15E , and ligand binding domain for 15E/CviR , respectively.
Figure S28. Overlap of 2 with 16E , and ligand binding domain for 16E/CviR , respectively.
Figure S29. Overlap of 2 with 17E , and ligand binding domain for 17E/CviR , respectively.
Figure S30. Overlap of 2 with 18E , and ligand binding domain for 18E/CviR , respectively.
Figure S31. Overlap of 2 with 19E , and ligand binding domain for 19E/CviR , respectively.
Figure S32. (A): Chemical structure of 21 .; B: CviR (PDB ID: 3PQ5) complex with 21 (blue), in yellow is shown HHL to exemplify the LBD.; (C): LBD complex with 21 (blue), in yellow is shown HHL (2) to exemplify the LBD.

S2.1. ¹ H NMR spectrum of 8 (E/Z) R = Methyl in CDCl ₃ .	S2.2. ¹³ C NMR spectrum of 8 (E/Z) R = Methyl in CDCl ₃ .
S2.3. ¹ H NMR spectrum of 8 (E/Z) R = Ethyl in CDCl ₃ .	S2.4. ¹³ C NMR spectrum of 8 (E/Z) R = Ethyl in CDCl ₃ .
S2.5. ¹ H NMR spectrum of 8 (E/Z) R = n-Hexyl in CDCl ₃ .	S2.6. ¹³ C NMR spectrum of 8 (E/Z) R = n-Hexyl in CDCl ₃ .
S2.7. ¹ H NMR spectrum of 8 (E/Z) R = n-Heptyl in CDCl ₃ .	S2.8. ¹³ C NMR spectrum of 8 (E/Z) R = n-Heptyl in CDCl ₃ .
S2.9. ¹ H NMR spectrum of 8 (E/Z) R = iso-Propyl in CDCl ₃ .	S2.10. ¹³ C NMR spectrum of 8 (E/Z) R = iso-Propyl in CDCl ₃ .
S2.11. ¹ H NMR spectrum of 8 (E) R = Phenyl in CDCl ₃ .	S2.12. ¹³ C NMR spectrum of 8 (E) R = Phenyl in CDCl ₃ .
S2.13. ¹ H NMR spectrum of 8 (E) R = 4-Cl-Phenyl in CDCl ₃ .	S2.14. ¹³ C NMR spectrum of 8 (E) R = 4-Cl-Phenyl in CDCl ₃ .
S2.15. ¹ H NMR spectrum of 8 (E) R = 4-Br-Phenyl in CDCl ₃ .	S2.16. ¹³ C NMR spectrum of 8 (E) R = 4-Br-Phenyl in CDCl ₃ .
S2.17. ¹ H NMR spectrum of 8 (E) R = 3,4-methylenedioxyphenyl in CDCl ₃ .	S2.18. ¹³ C NMR spectrum of 8 (E) R = 3,4-methylenedioxyphenyl in CDCl ₃ .
S2.19. ¹ H NMR spectrum of 8 (E) R = 4-NO₂-Phenyl in CDCl ₃ .	S2.20. ¹³ C NMR spectrum of 8 (E) R = 4-NO₂-Phenyl in CDCl ₃ .
S2.21. ¹ H NMR spectrum of 10E in CDCl ₃ .	S2.22. ¹³ C NMR spectrum of 10E in CDCl ₃ .
S2.23. ¹ H NMR spectrum of 10Z in CDCl ₃ .	S2.24. ¹³ C NMR spectrum of 10Z in CDCl ₃ .
S2.25. ¹ H NMR spectrum of 11E in CDCl ₃ .	S2.26. ¹³ C NMR spectrum of 11E in CDCl ₃ .
S2.27. ¹ H NMR spectrum of 11Z in CDCl ₃ .	S2.28. ¹³ C NMR spectrum of 11Z in CDCl ₃ .
S2.29. ¹ H NMR spectrum of 12E in CDCl ₃ .	S2.30. ¹³ C NMR spectrum of 12E in CDCl ₃ .
S2.31. ¹ H NMR spectrum of 12Z in CDCl ₃ .	S2.32. ¹³ C NMR spectrum of 12Z in CDCl ₃ .
S2.33. ¹ H NMR spectrum of 13E in CDCl ₃ .	S2.34. ¹³ C NMR spectrum of 13E in CDCl ₃ .
S2.35. ¹ H NMR spectrum of 13Z in CDCl ₃ .	S2.36. ¹³ C NMR spectrum of 13Z in CDCl ₃ .
S2.37. ¹ H NMR spectrum of 14E in CDCl ₃ .	S2.38. ¹³ C NMR spectrum of 14E in CDCl ₃ .
S2.39. ¹ H NMR spectrum of 15E in CDCl ₃ .	S2.40. ¹³ C NMR spectrum of 15E in CDCl ₃ .
S2.41. ¹ H NMR spectrum of 16E in CDCl ₃ .	S2.42. ¹³ C NMR spectrum of 16E in CDCl ₃ .
S2.43. ¹ H NMR spectrum of 17E in CDCl ₃ .	S2.44. ¹³ C NMR spectrum of 17E in CDCl ₃ .
S2.45. ¹ H NMR spectrum of 18E in CDCl ₃ .	S2.46. ¹³ C NMR spectrum of 18E in CDCl ₃ .
S2.47. ¹ H NMR spectrum of 19E in CDCl ₃ .	S2.48. ¹³ C NMR spectrum of 19E in CDCl ₃ .
S2.49. ¹ H NMR spectrum of 20 in CDCl ₃ .	S2.50. ¹³ C NMR spectrum of 20 in CDCl ₃ .

S3.1. IR (ATR) spectrum of 10E .	S3.2. IR (ATR) spectrum of 10Z .
S3.3. IR (ATR) spectrum of 11E .	S3.4. IR (ATR) spectrum of 11Z .
S3.5. IR (ATR) spectrum of 12E .	S3.6. IR (ATR) spectrum of 12Z .
S3.7. IR (ATR) spectrum of 13E .	S3.8. IR (ATR) spectrum of 13Z .

S3.9. IR (ATR) spectrum of 14E .	S3.10. IR (ATR) spectrum of 15E .
S3.11. IR (ATR) spectrum of 16E .	S3.12. IR (ATR) spectrum of 17E .
S3.13. IR (ATR) spectrum of 18E	S3.14. IR (ATR) spectrum of 19E .
S3.15. IR (ATR) spectrum of 20 .	

4. HRMS spectra of compounds 10 – 19.

Page 78–91

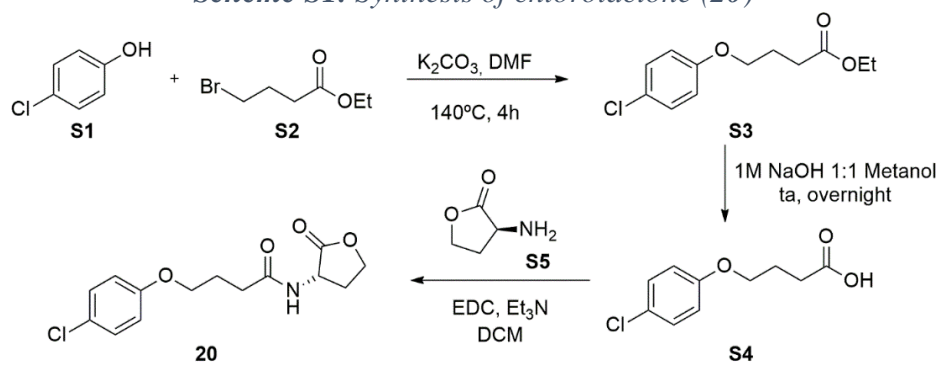
S4.1. HRMS data of 10E .	S4.2. HRMS data of 10Z .
S4.3. HRMS data of 11E .	S4.4. HRMS data of 11Z .
S4.5. HRMS data of 12E .	S4.6. HRMS data of 12Z .
S4.7. HRMS data of 13E .	S4.8. HRMS data of 13Z .
S4.9. HRMS data of 14E .	S4.10. HRMS data of 15E .
S4.11. HRMS data of 16E .	S4.12. HRMS data of 17E .
S4.13. HRMS data of 18E	S4.14. HRMS data of 19E .

5. Purity analyses of compounds 10-20 by GC-MS.

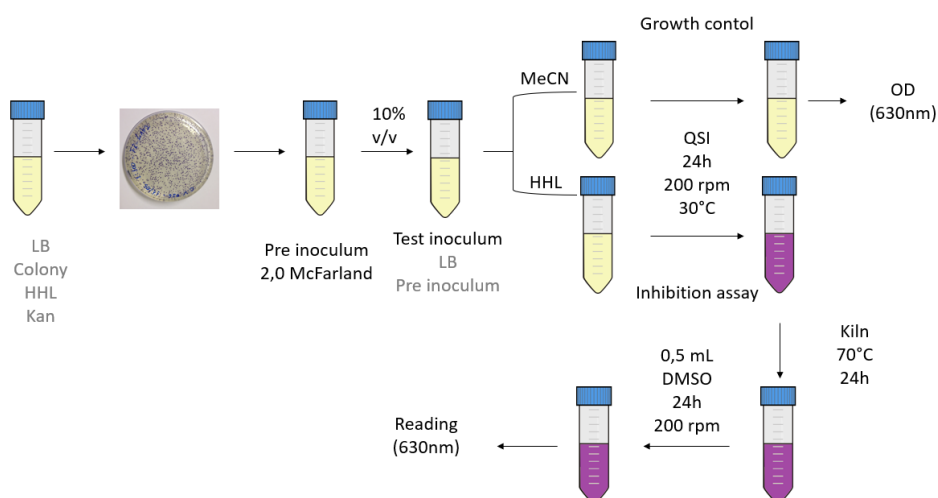
Page 92-105

S5.1. GC-MS data of 10E .	S5.2. GC-MS data of 10Z .
S5.3. GC-MS data of 11E .	S5.4. GC-MS data of 11Z .
S5.5. GC-MS data of 12E .	S5.6. GC-MS data of 12Z .
S5.7. GC-MS data of 13E .	S5.8. GC-MS data of 13Z .
S5.9. GC-MS data of 14E .	S5.10. GC-MS data of 15E .
S5.11. GC-MS data of 16E .	S5.12. GC-MS data of 17E .
S5.13. GC-MS data of 18E	S5.14. GC-MS data of 19E .
S5.15. GC-MS data of 20 .	

Scheme S1. Synthesis of chlorolactone (20)



Scheme S2. Violacein quantification assay.



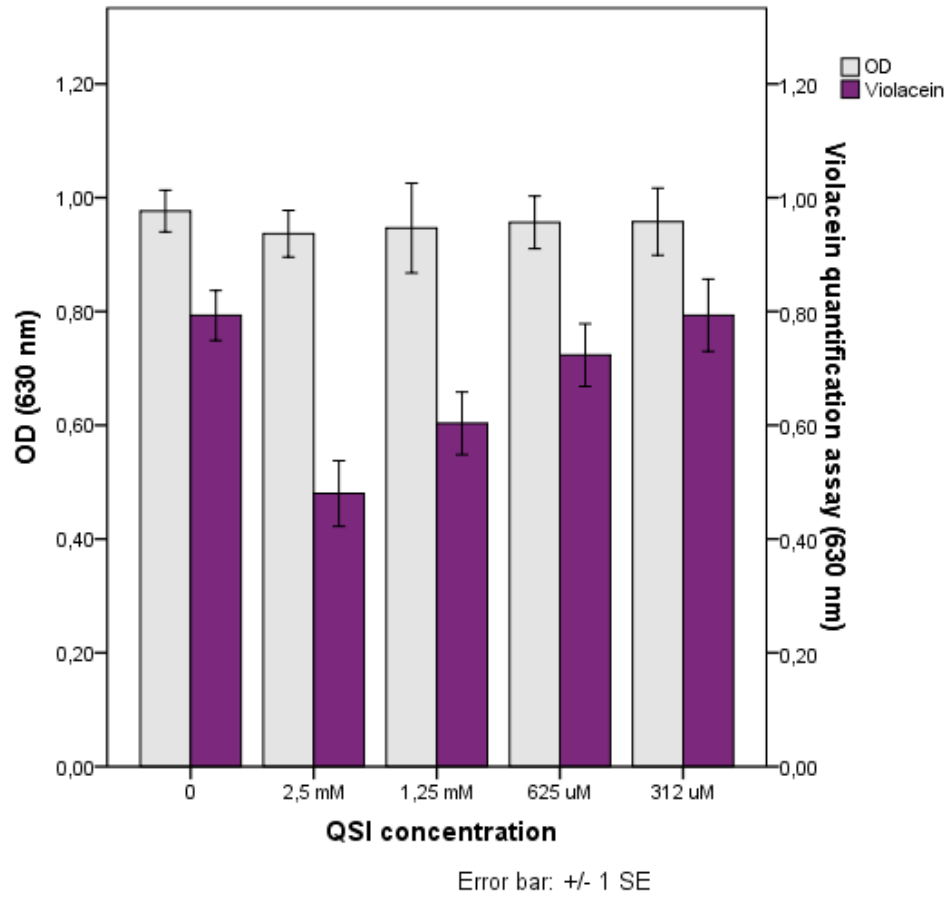


Figure S1. Violacein quantification assay for **10E**.

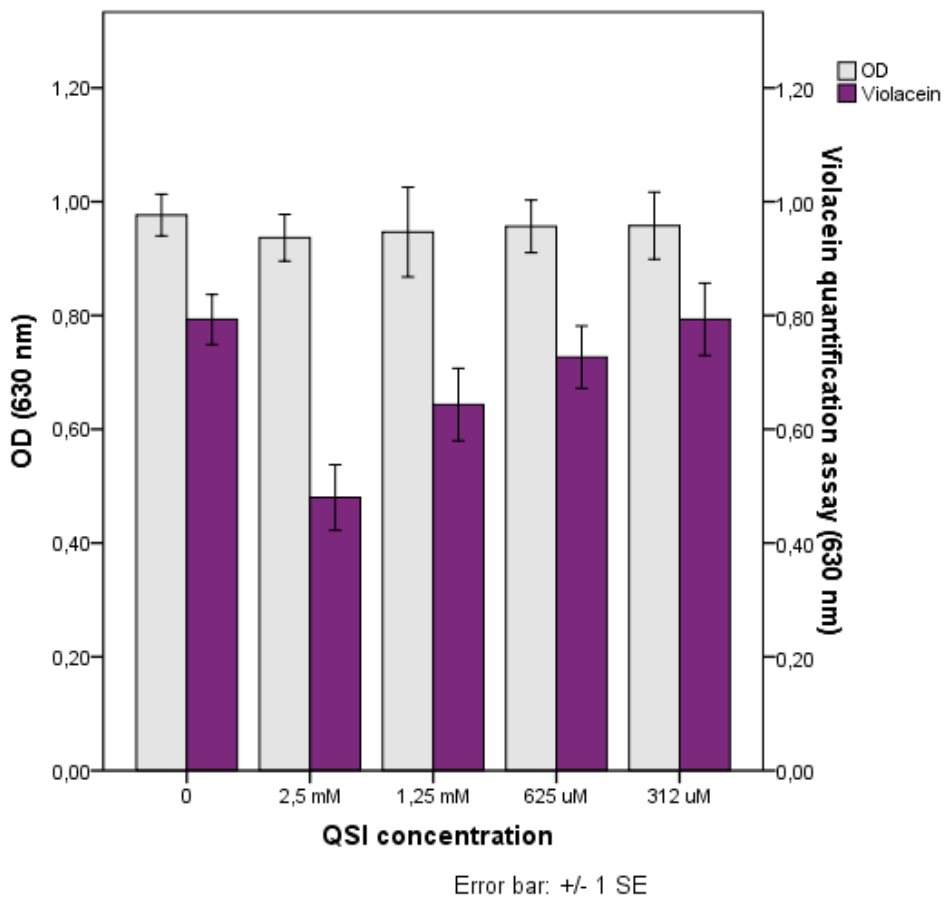


Figure S2. Violacein quantification assay for **10Z**.

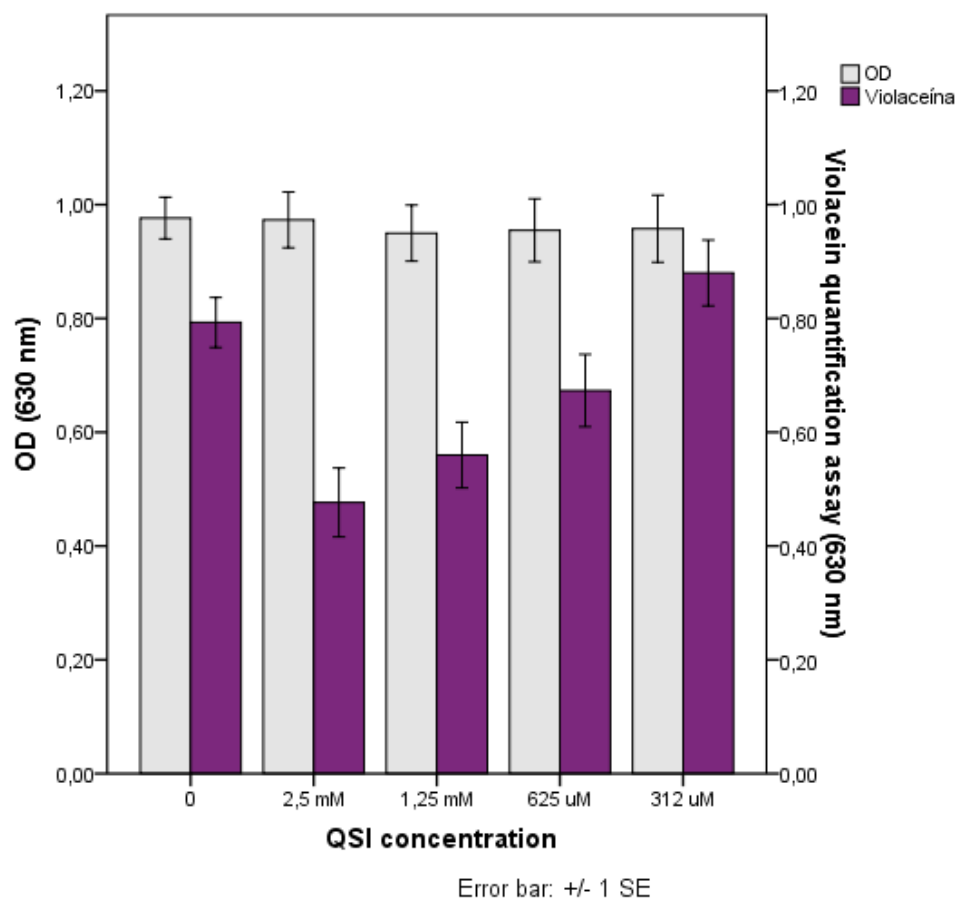


Figure S3. Violacein quantification assay for **11E**.

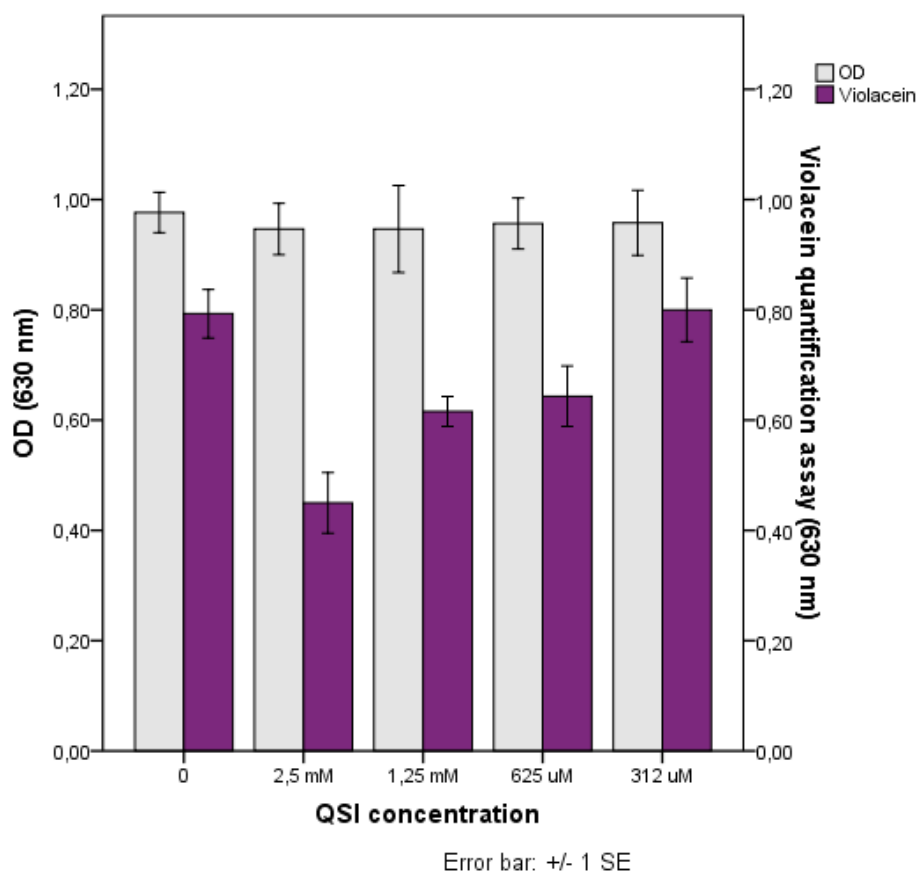


Figure S4. Violacein quantification assay for **11Z**.

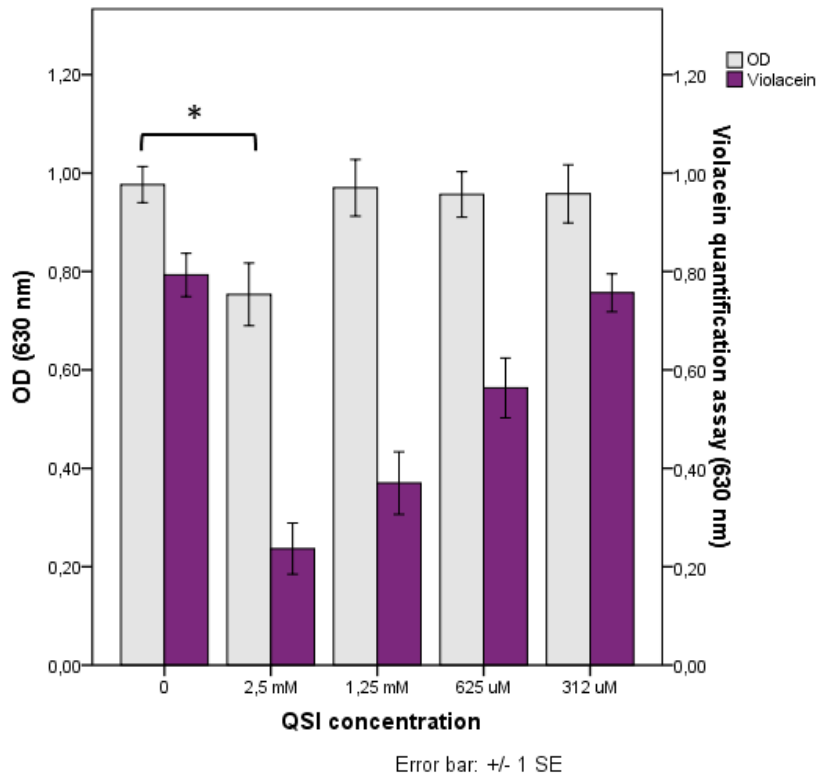


Figure S5. Violacein quantification assay for **12E**.

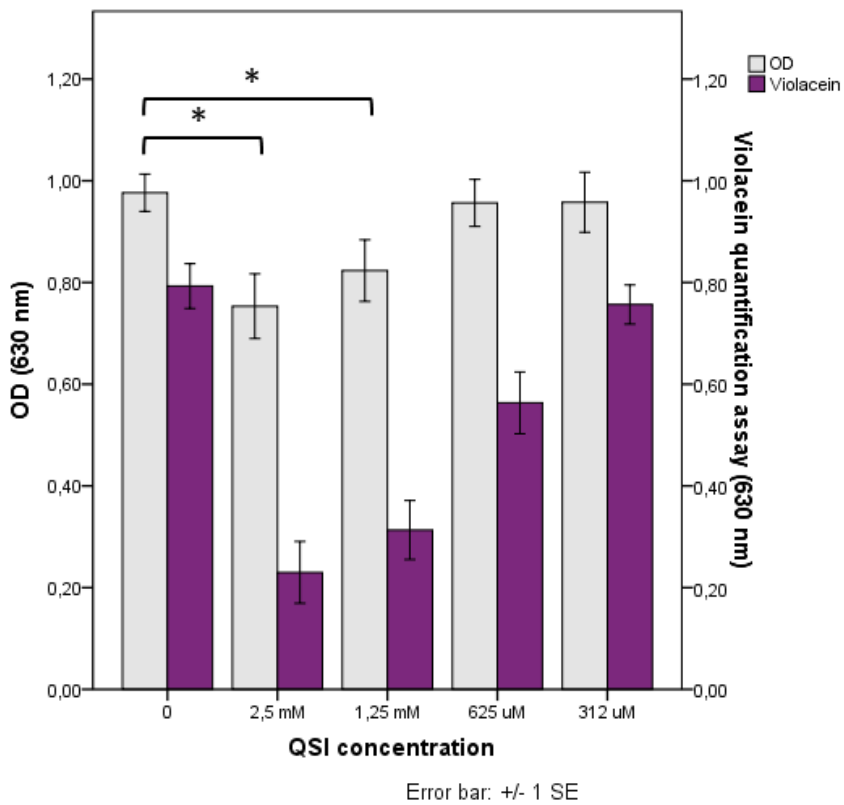


Figure S6. Violacein quantification assay for **12Z**.

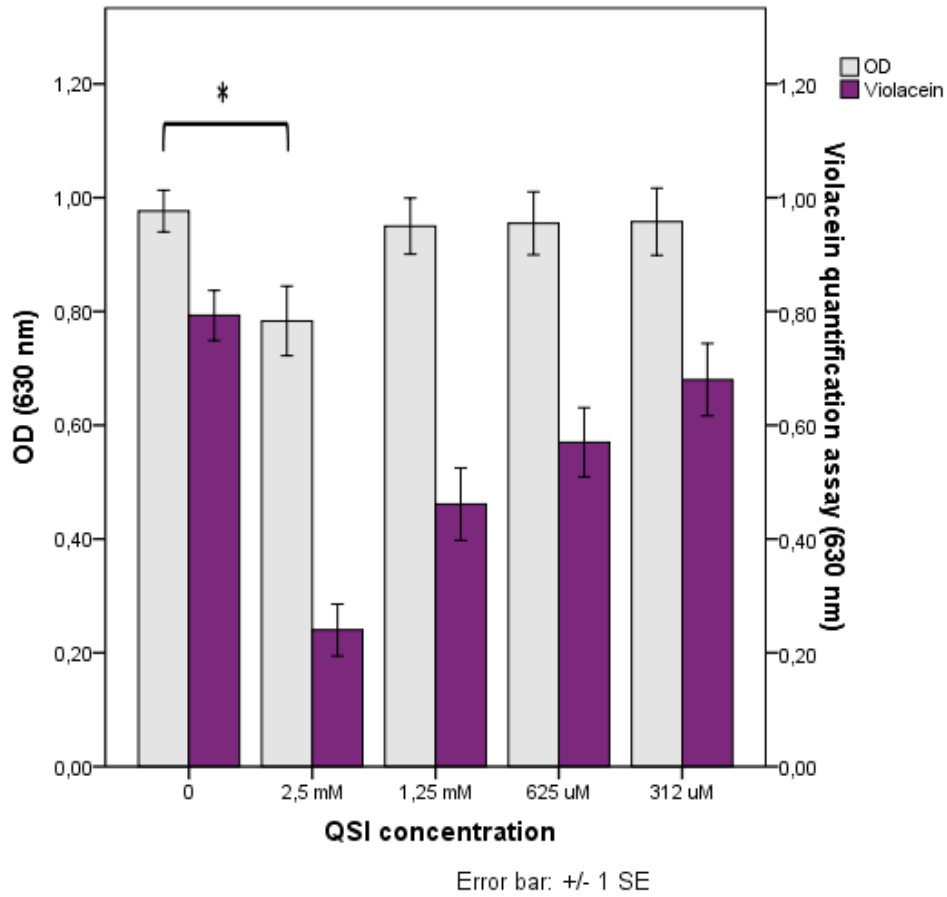


Figure S7. Violacein quantification assay for **13E**.

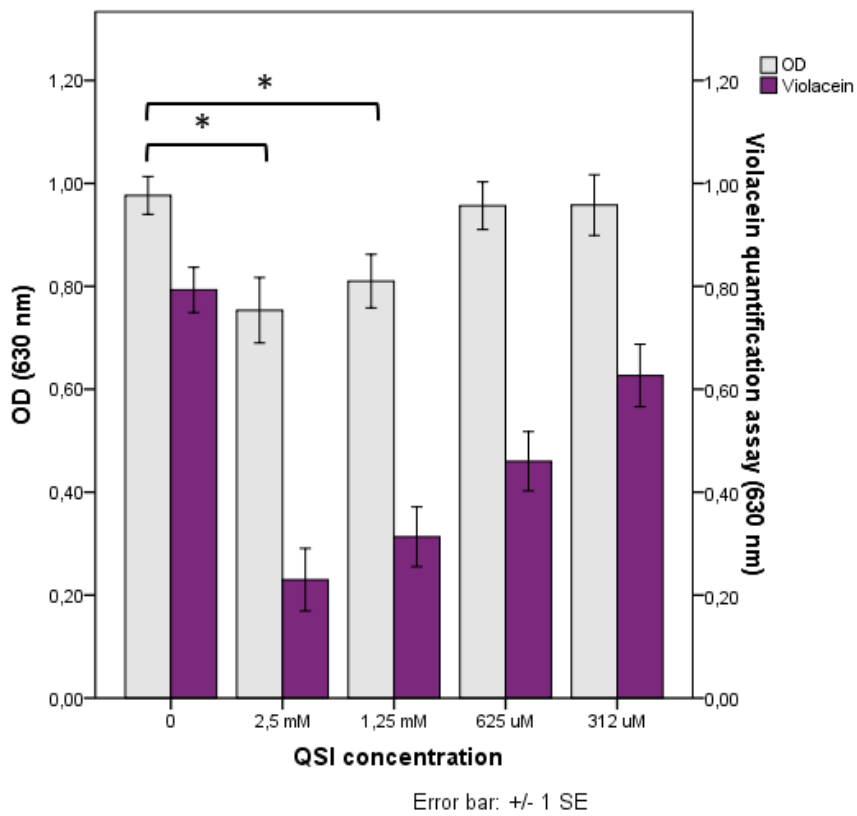


Figure S8. Violacein quantification assay for **13Z**.

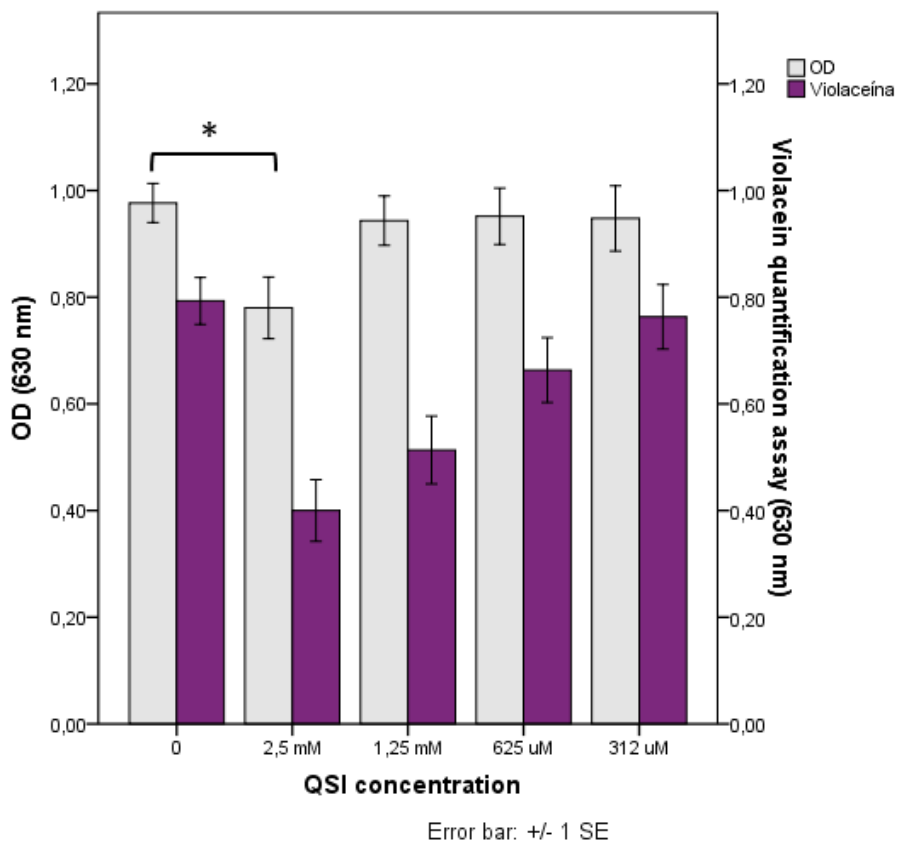


Figure S9. Violacein quantification assay for **14E**.

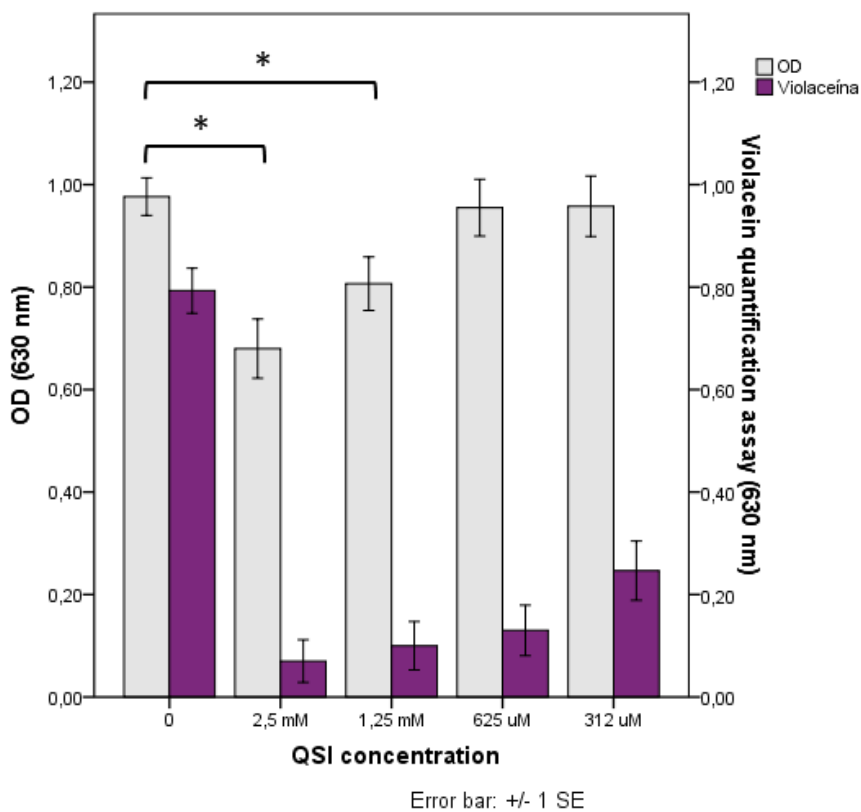


Figure S10. Violacein quantification assay for **15E**.

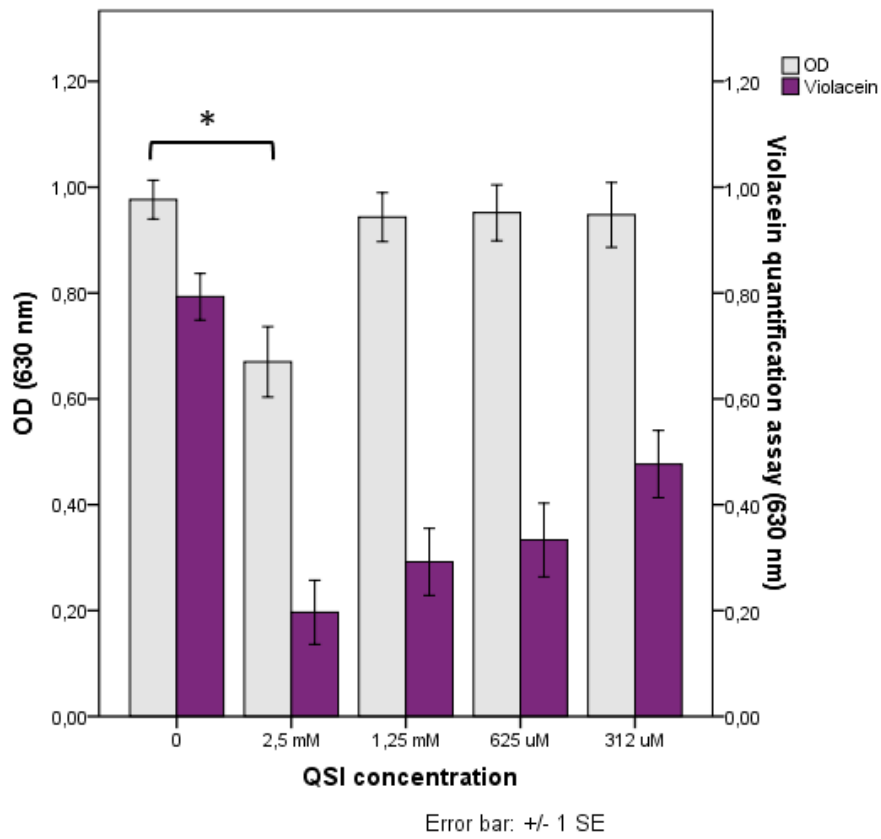


Figure S11. Violacein quantification assay for **16E**.

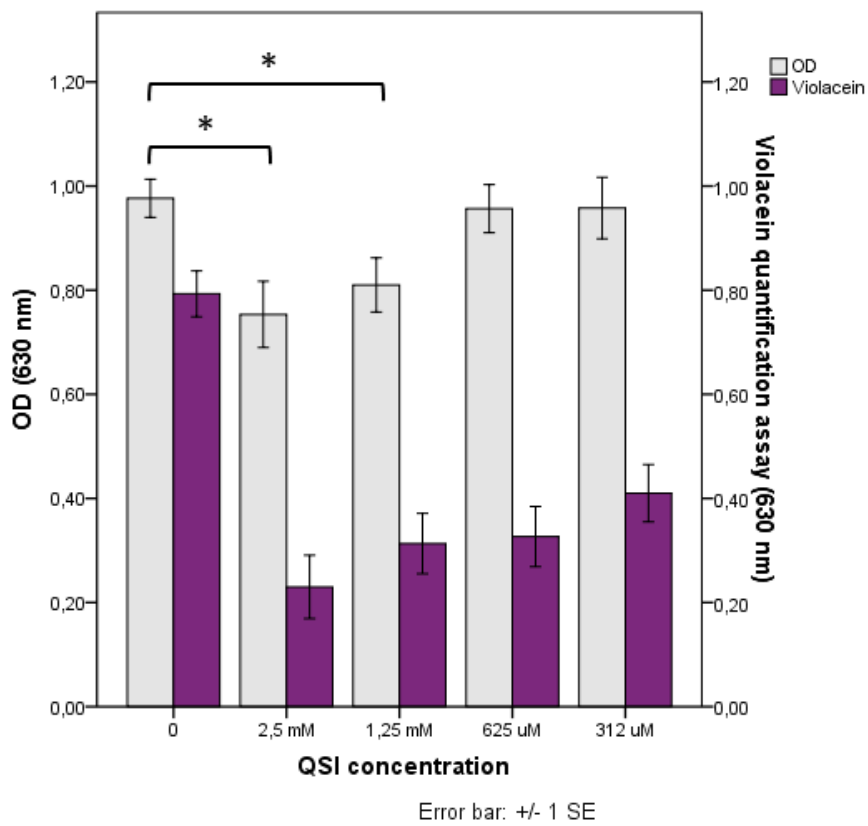


Figure S12. Violacein quantification assay for **17E**.

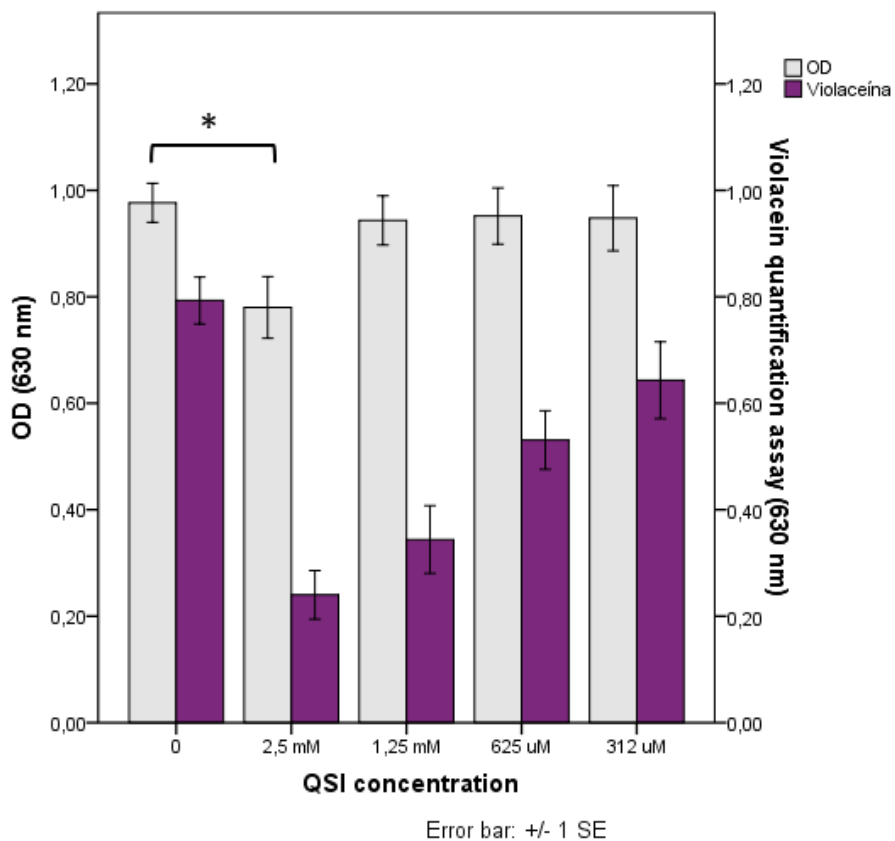


Figure S13. Violacein quantification assay for **18E**.

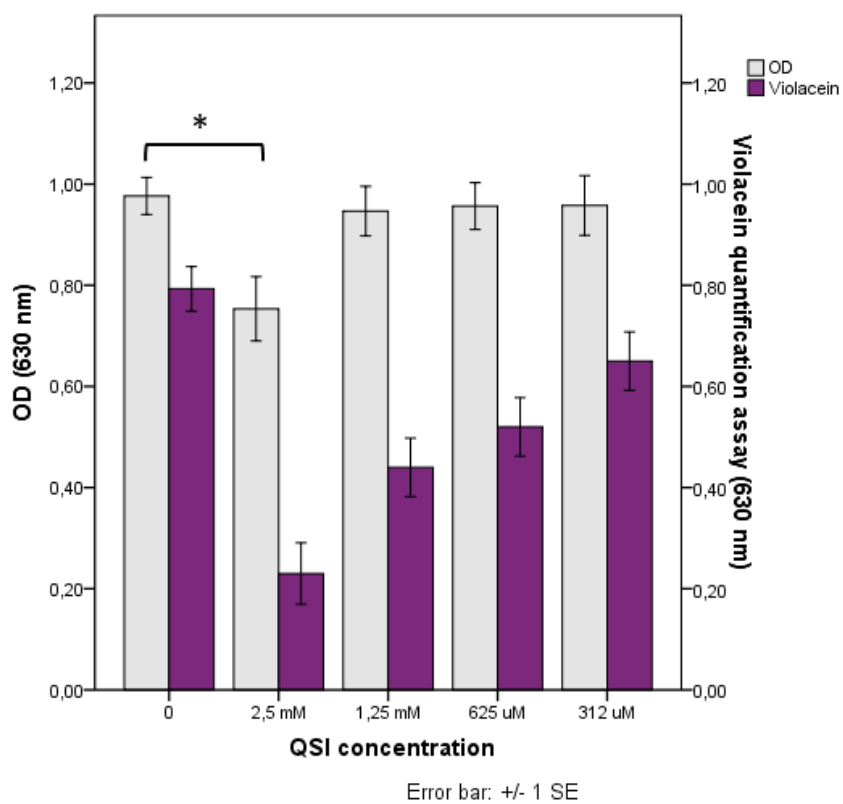


Figure S14. Violacein quantification assay for **19E**.

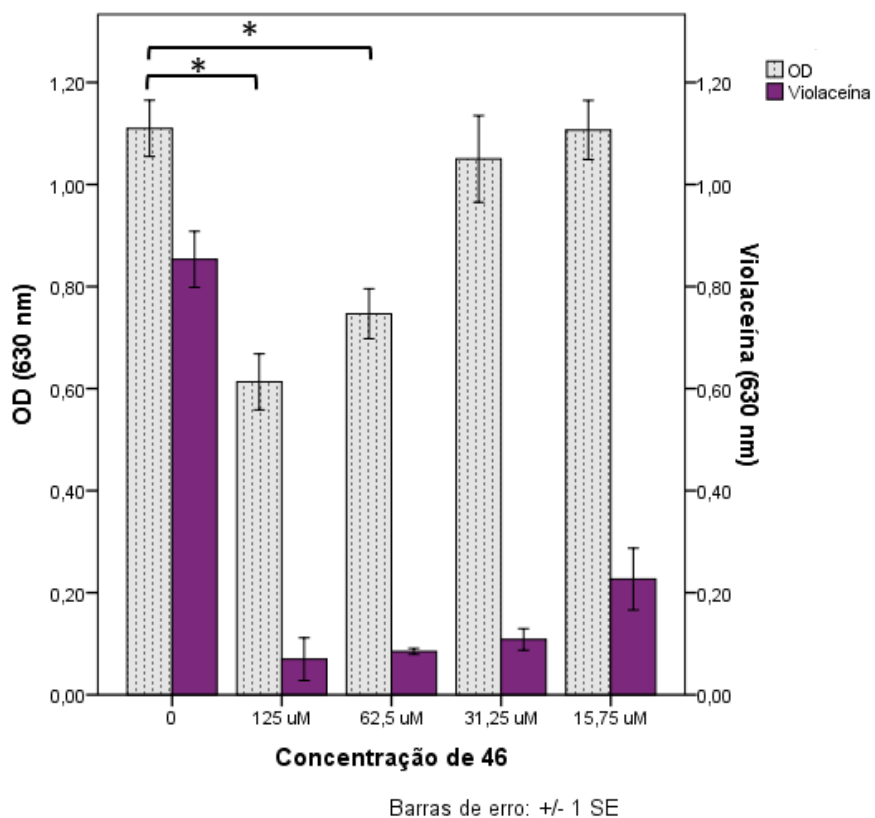


Figure S15. Violacein quantification assay for **20**.

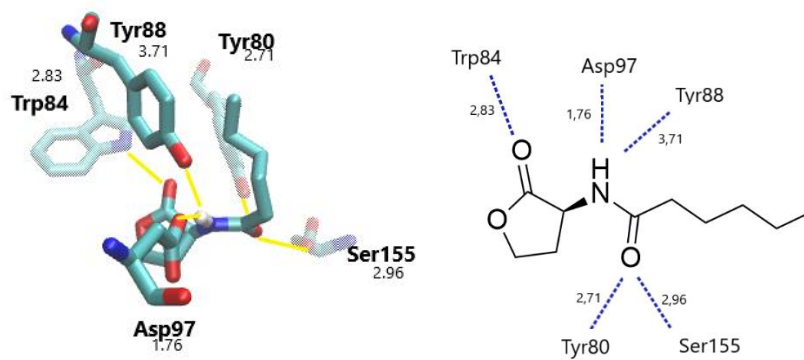


Figure S16. Ligand binding domain for **2/CviR**.

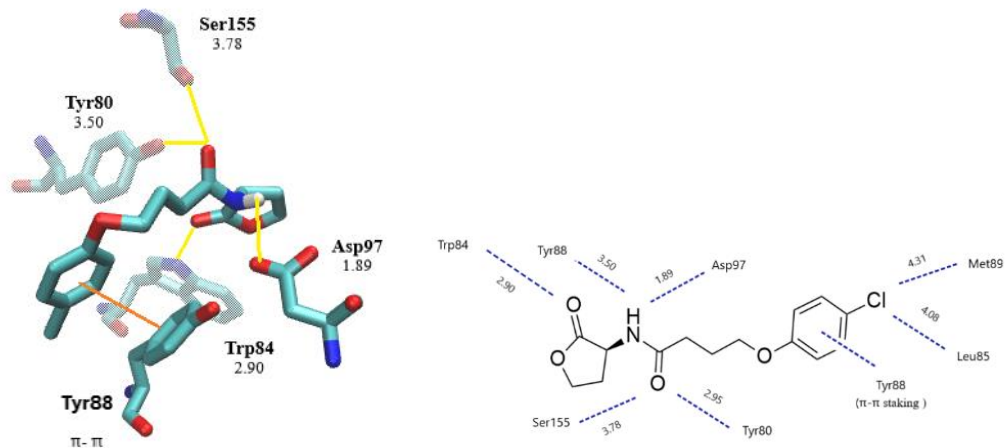


Figure S17. Ligand binding domain for **20/CviR**.

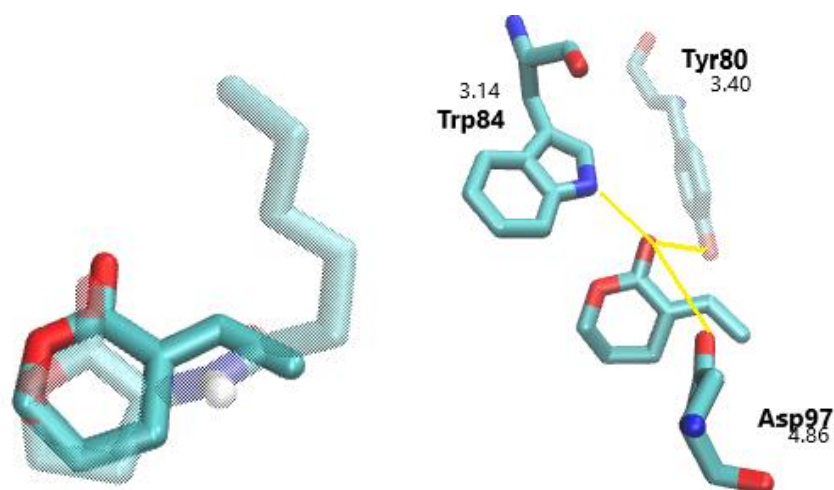


Figure S18. Overlap of **2** with **10E**, and ligand binding domain for **10E/CviR**, respectively.

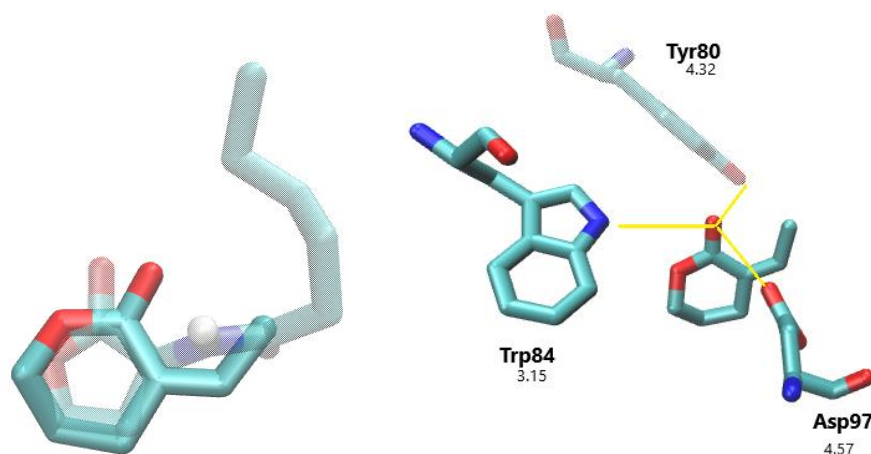


Figure S19. Overlap of **2** with **10Z**, and ligand binding domain for **10Z/CviR**, respectively.

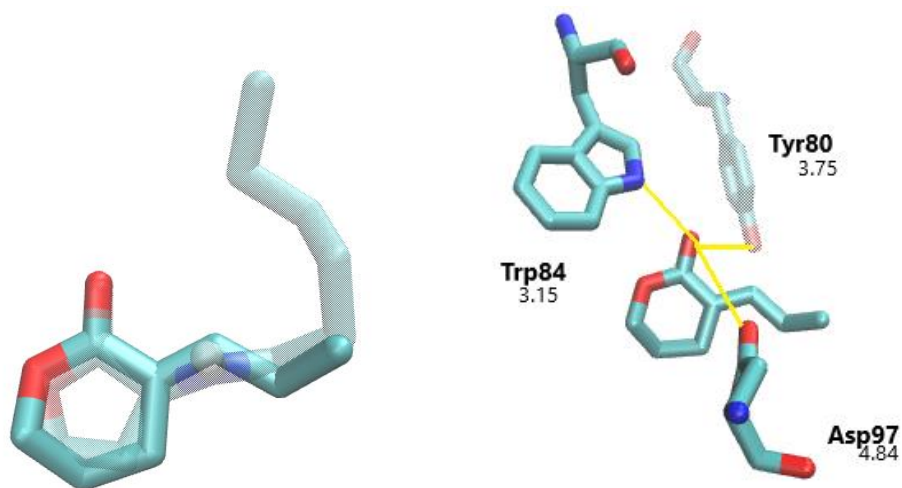


Figure S20. Overlap of **2** with **11E**, and ligand binding domain for **11E/CviR**, respectively.

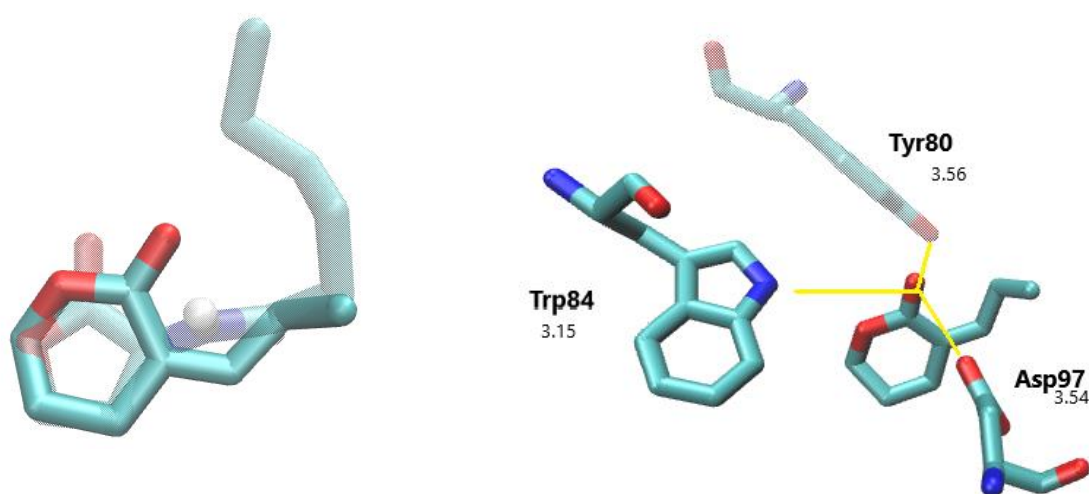


Figure S21. Overlap of **2** with **11Z**, and ligand binding domain for **11Z/CviR**, respectively.

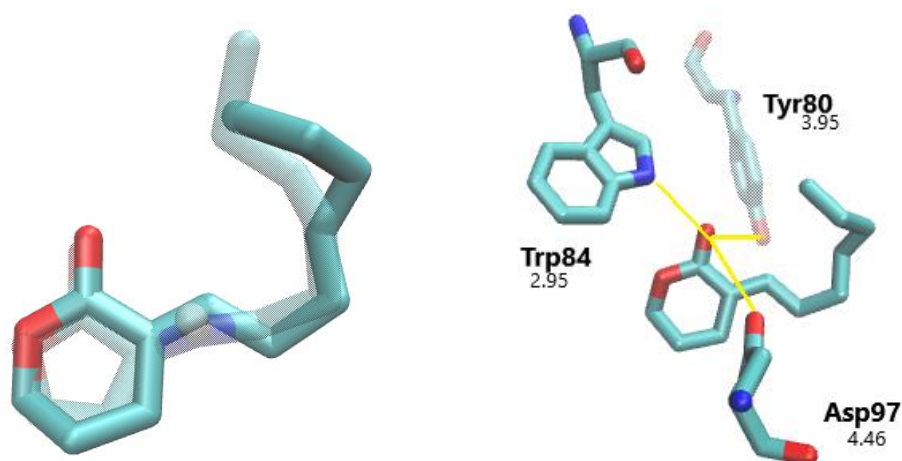


Figure S22. Overlap of **2** with **12E**, and ligand binding domain for **12E/CviR**, respectively.

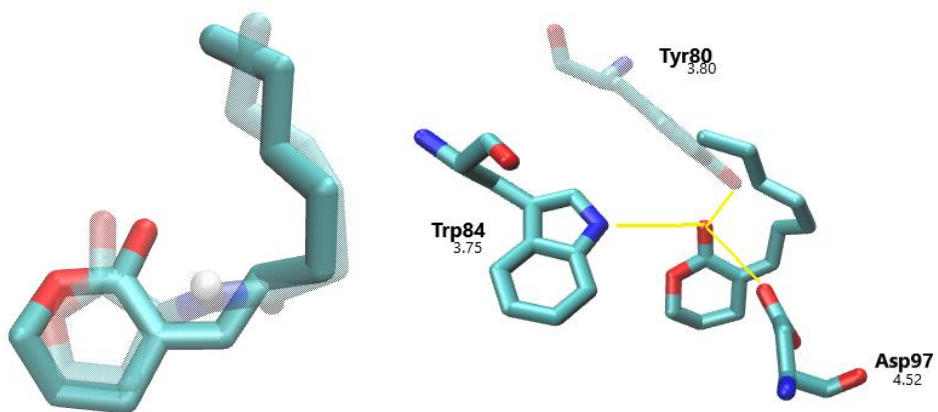


Figure S23. Overlap of 2 with 12Z, and ligand binding domain for 12Z/CviR, respectively.

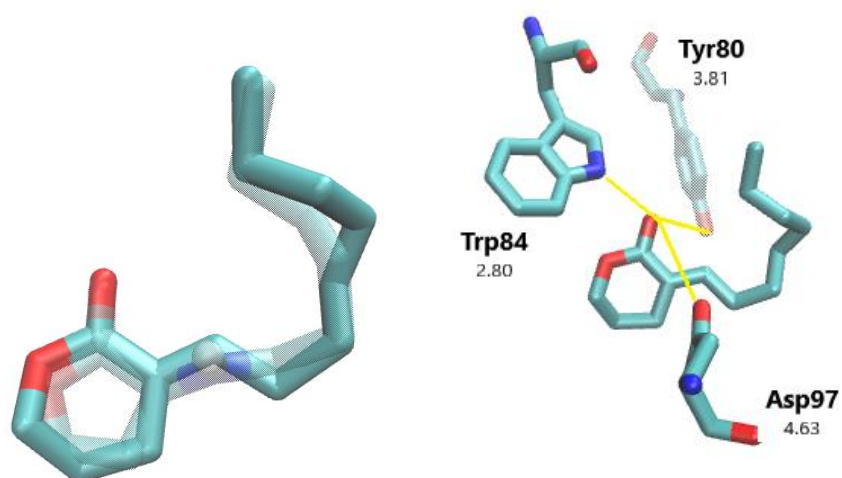


Figure S24. Overlap of 2 with 13E, and ligand binding domain for 13E/CviR, respectively.

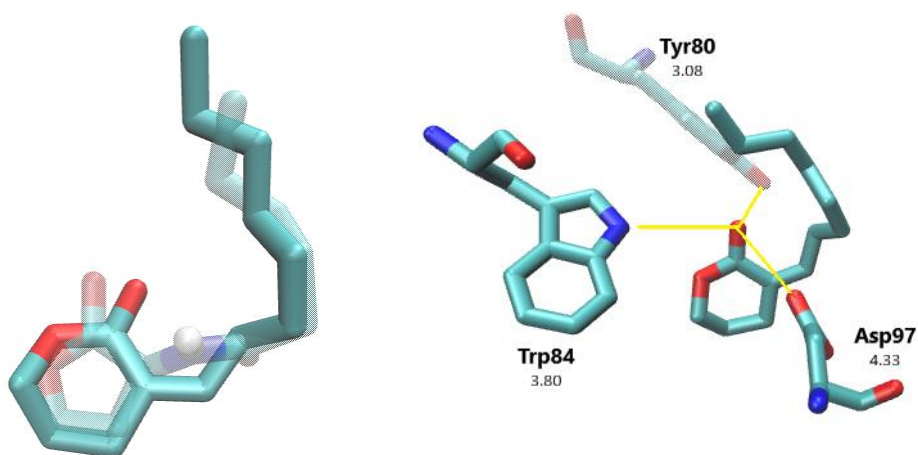


Figure S25. Overlap of 2 with 13Z, and ligand binding domain for 13Z/CviR, respectively.

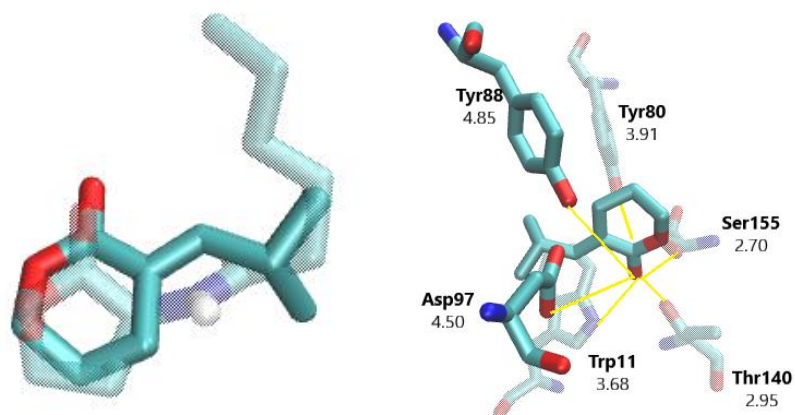


Figure S26. Overlap of **2** with **14E**, and ligand binding domain for **14E/CviR**, respectively.

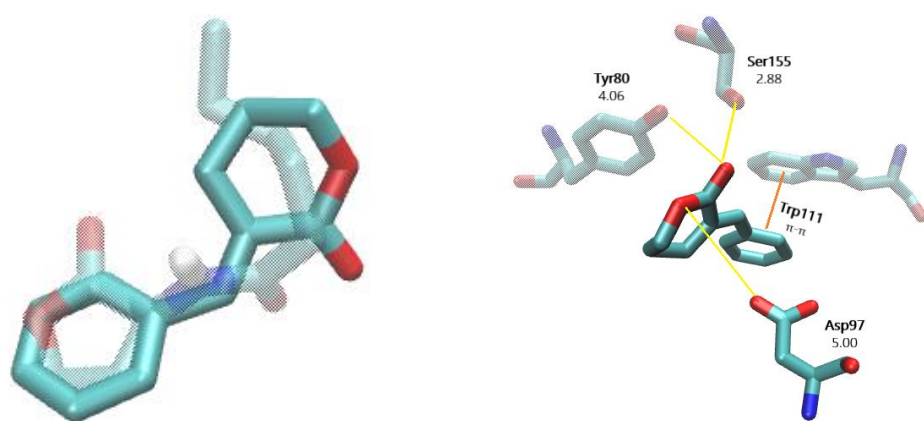


Figure S27. Overlap of **2** with **15E**, and ligand binding domain for **15E/CviR**, respectively.

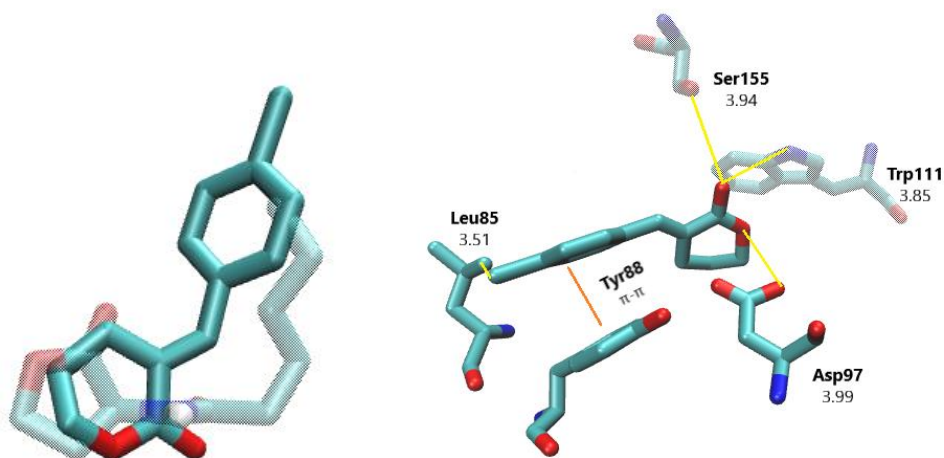


Figure S28. Overlap of **2** with **16E**, and ligand binding domain for **16E/CviR**, respectively.

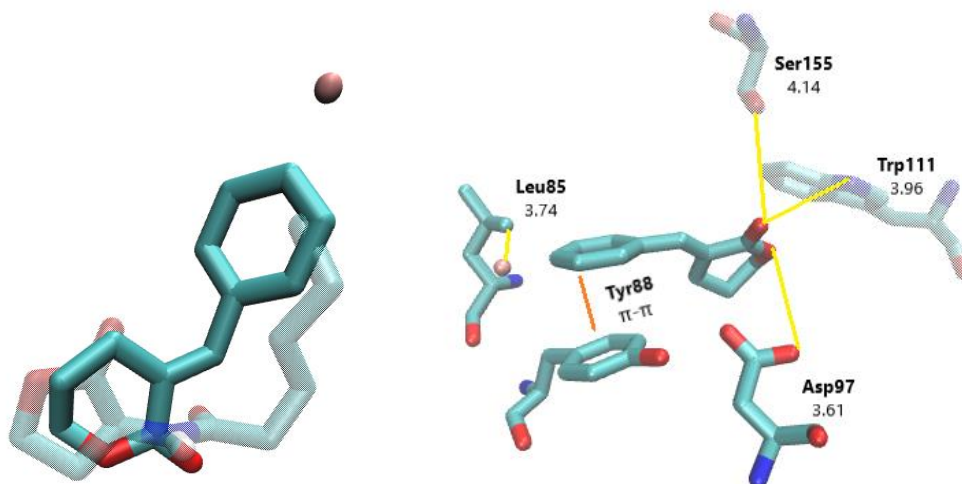


Figure S29. Overlap of **2** with **17E**, and ligand binding domain for **17E/CviR**, respectively.

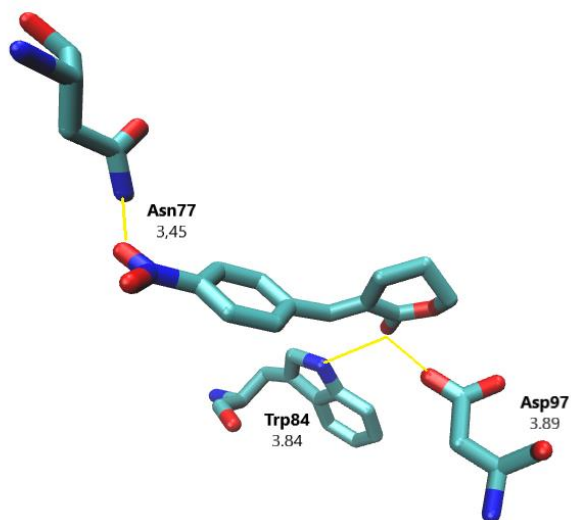


Figure S30. Overlap of **2** with **18E**, and ligand binding domain for **18E/CviR**, respectively.

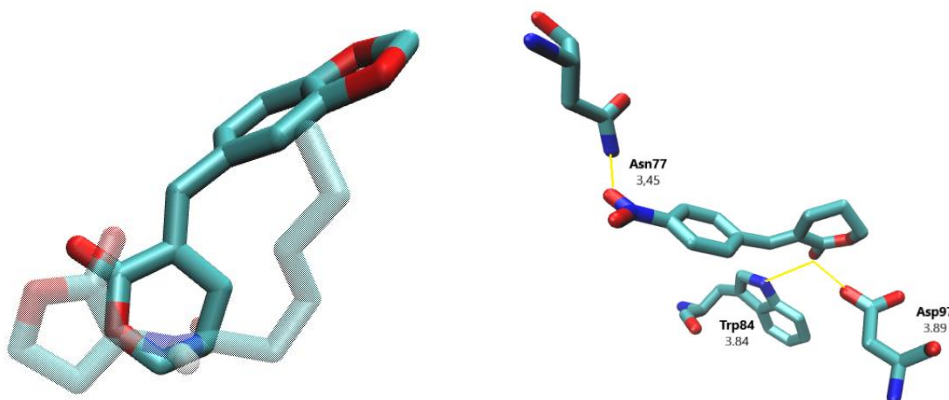


Figure S31. Overlap of **2** with **19E**, and ligand binding domain for **19E/CviR**, respectively.

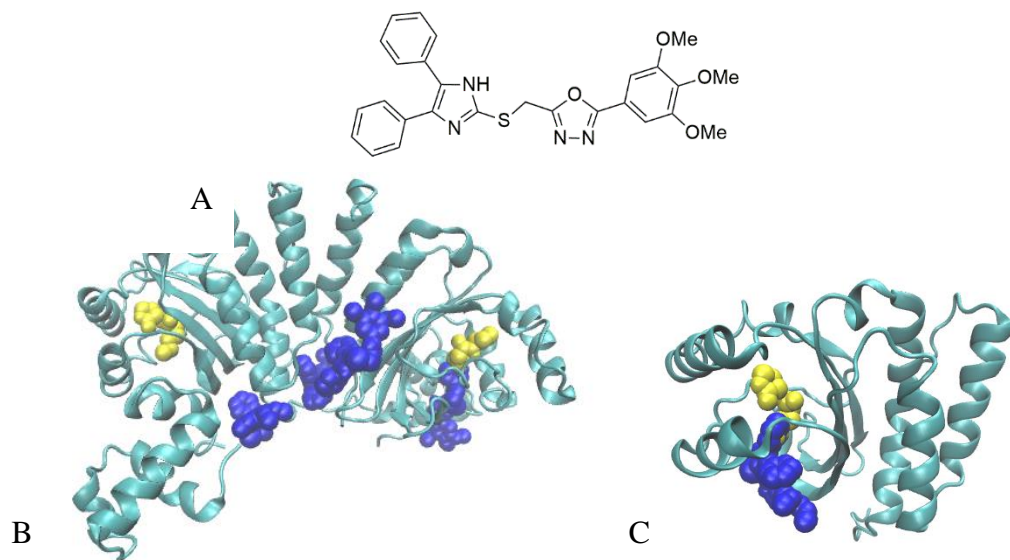
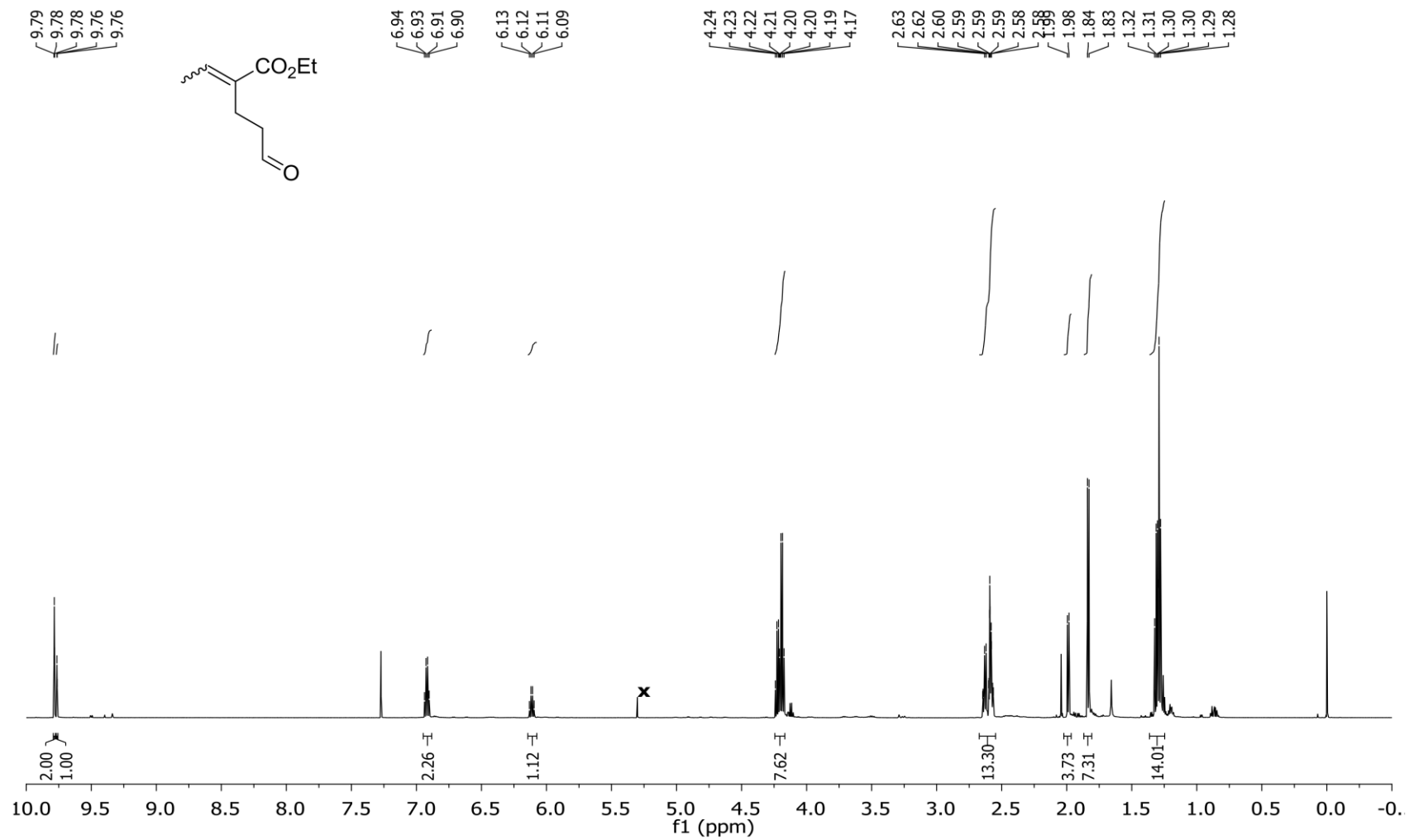


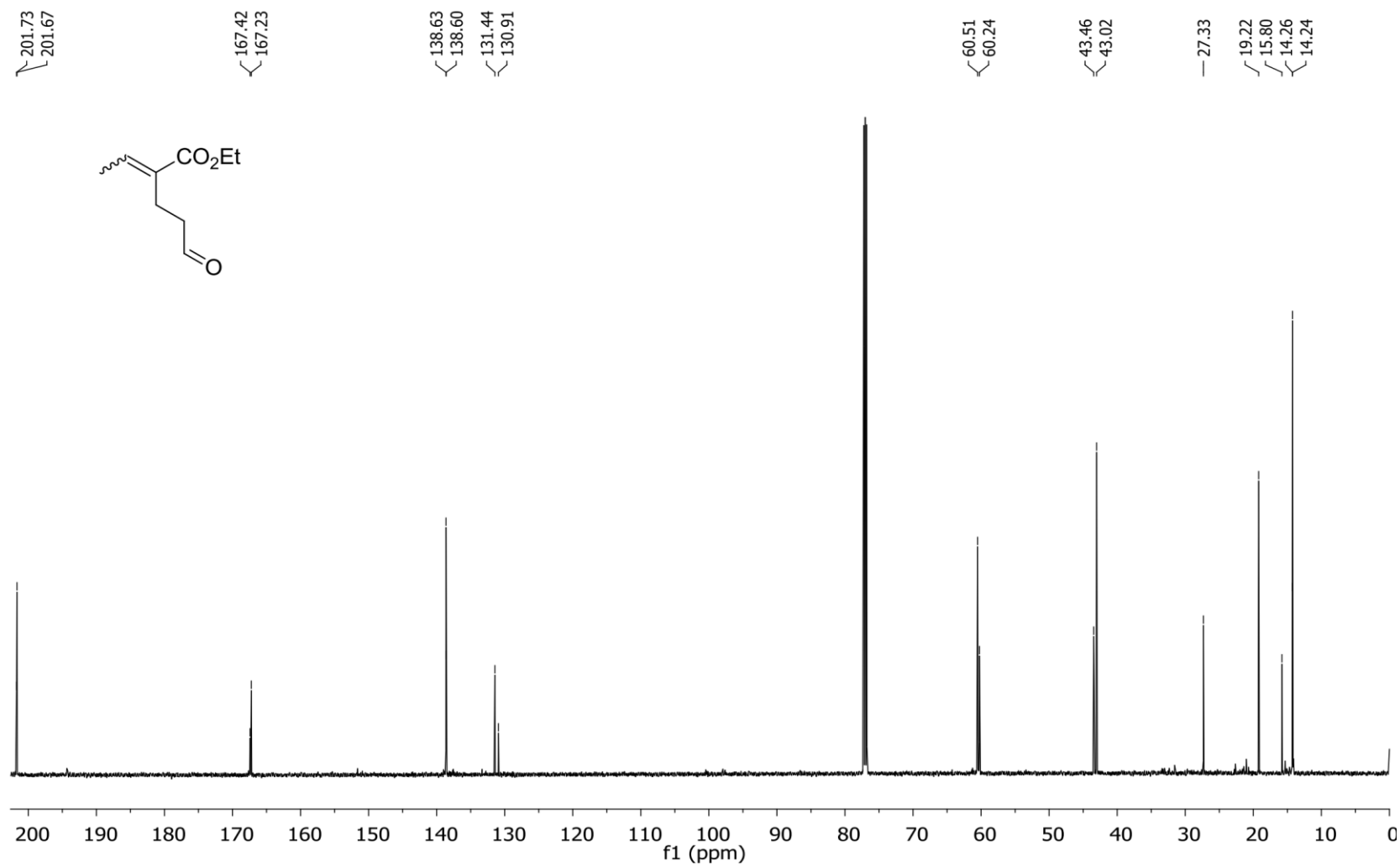
Figure S32. (A): Chemical structure of **21**.; B: CviR (PDB ID: 3PQ5) complex with **21**(blue), in yellow is shown HHL to exemplify the LBD.; (C): LBD complex with **21**(blue), in yellow is shown HHL (**2**) to exemplify the LBD.

2. NMR spectrums:

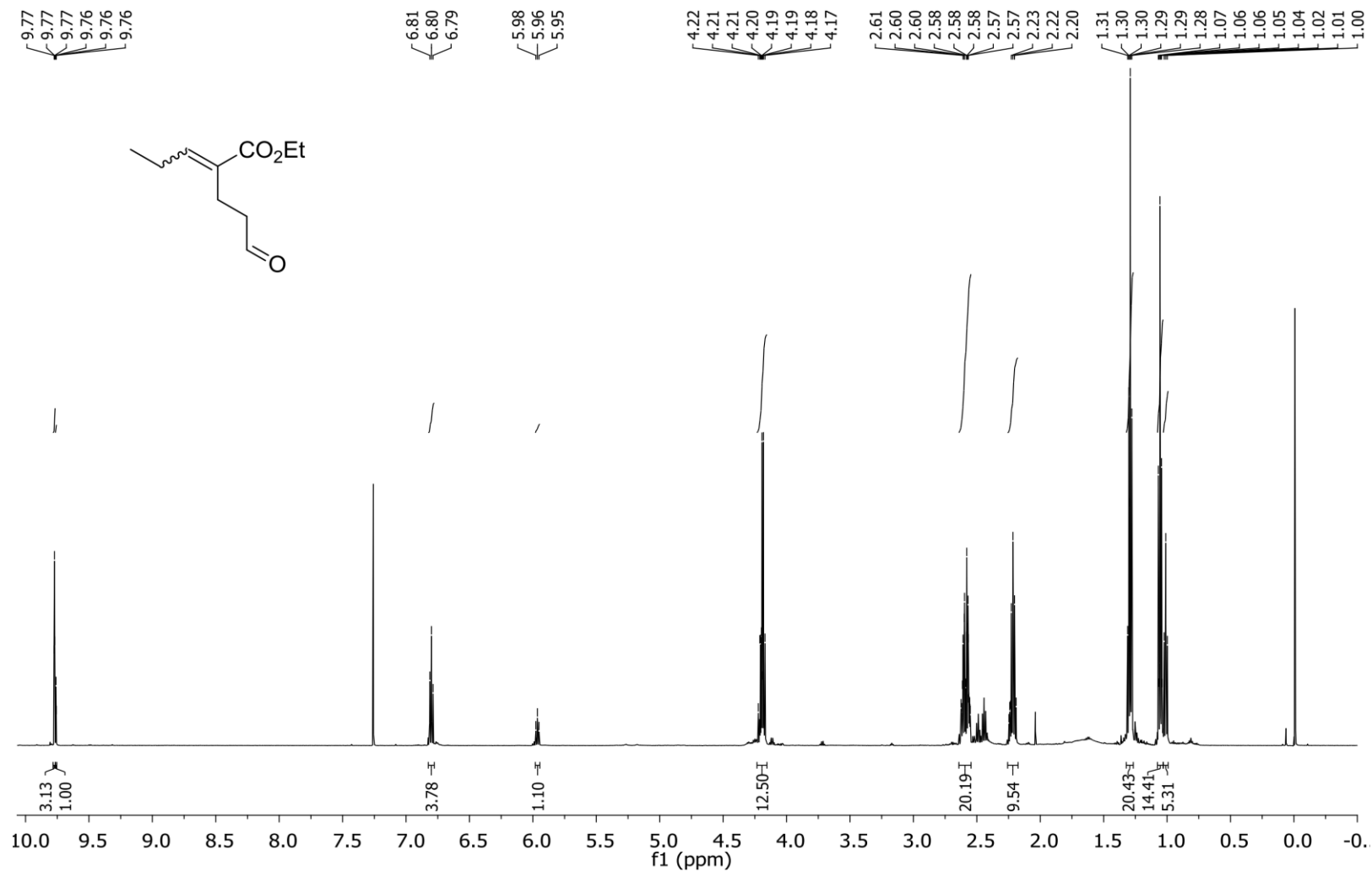
S2.1. ^1H NMR (600 MHz) spectrum of **8** (*E/Z*) **R** = **Methyl** in CDCl_3 .



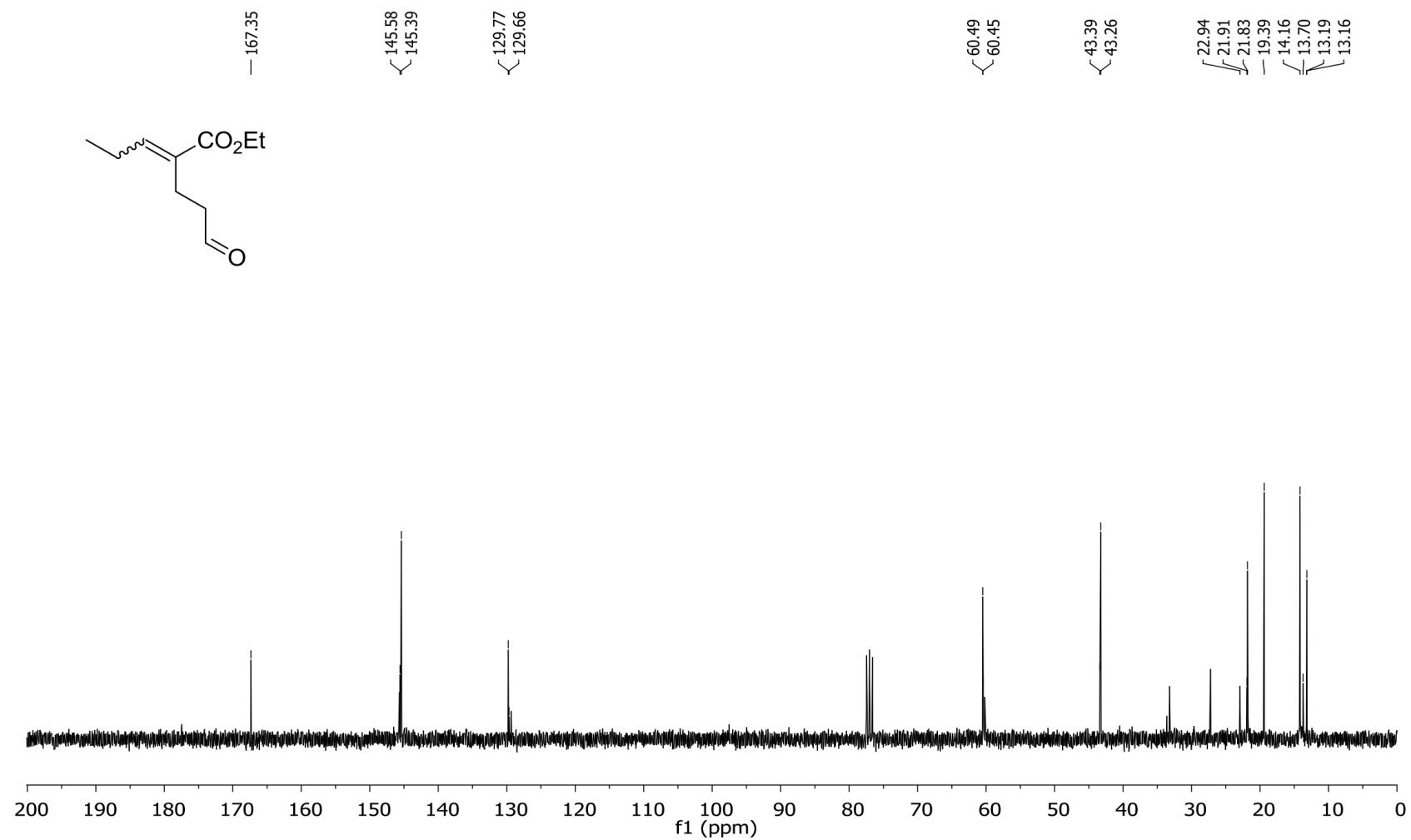
S2.2. ^{13}C NMR (75 MHz) spectrum of **8** (*E/Z*) **R** = Methyl in CDCl_3



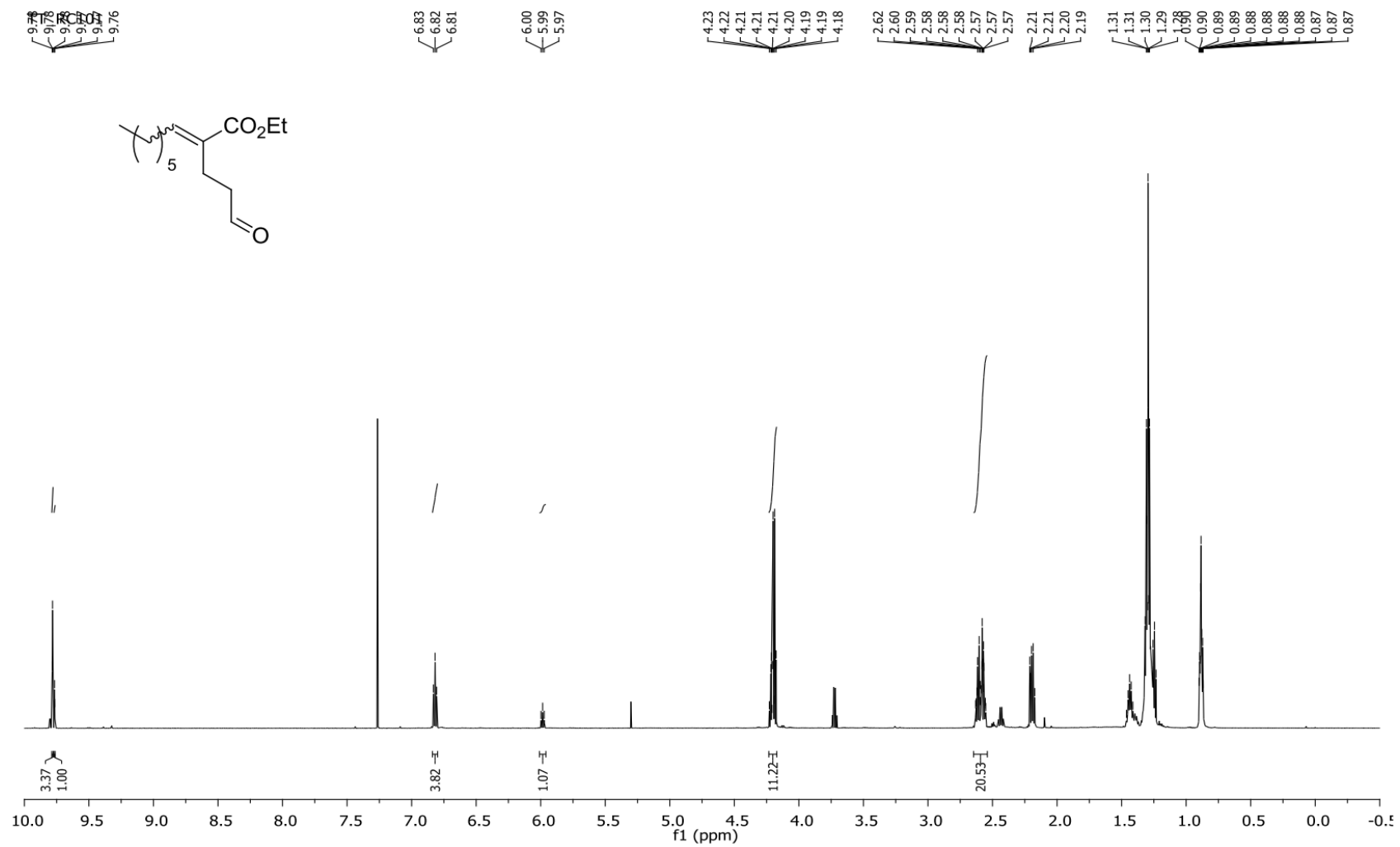
S2.3. ^1H NMR (600 MHz) spectrum of **8** (*E/Z*) **R** = Ethyl in CDCl_3 .



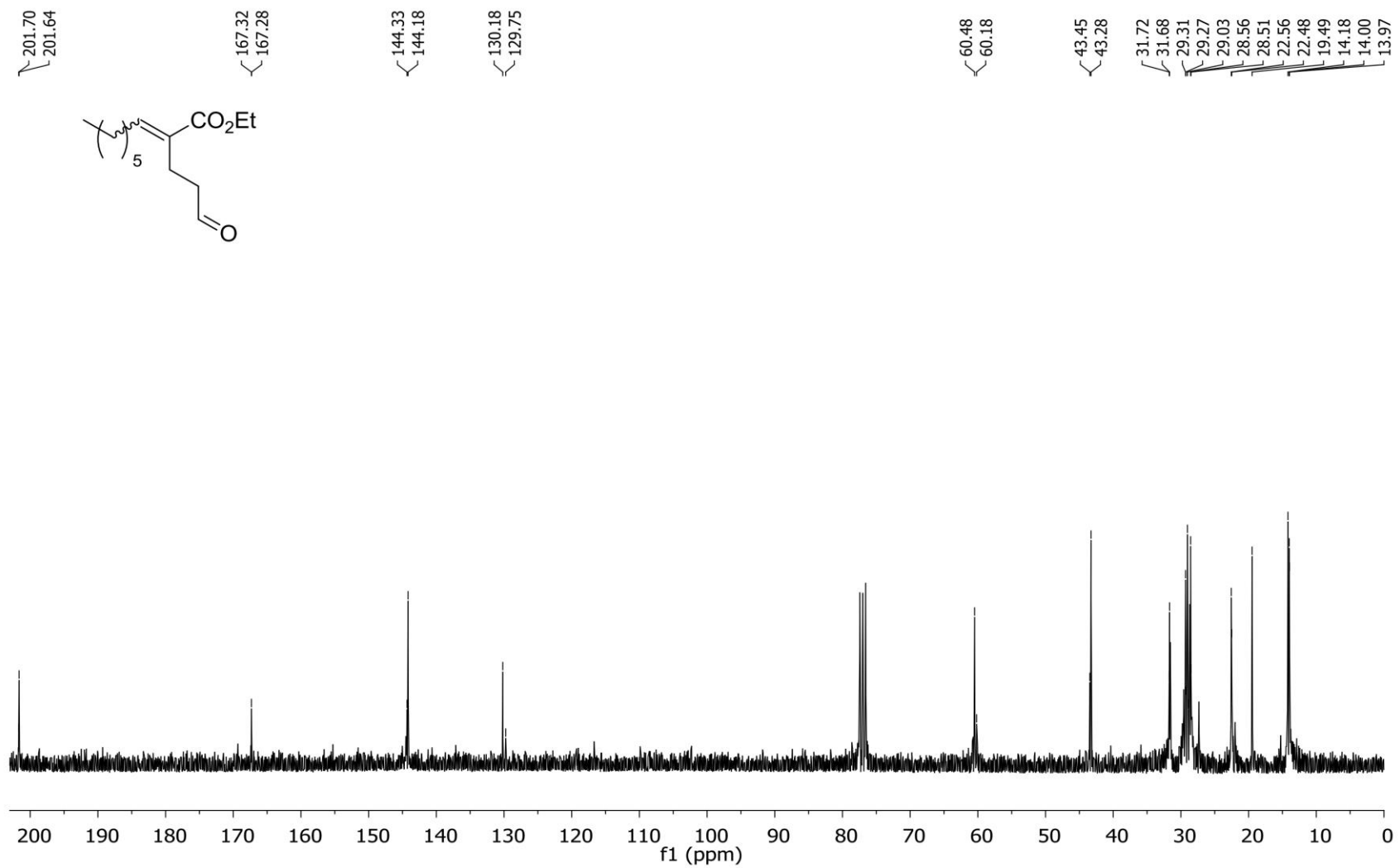
S2.4. ^{13}C NMR (75 MHz) spectrum of **8** (*E/Z*) **R** = Ethyl in CDCl_3 .



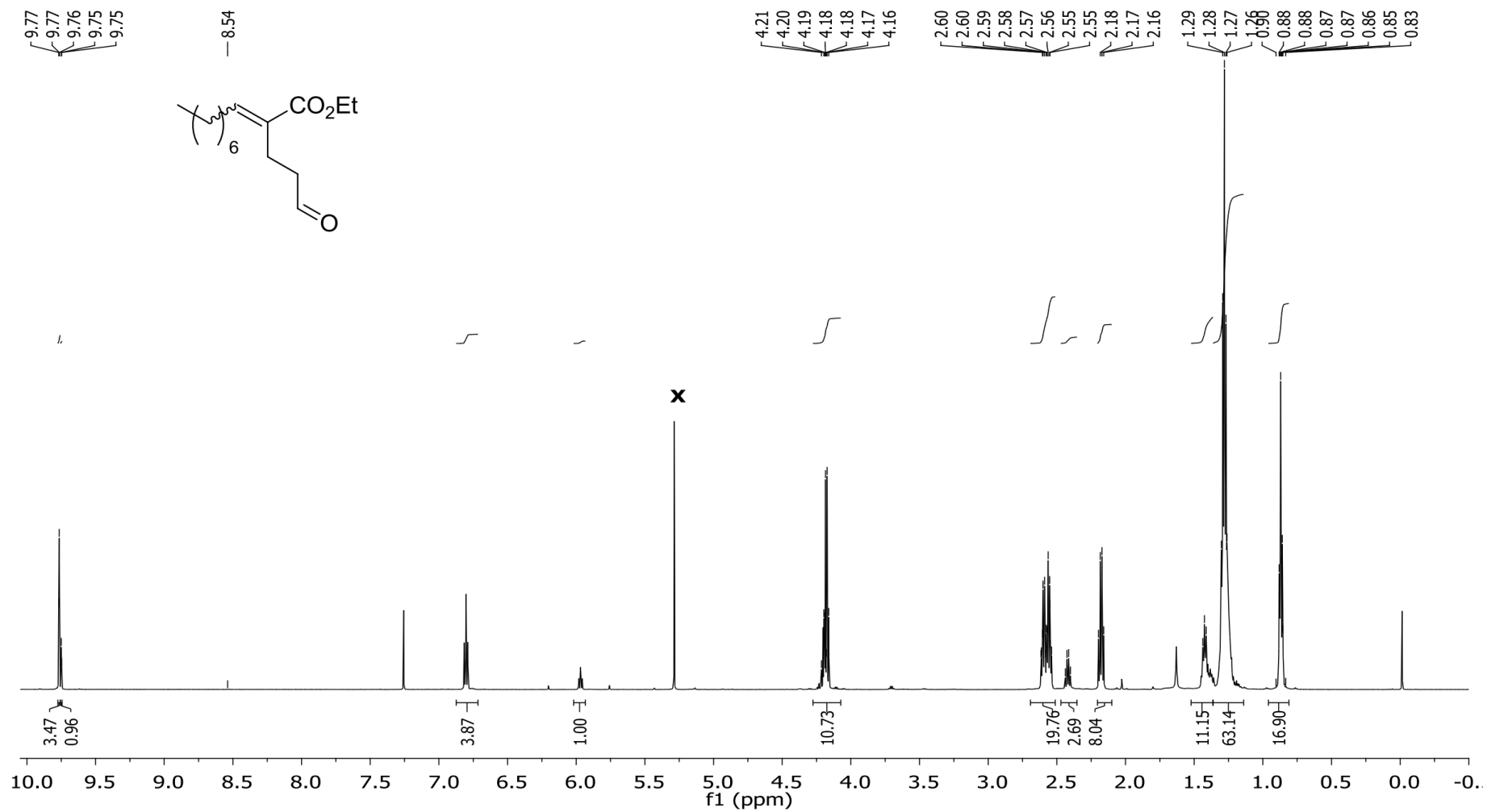
S2.5. ^1H NMR (600 MHz) spectrum of **8** (*E/Z*) **R** = *n*-Hexyl in CDCl_3 .



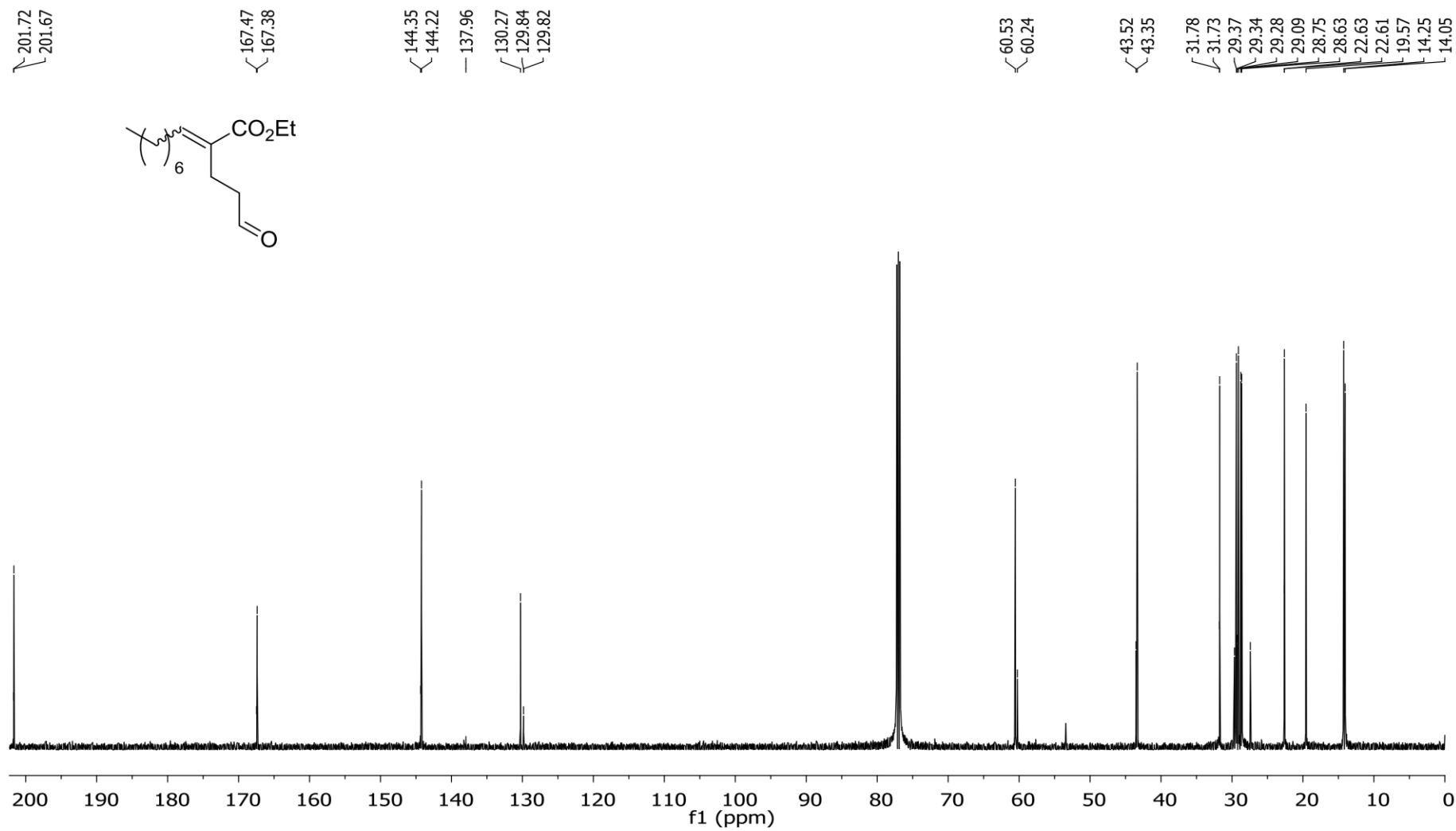
S2.6. ^{13}C NMR (151 MHz) spectrum of **8** (*E/Z*) **R** = *n*-Hexyl in CDCl_3 .



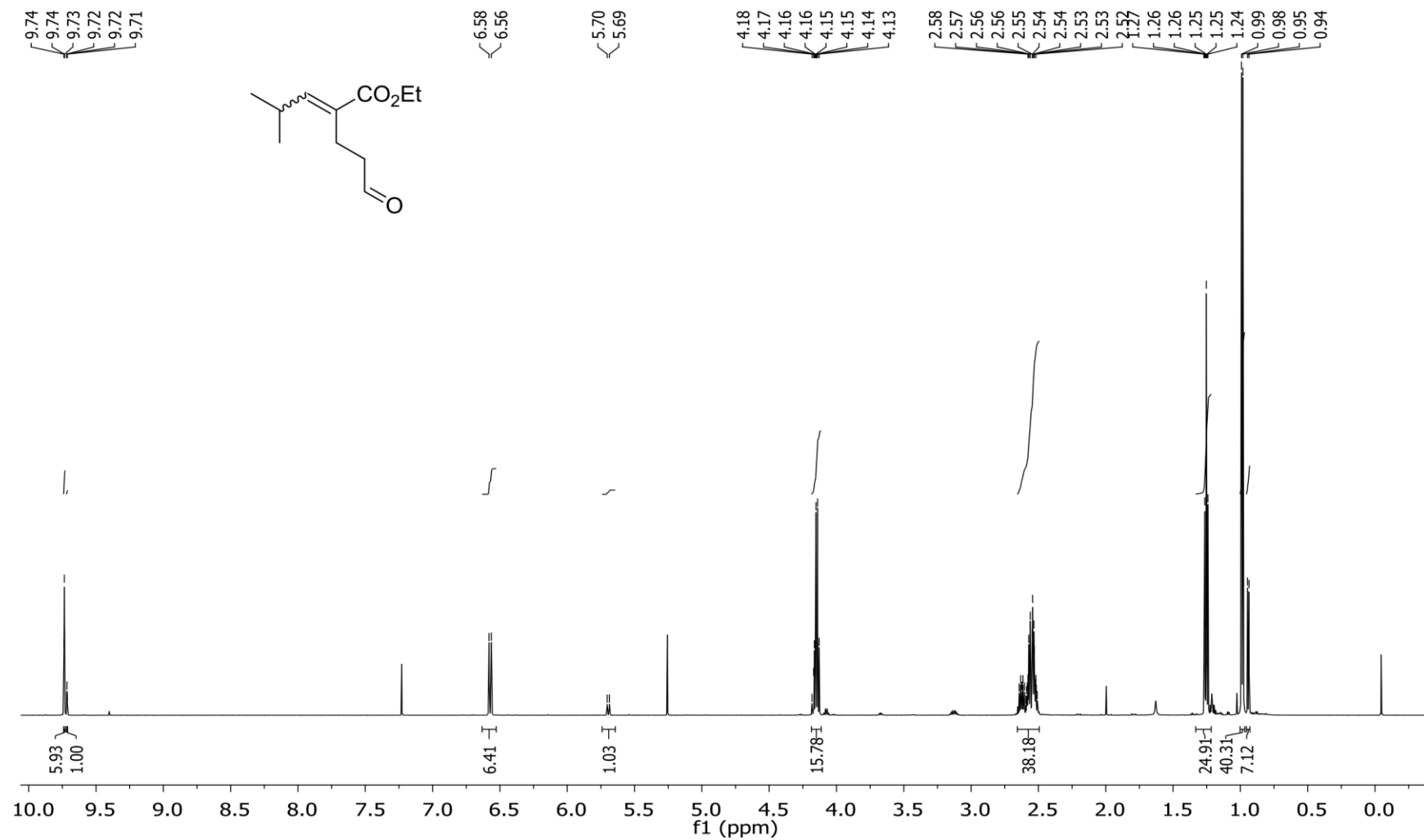
S2.7. ^1H NMR (600 MHz) spectrum of **8** (*E/Z*) **R** = *n*-Heptyl in CDCl_3 .



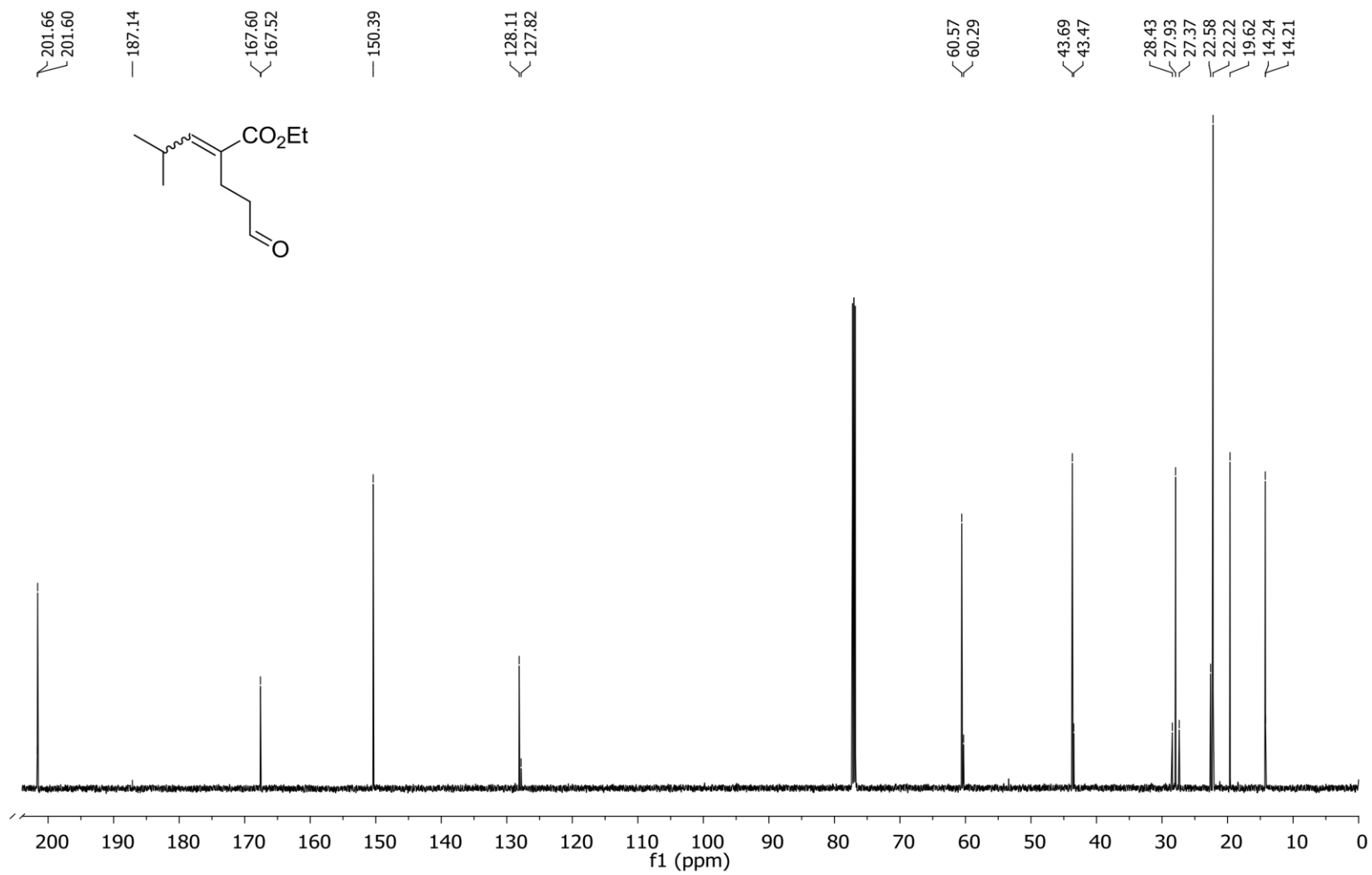
S2.8. ^{13}C NMR (151 MHz) spectrum of **8** (*E/Z*) **R** = *n*-Heptyl in CDCl_3 .



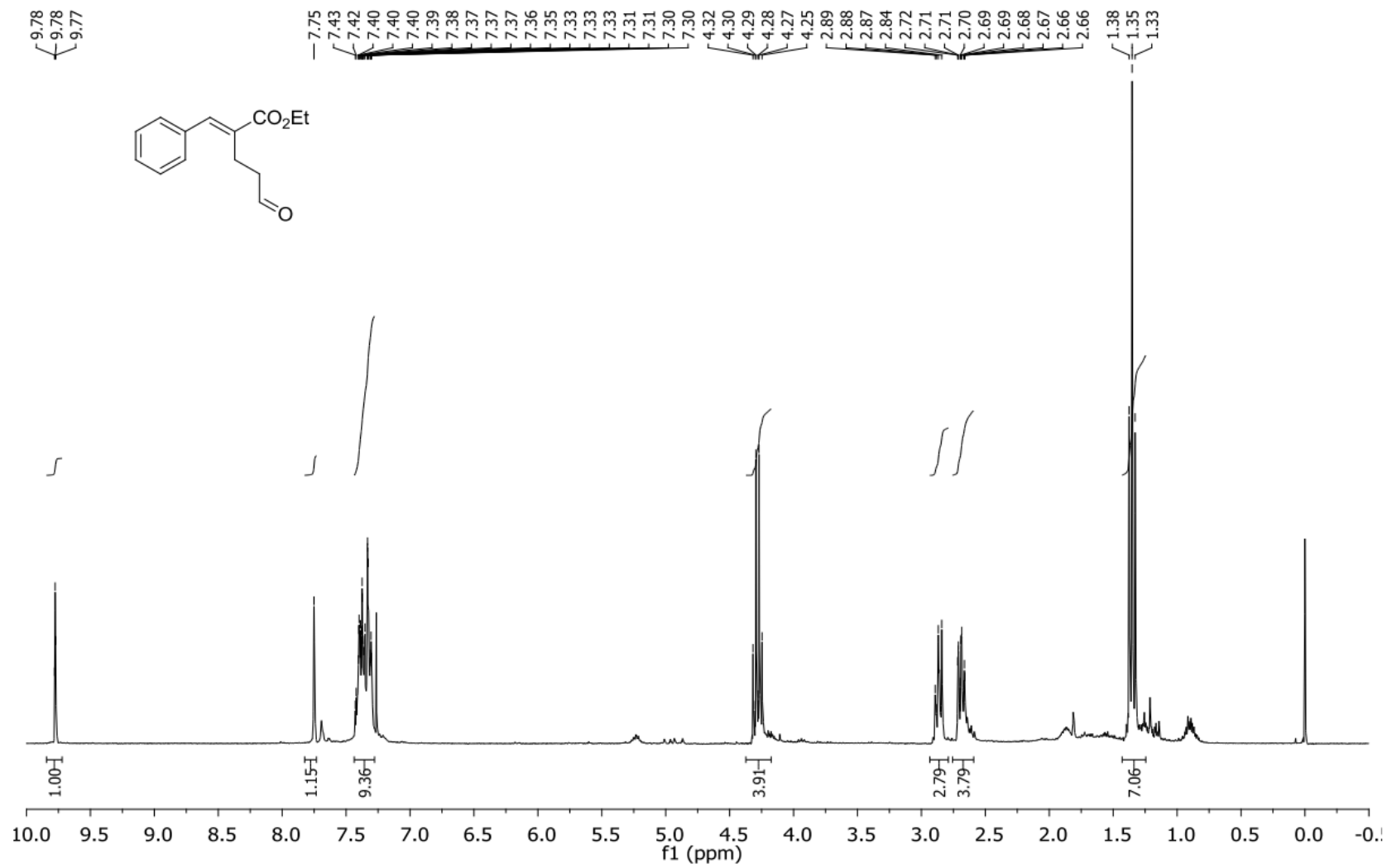
S2.9. ^1H NMR (600 MHz) spectrum of **8** (*E/Z*) **R** = *iso*-Propyl in CDCl_3 .



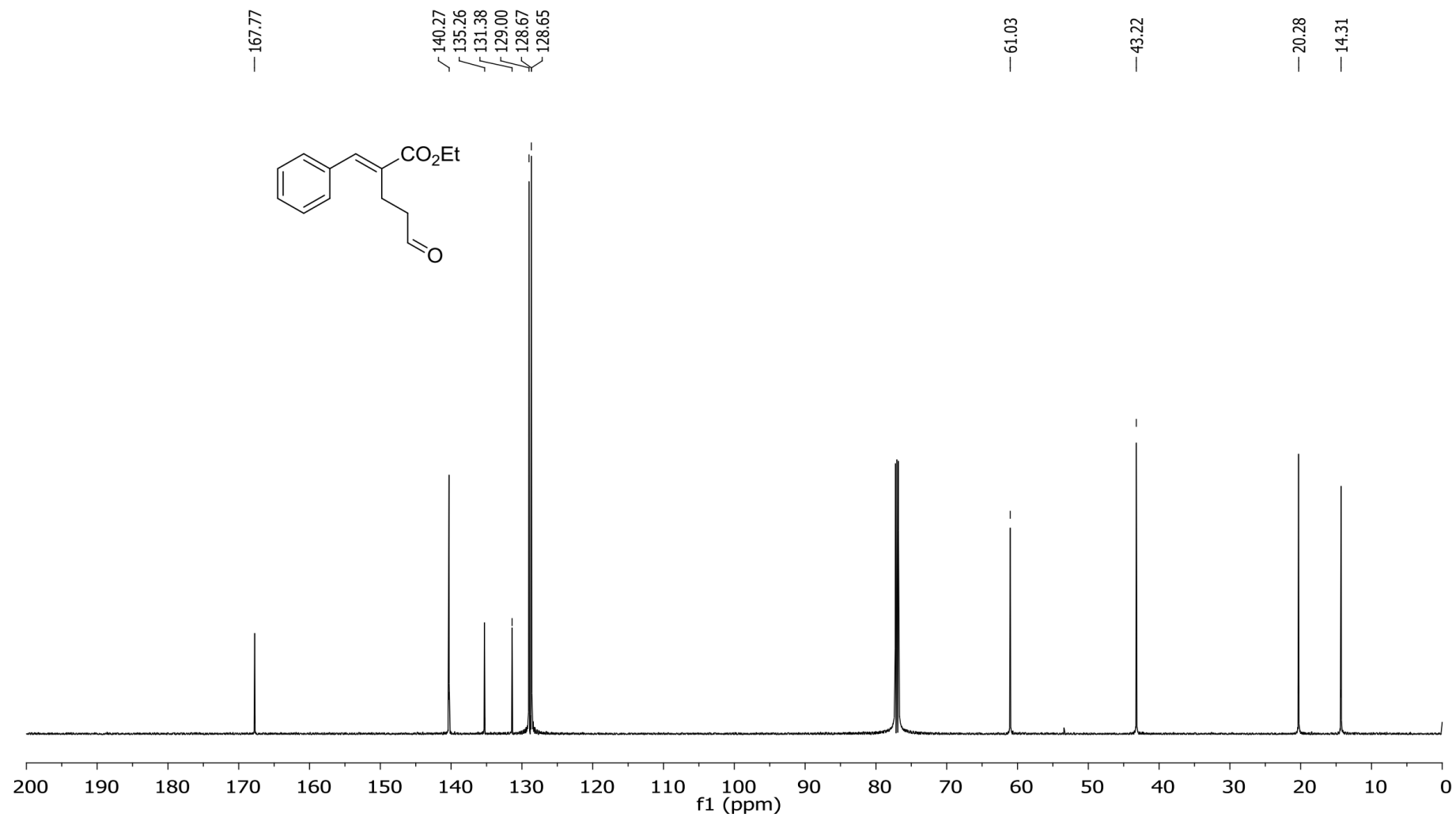
S2.10. ^{13}C NMR (151 MHz) spectrum of **8** (*E/Z*) **R** = *iso*-Propyl in CDCl_3 .



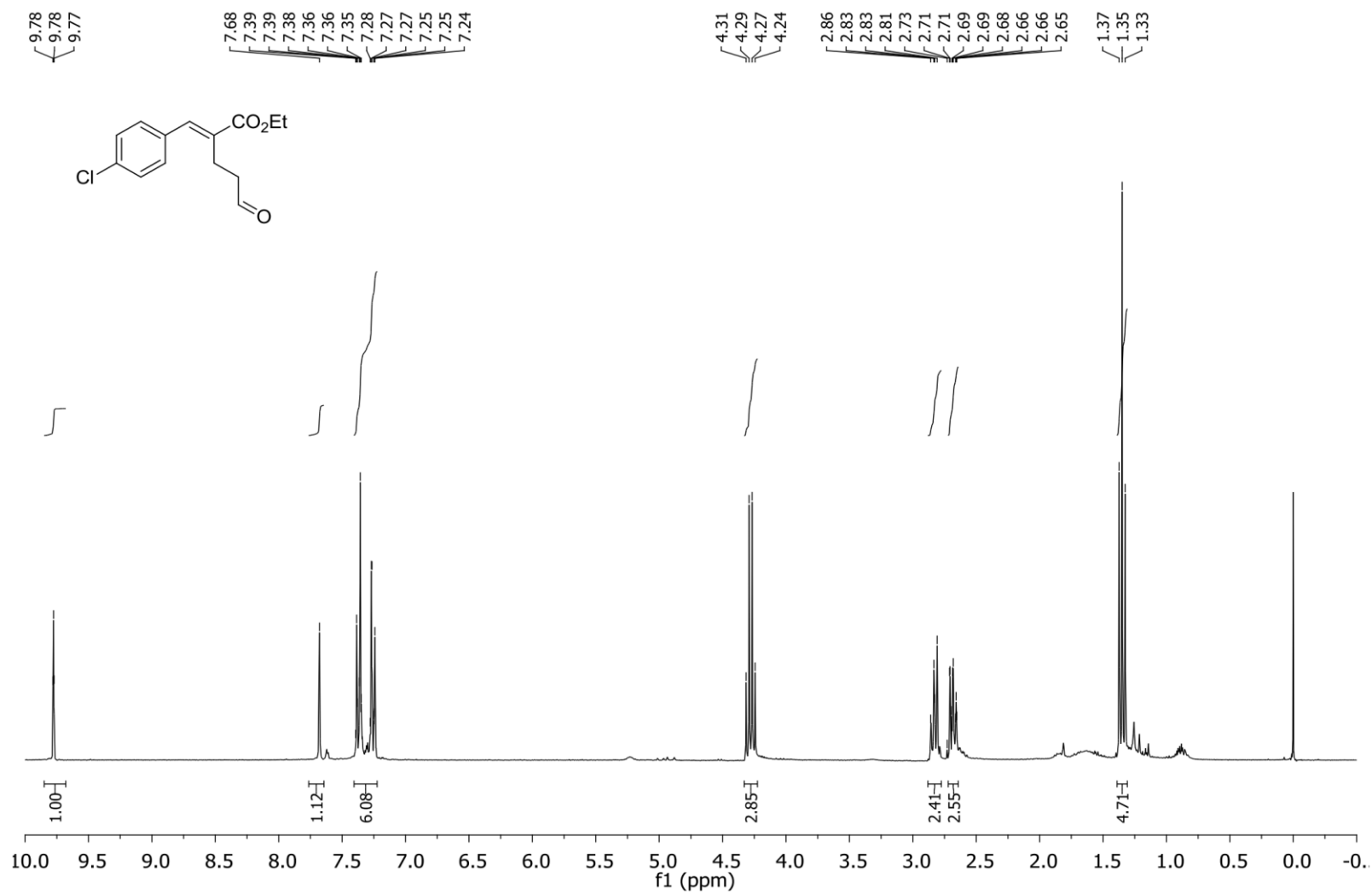
S2.11. ^1H NMR (600 MHz) spectrum of **8** (*E*) **R** = Phenyl in CDCl_3 .



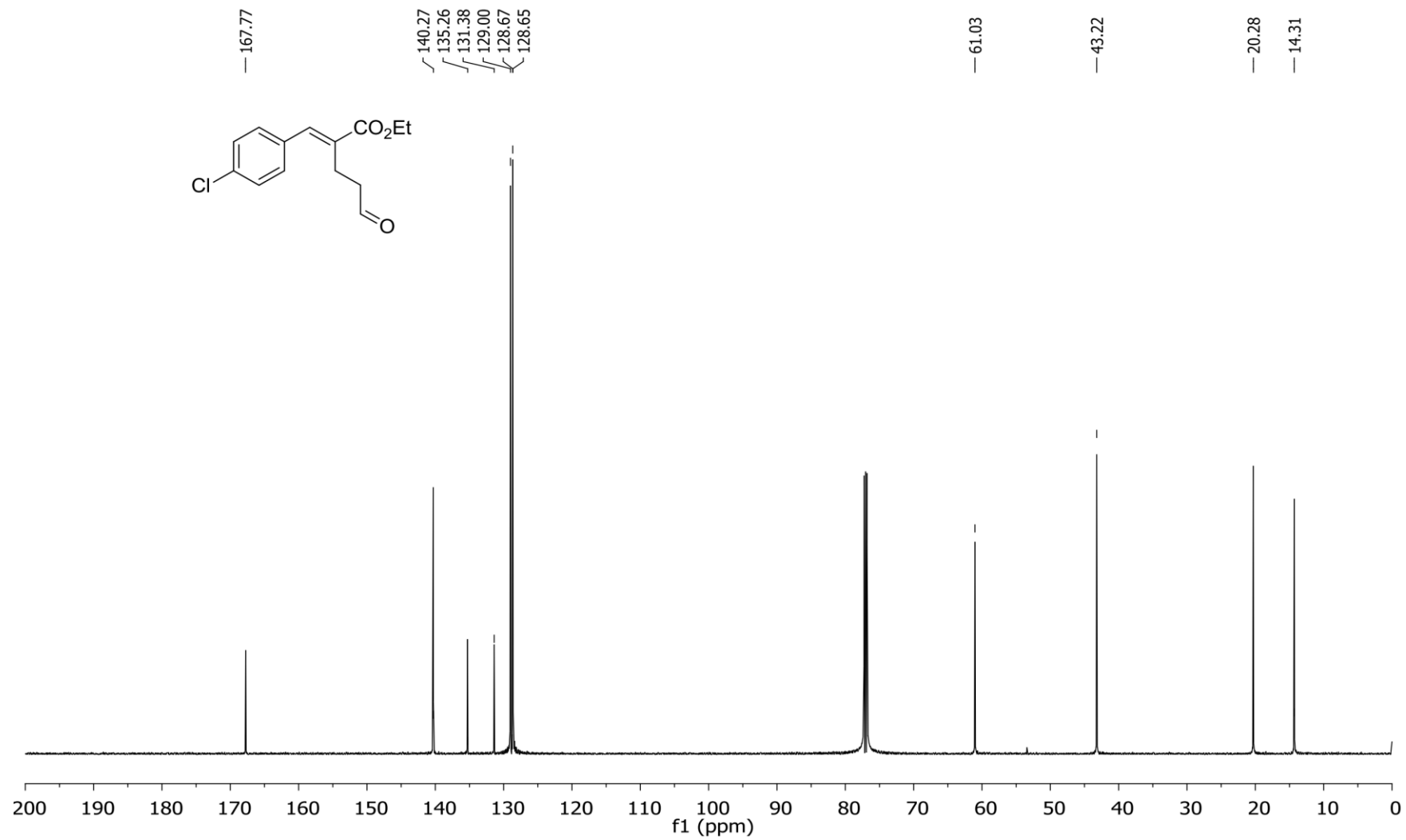
S2.12. ^{13}C NMR (151 MHz) spectrum of **8** (*E*) **R** = Phenyl in CDCl_3 .



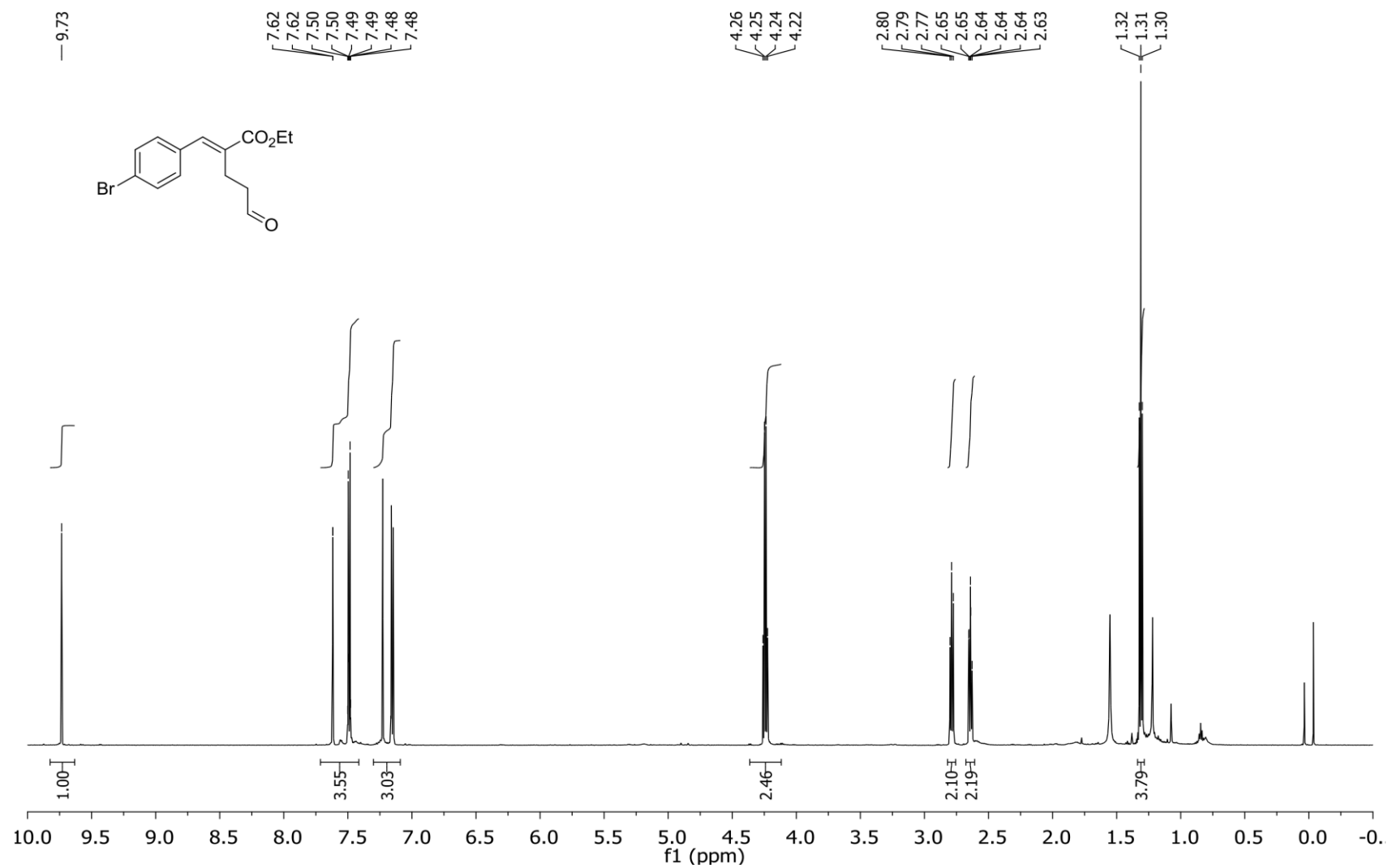
S2.13. ^1H NMR (300 MHz) spectrum of **8** (*E*) **R** = 4-Cl-Phenyl in CDCl_3 .



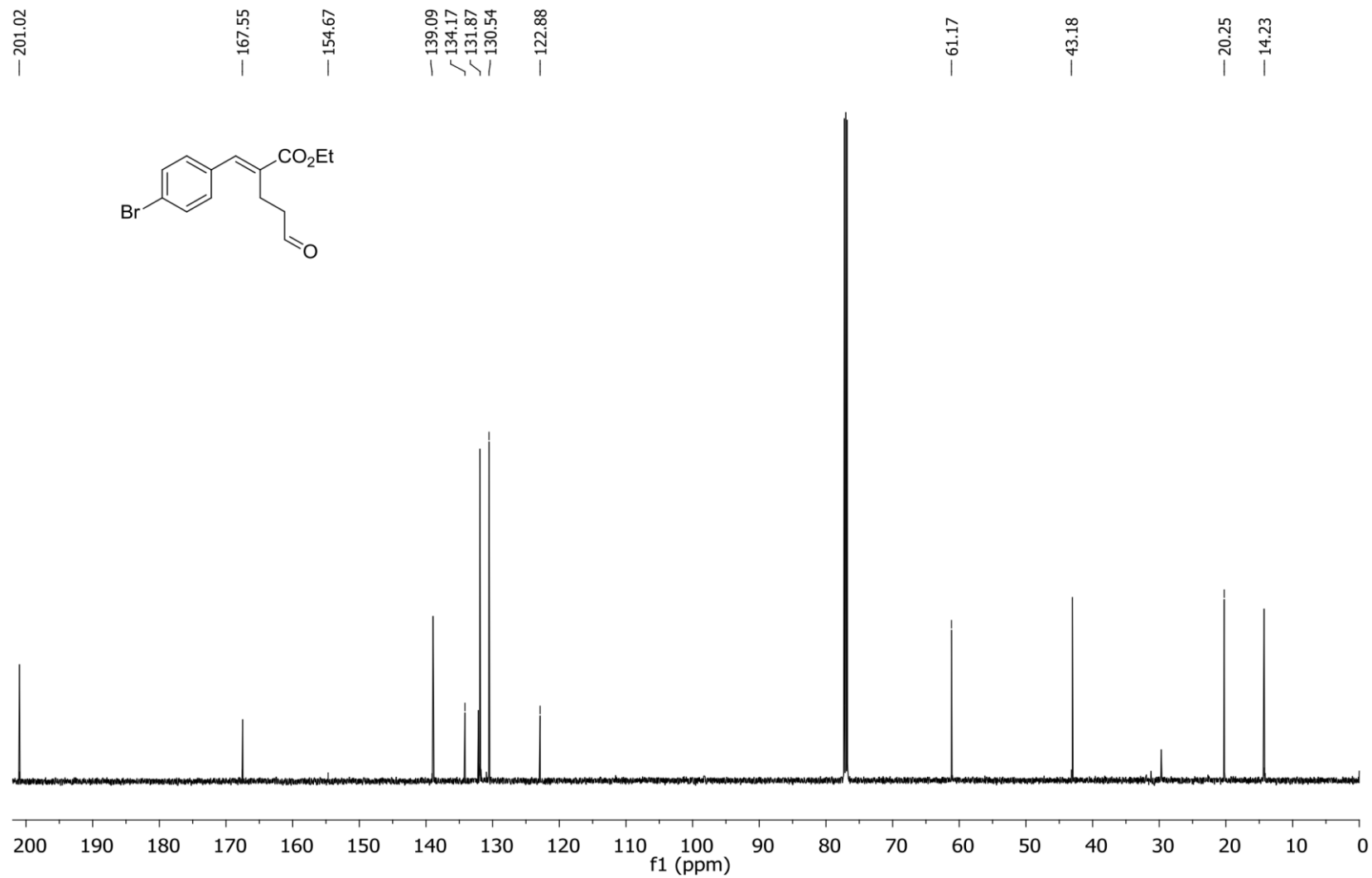
S2.14. ^{13}C NMR (151 MHz) spectrum of **8** (*E*) **R** = 4-Cl-Phenyl in CDCl_3 .



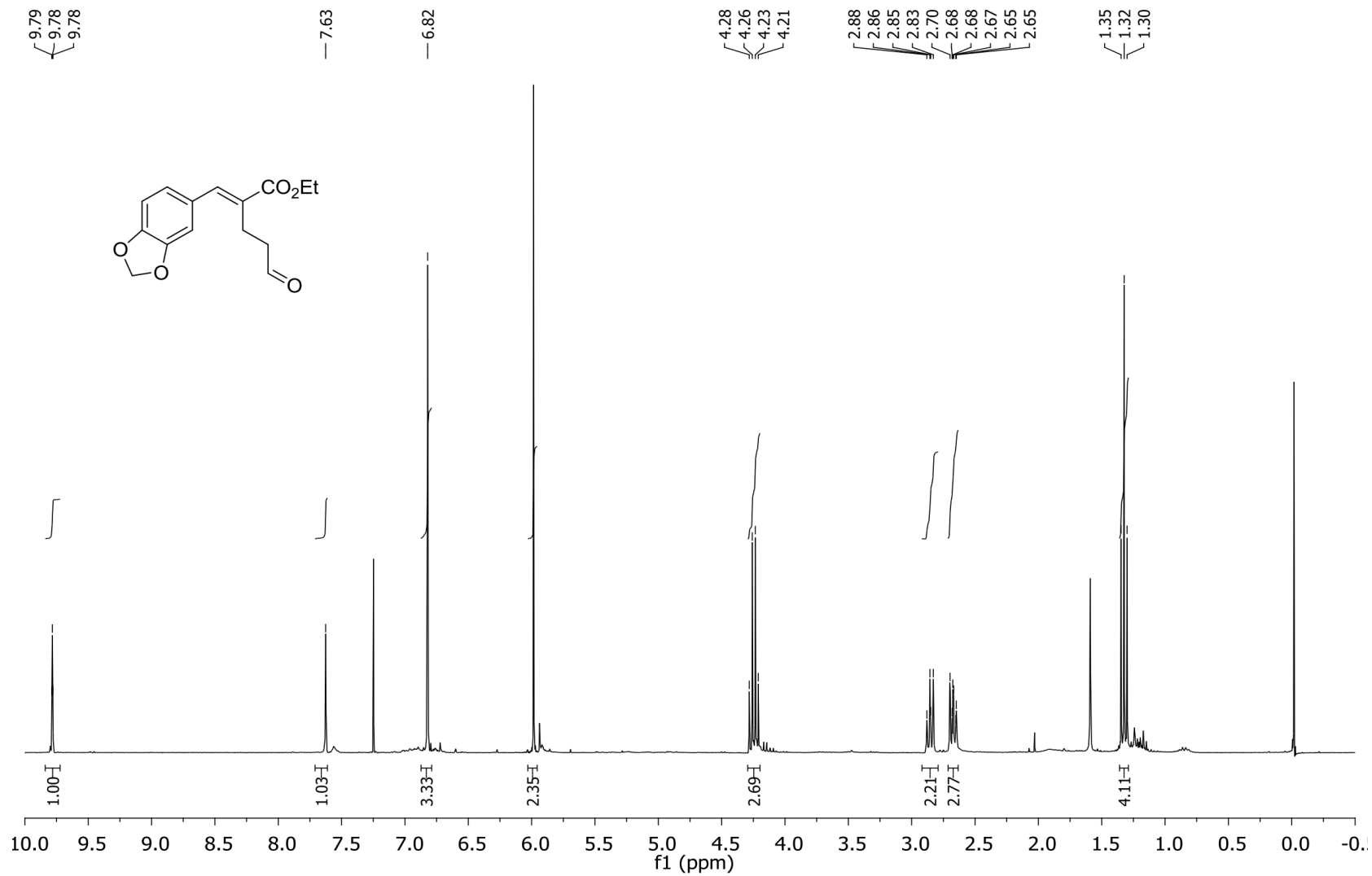
S2.15. ^1H NMR (600 MHz) spectrum of **8** (*E*) **R** = 4-Br-Phenyl in CDCl_3 .



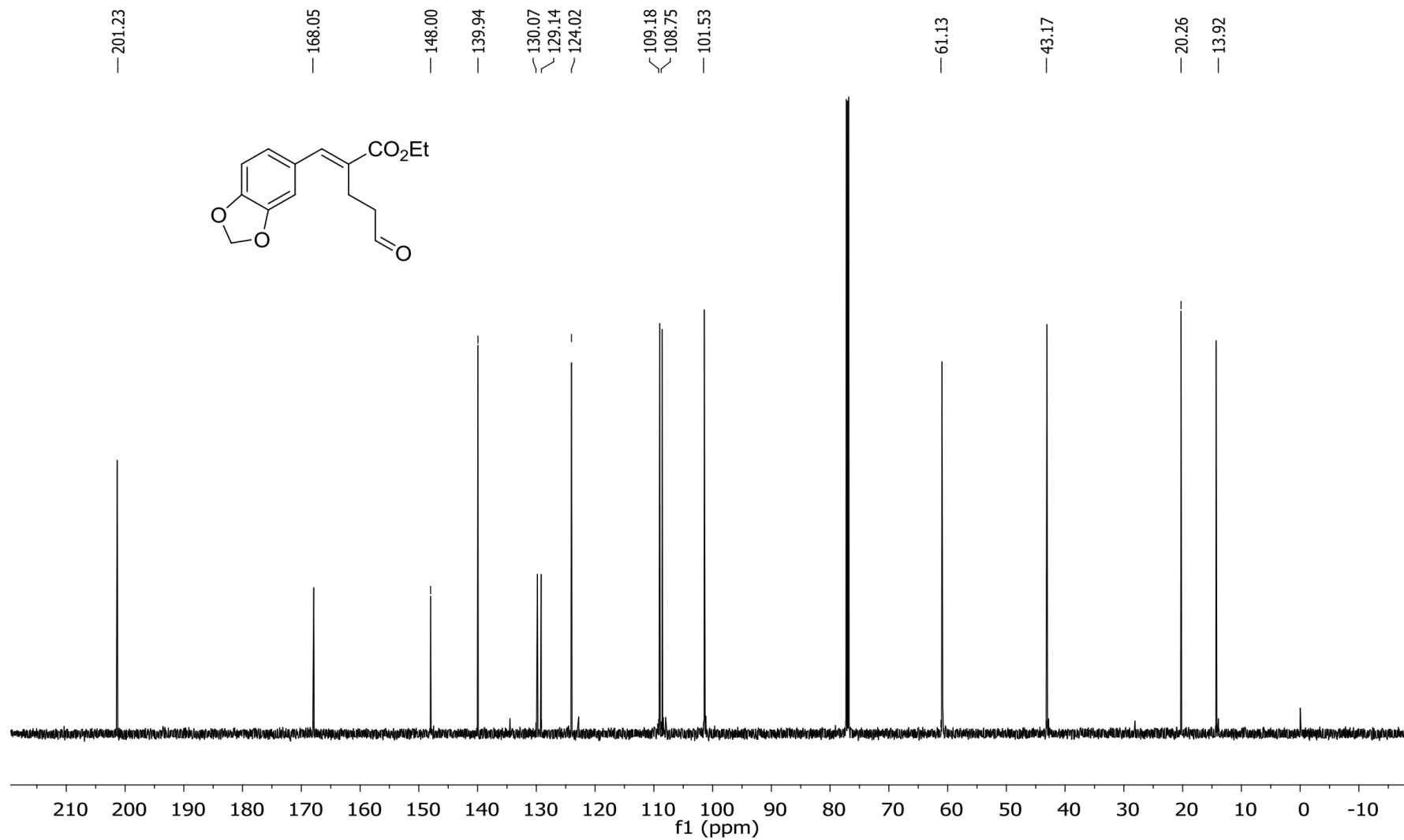
S2.16. ^{13}C NMR (151 MHz) spectrum of **8** (*E*) **R** = 4-Br-Phenyl in CDCl_3 .



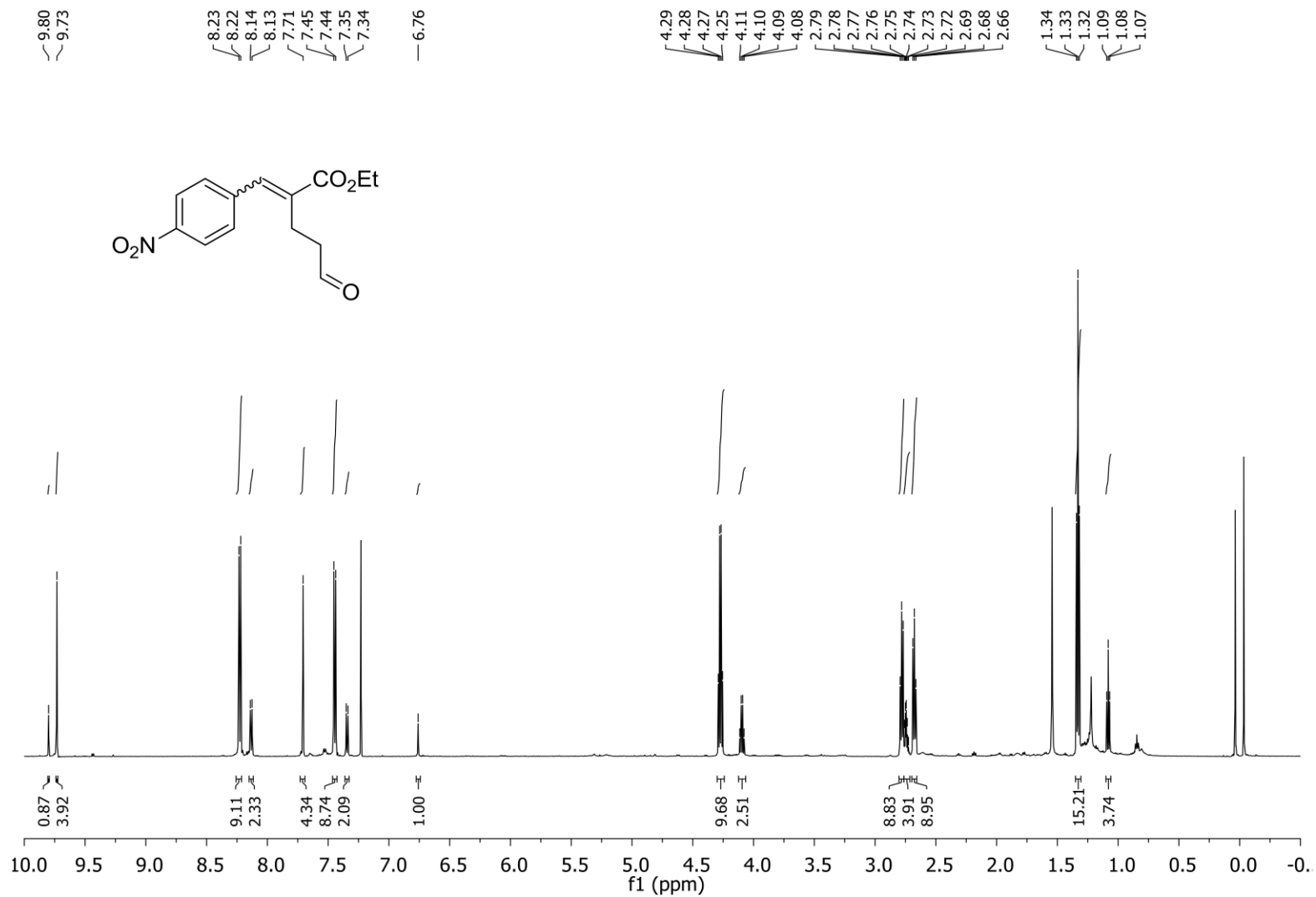
S2.17. ^1H NMR (600 MHz) spectrum of **8** (*E*) **R** = 3,4-Methylenedioxyphenyl in CDCl_3 .



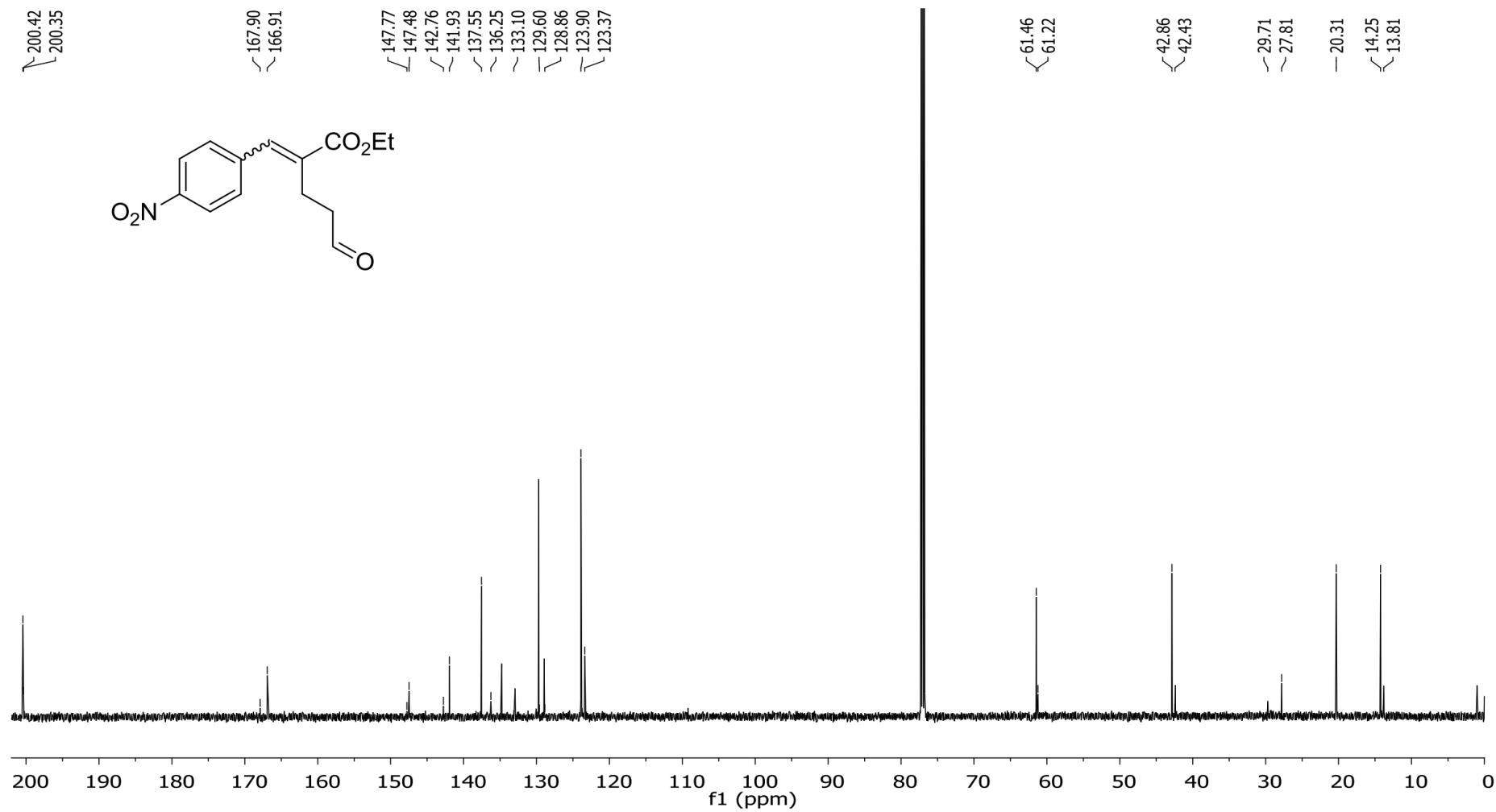
S2.18. ^{13}C NMR (151 MHz) spectrum of **8** (*E*) **R** = 3,4-Methylenedioxyphenyl in CDCl_3 .



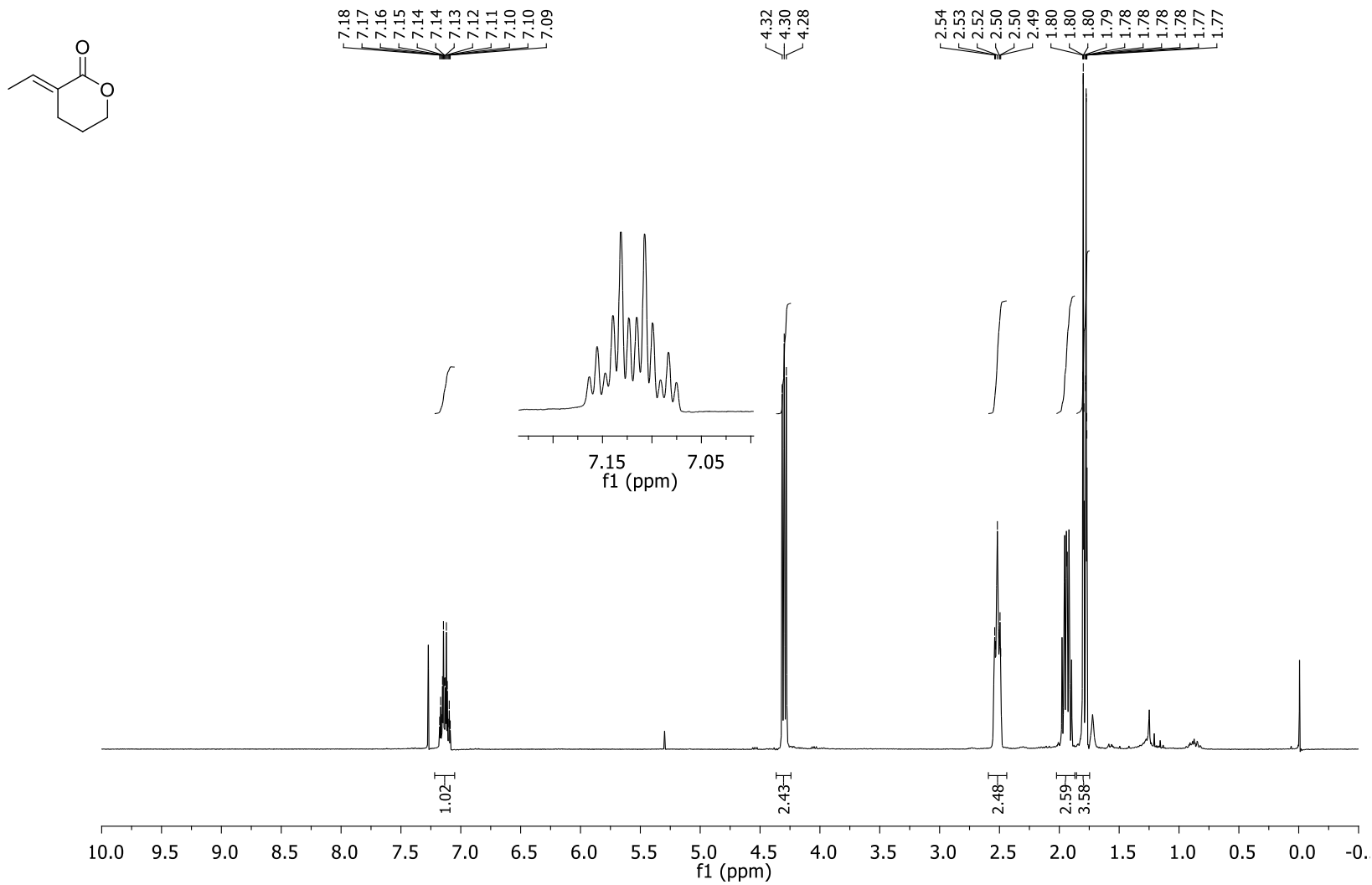
S2.19. ¹H NMR (600 MHz) spectrum of **8** (*E*) **R** = 4-NO₂-Phenyl in CDCl₃.



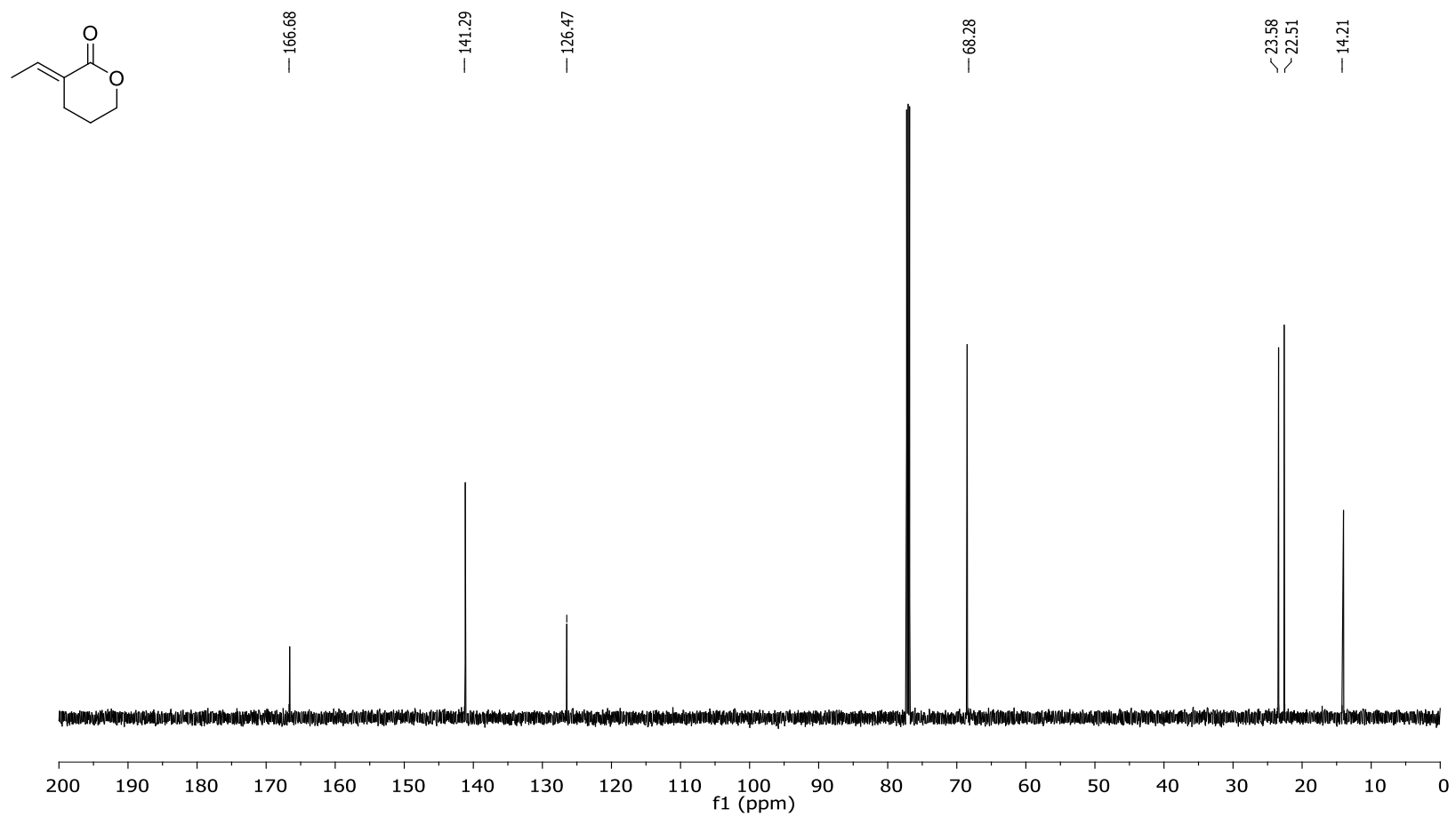
S2.20. ^{13}C NMR (151 MHz) spectrum of **8** (*E*) **R** = 4-NO₂-Phenyl in CDCl₃.



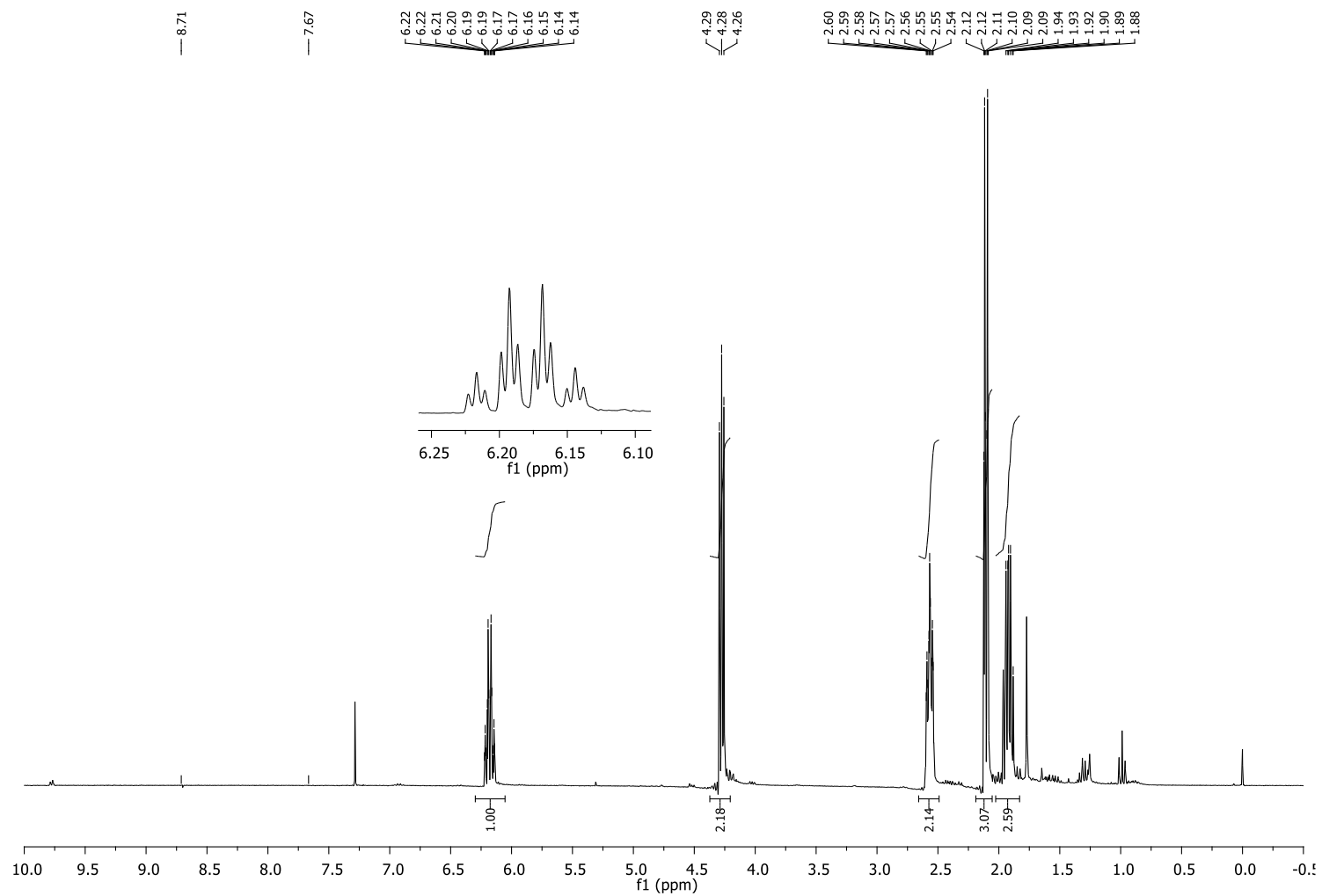
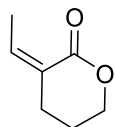
S2.21. ^1H NMR (600 MHz) spectrum of **10E** in CDCl_3 .



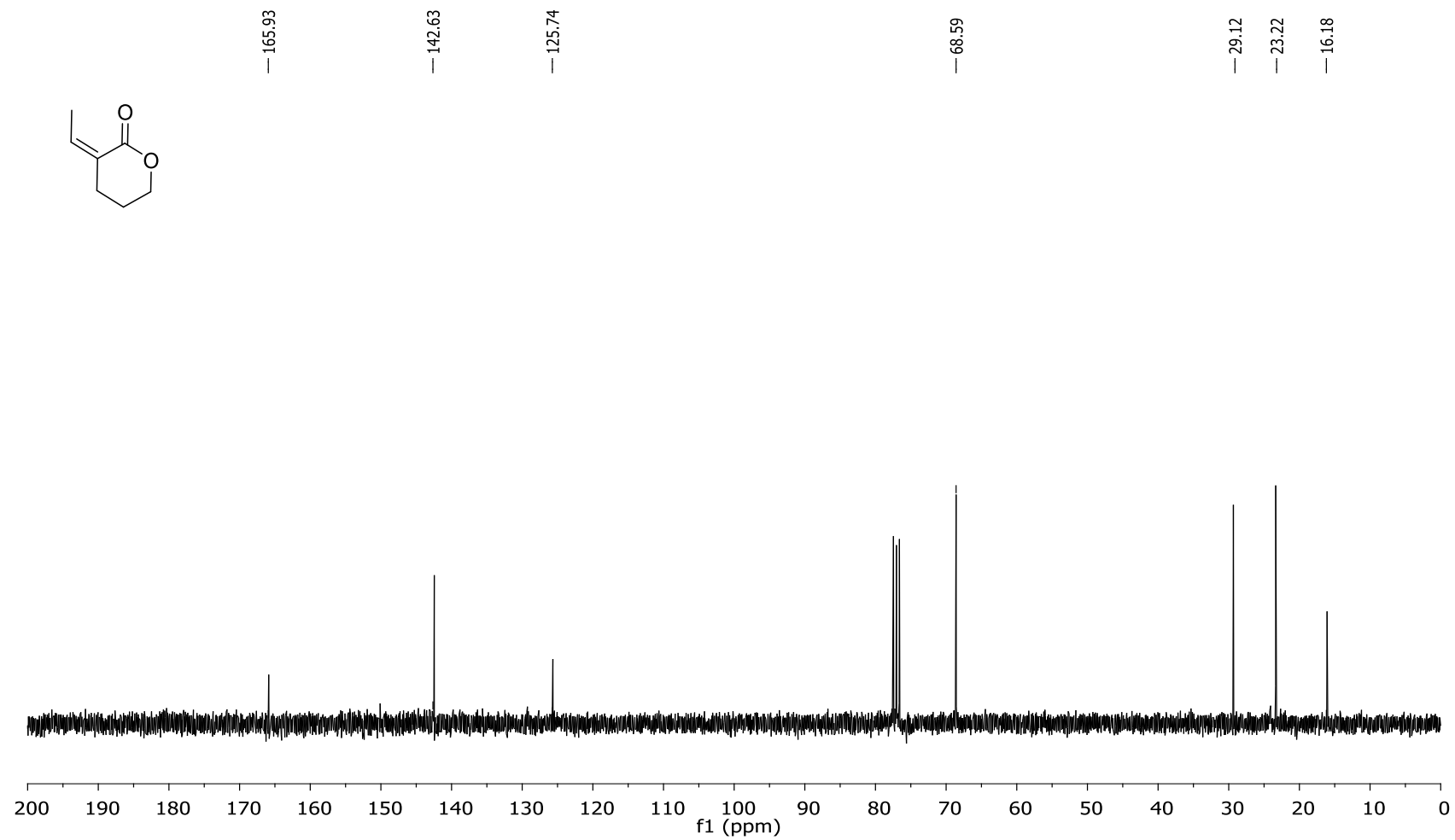
S2.22. ^{13}C NMR (151 MHz) spectrum of **10E** in CDCl_3 .



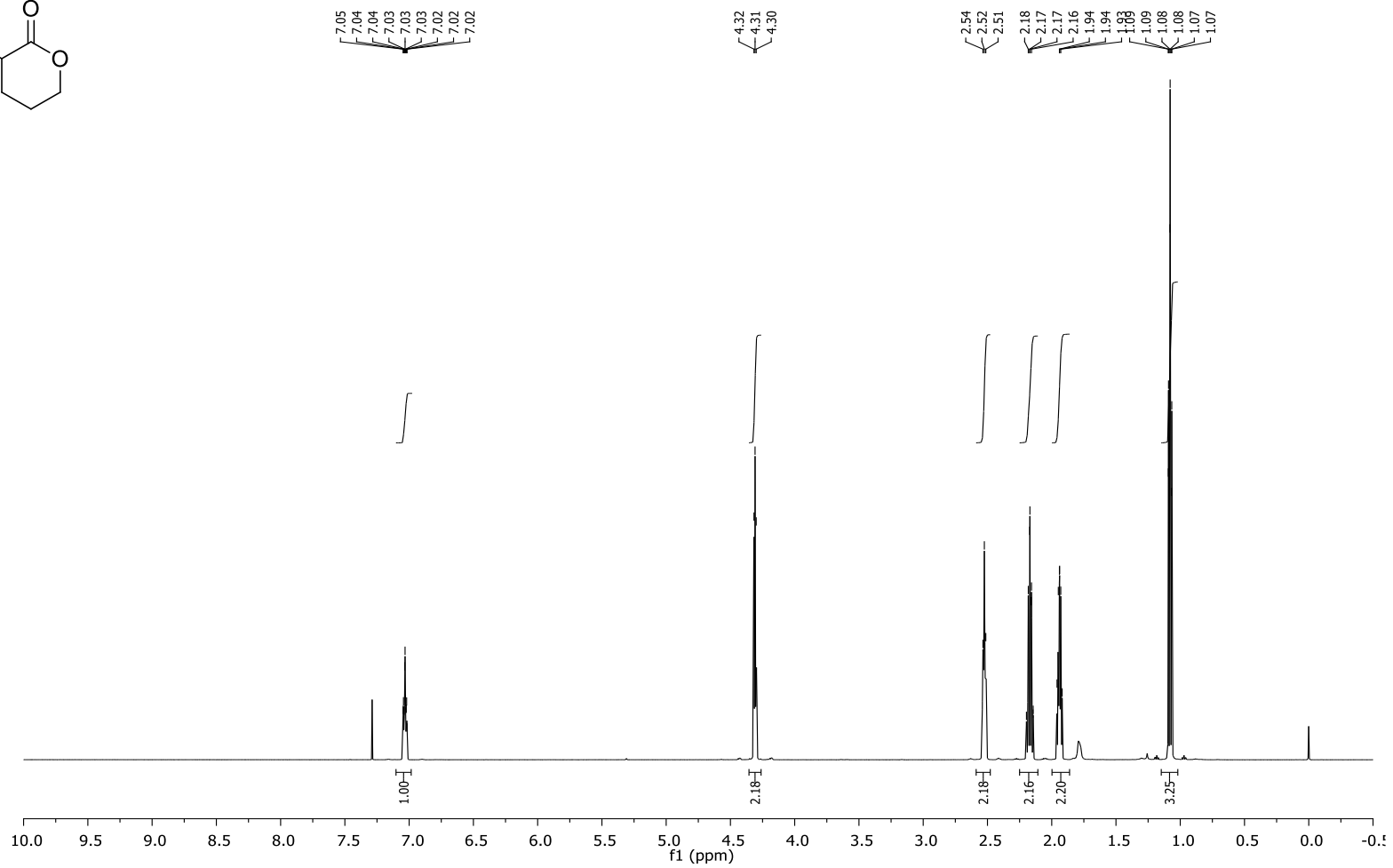
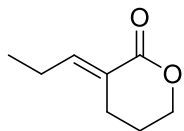
S2.23. ^1H NMR (300 MHz) spectrum of **10Z** in CDCl_3 .



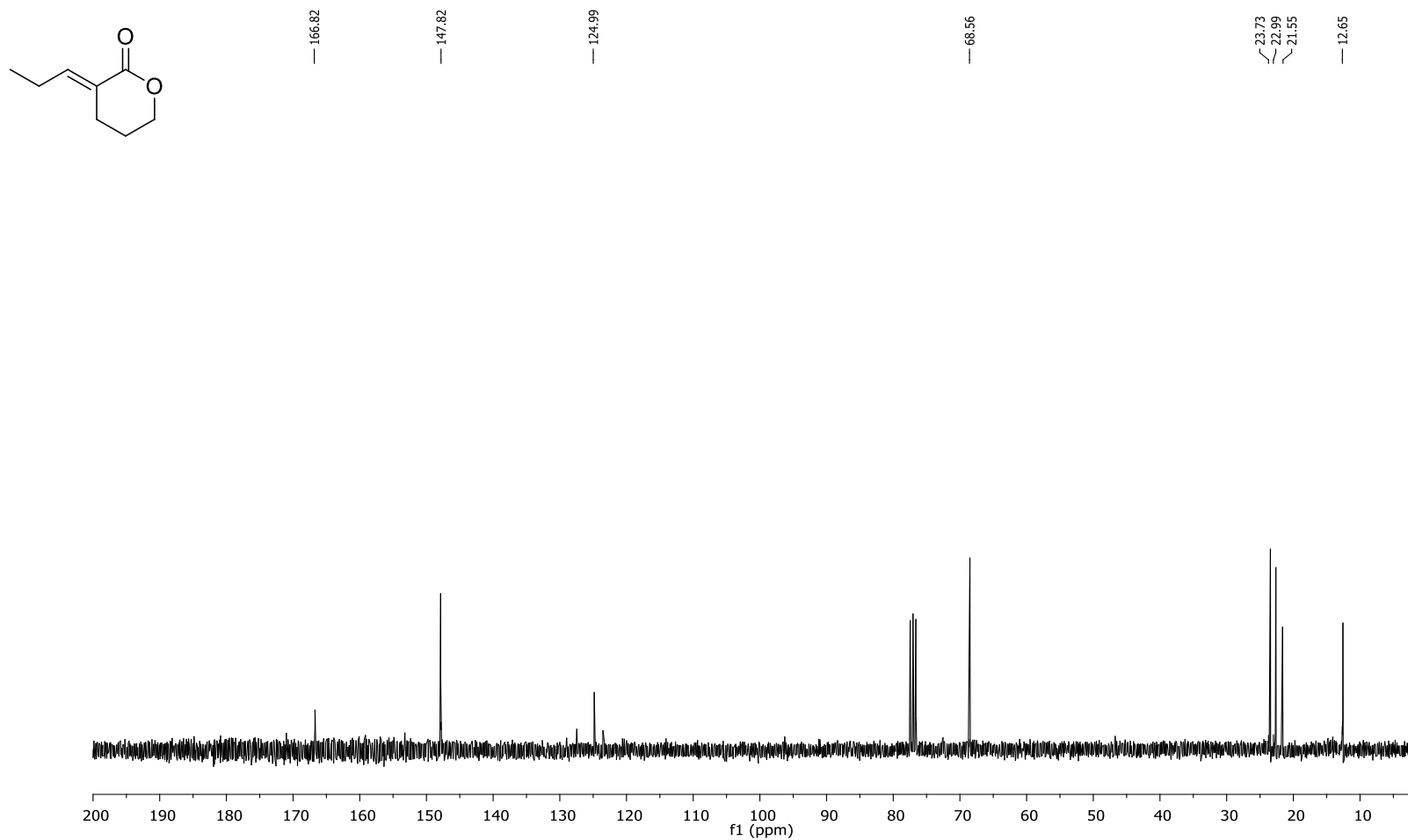
S2.24. ^{13}C NMR (75 MHz) spectrum of **10Z** in CDCl_3 .



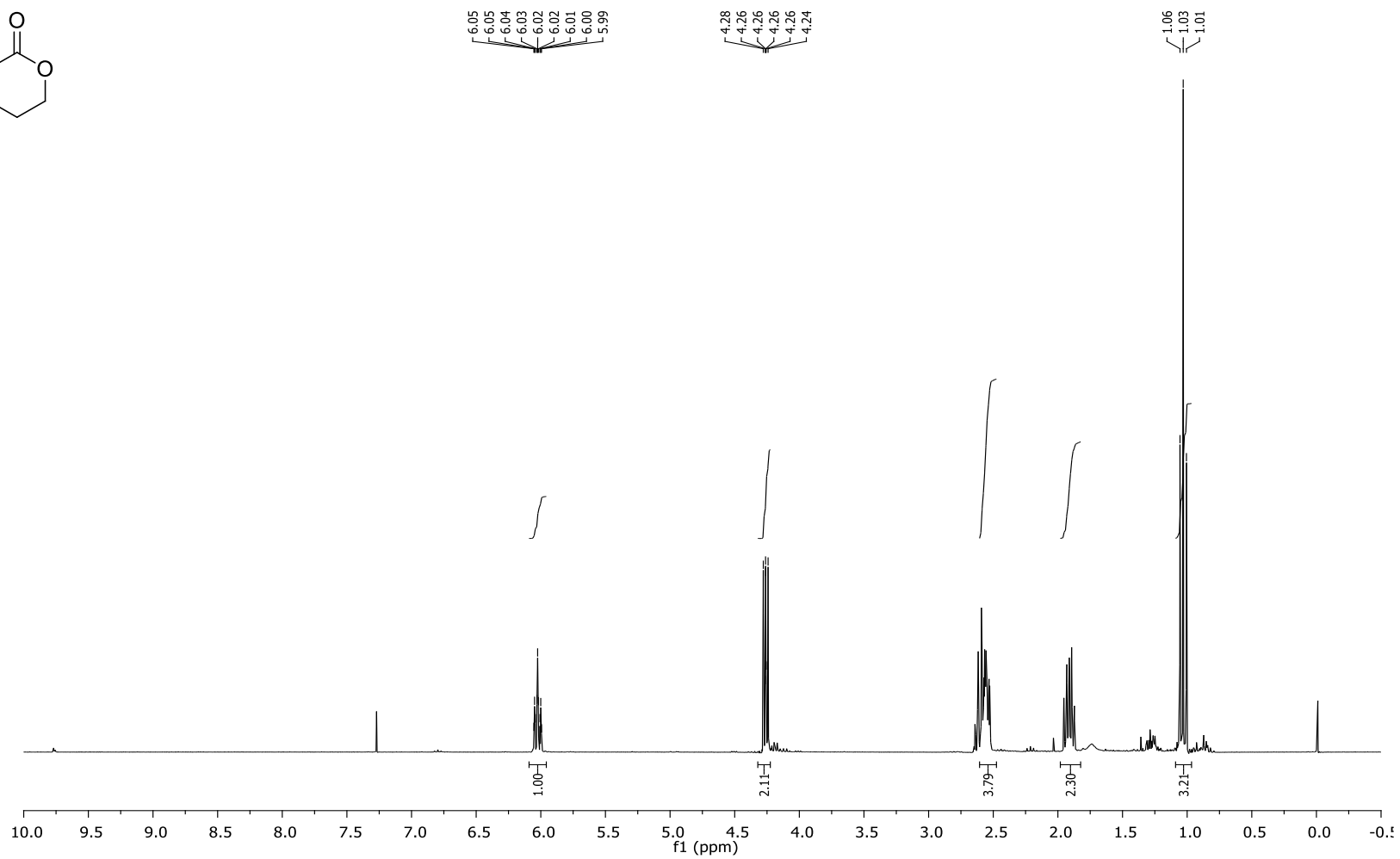
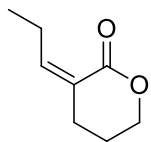
S2.25. ^1H NMR (600 MHz) spectrum of **11E** in CDCl_3 .



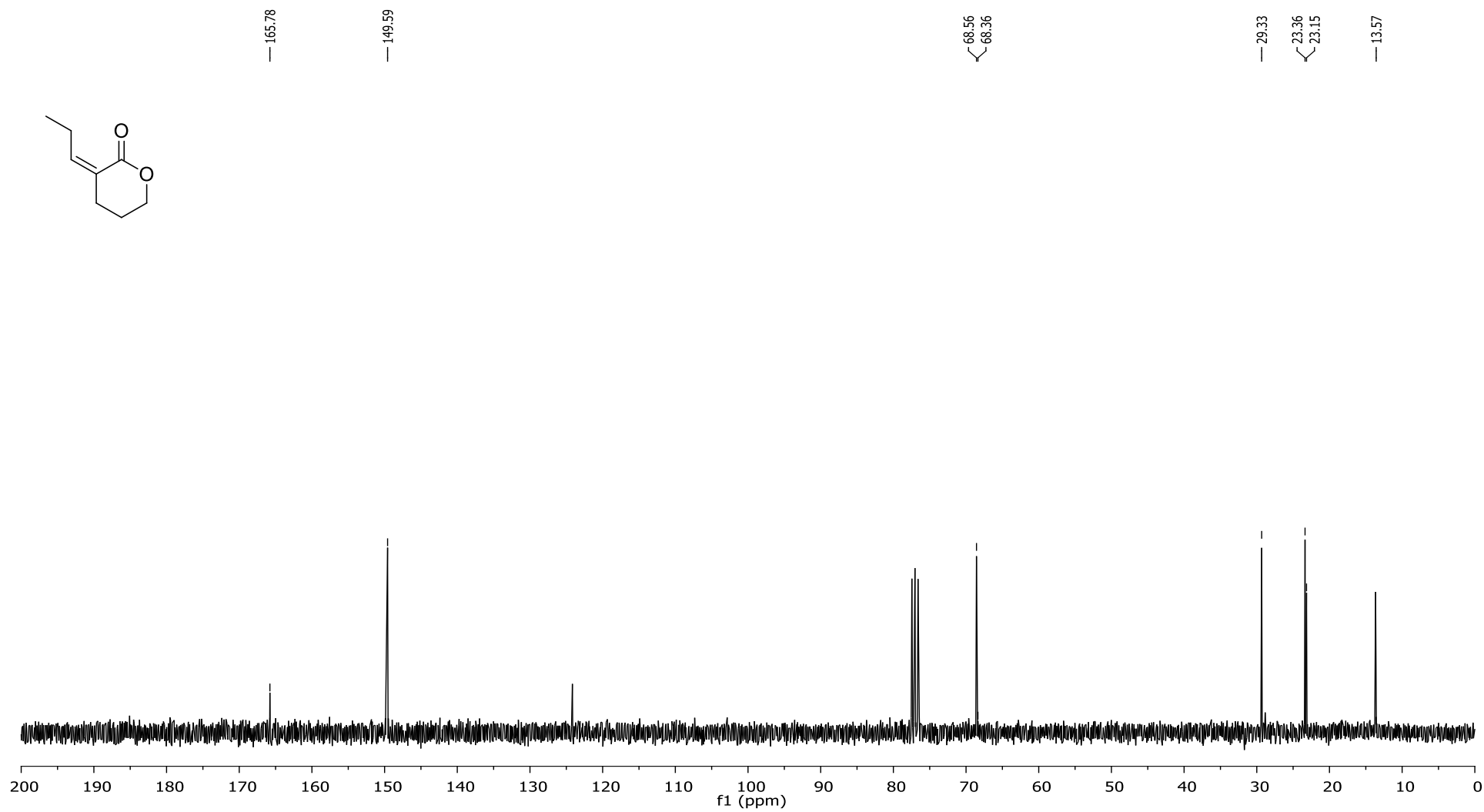
S2.26. ^{13}C NMR (75 MHz) spectrum of **11E** in CDCl_3 .



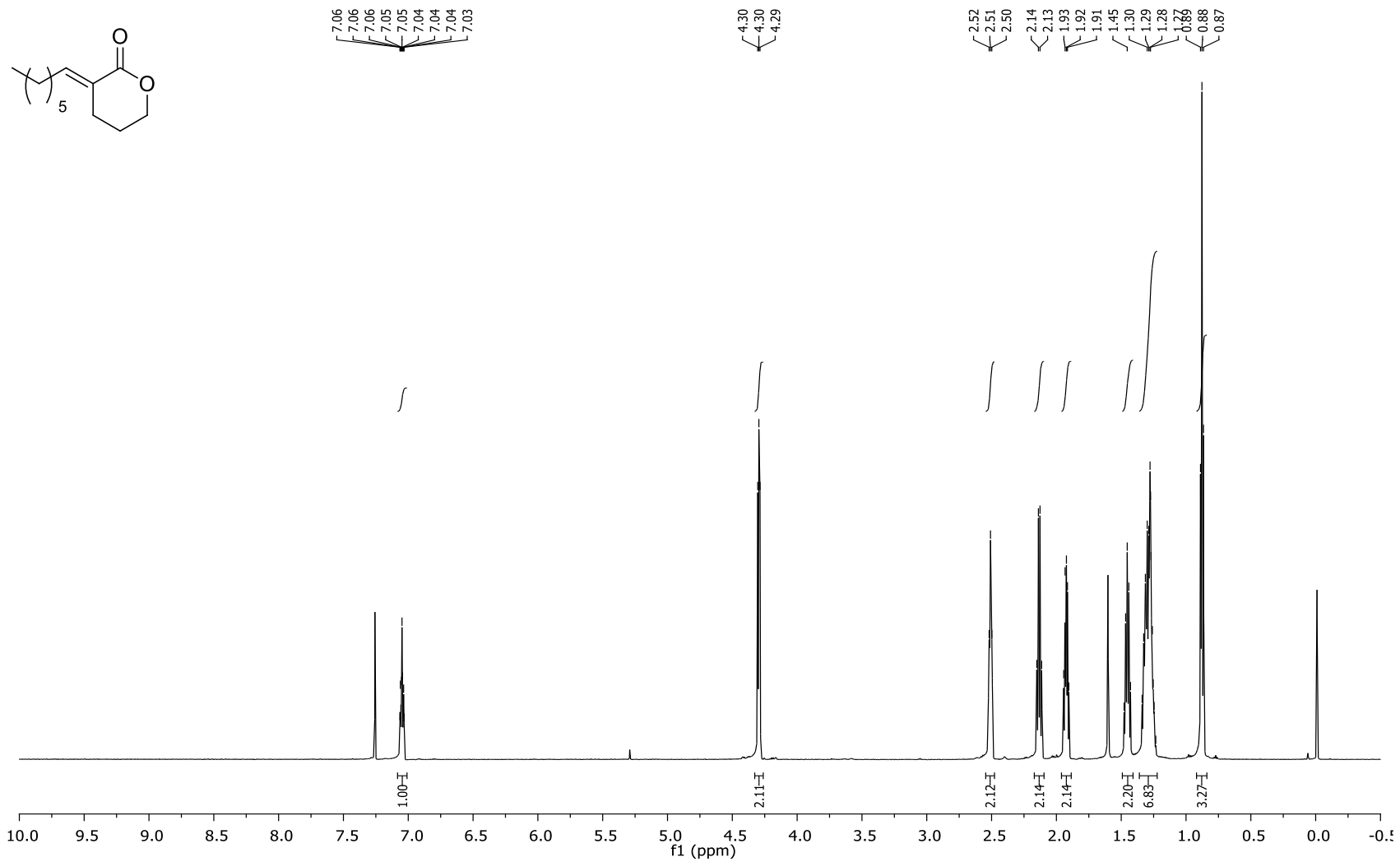
S2.27. ^1H NMR (300 MHz) spectrum of **11Z** in CDCl_3 .



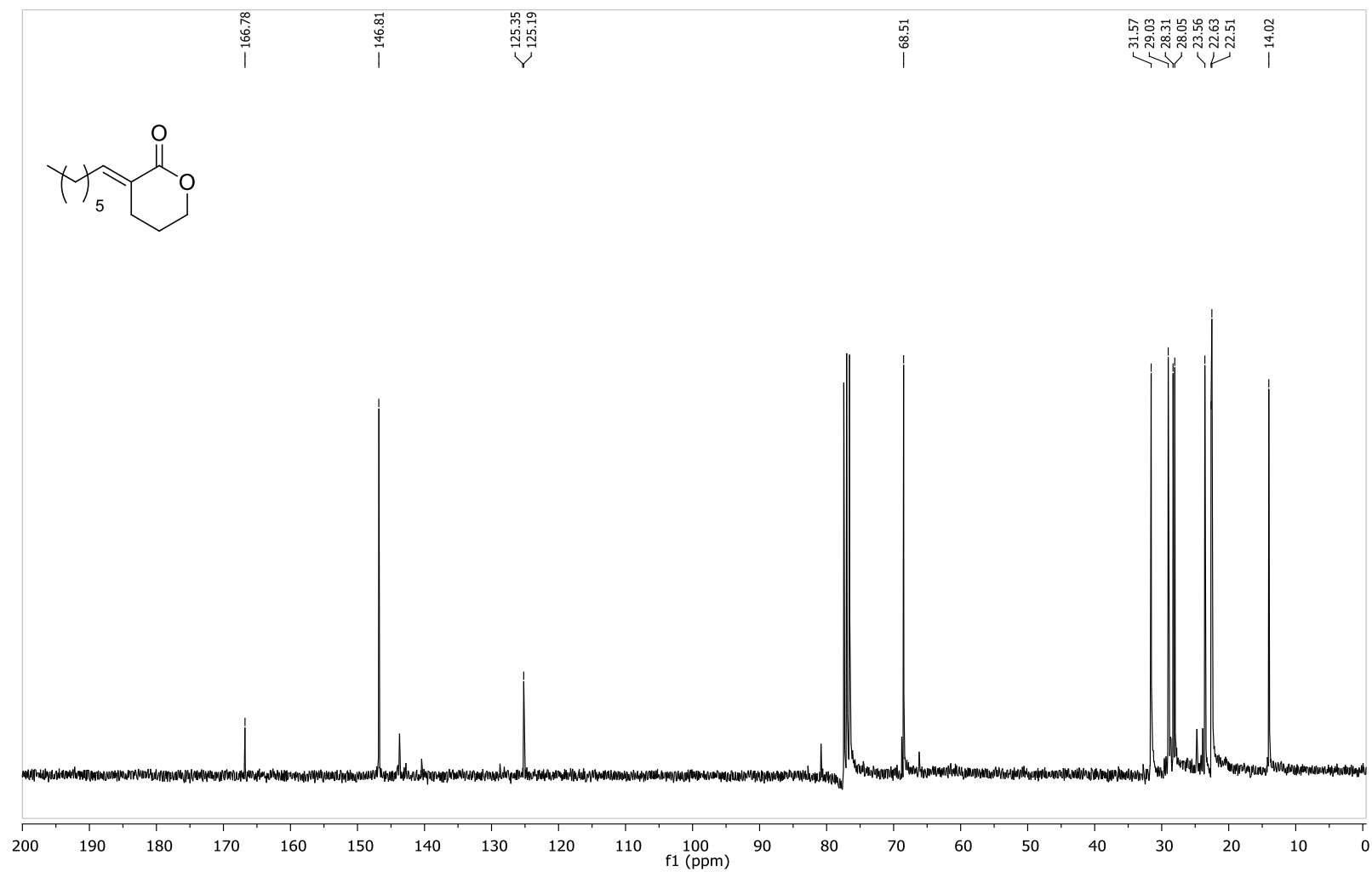
S2.28. ^{13}C NMR (75 MHz) spectrum of **11Z** in CDCl_3 .



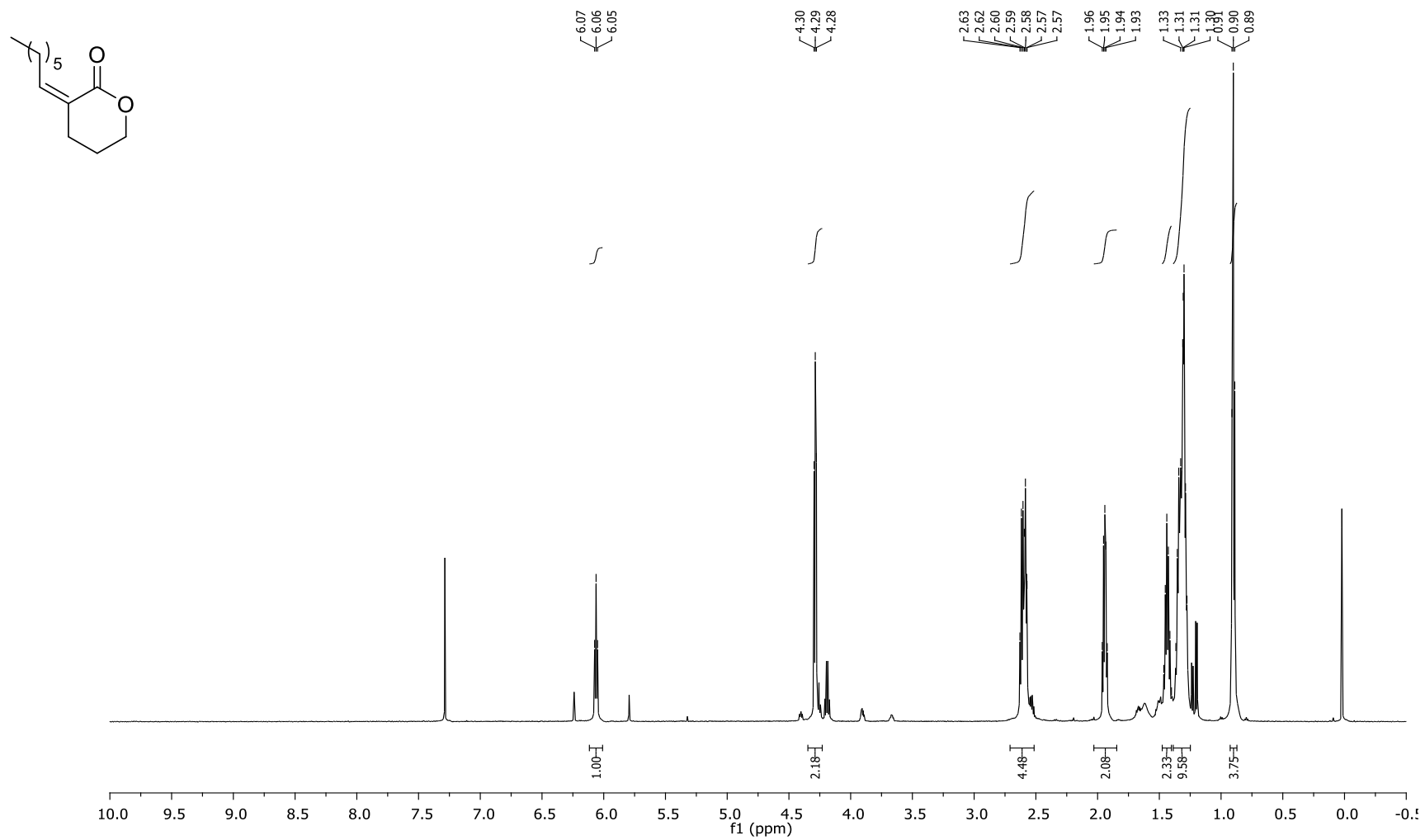
S2.29. ^1H NMR (600 MHz) spectrum of **12E** in CDCl_3 .



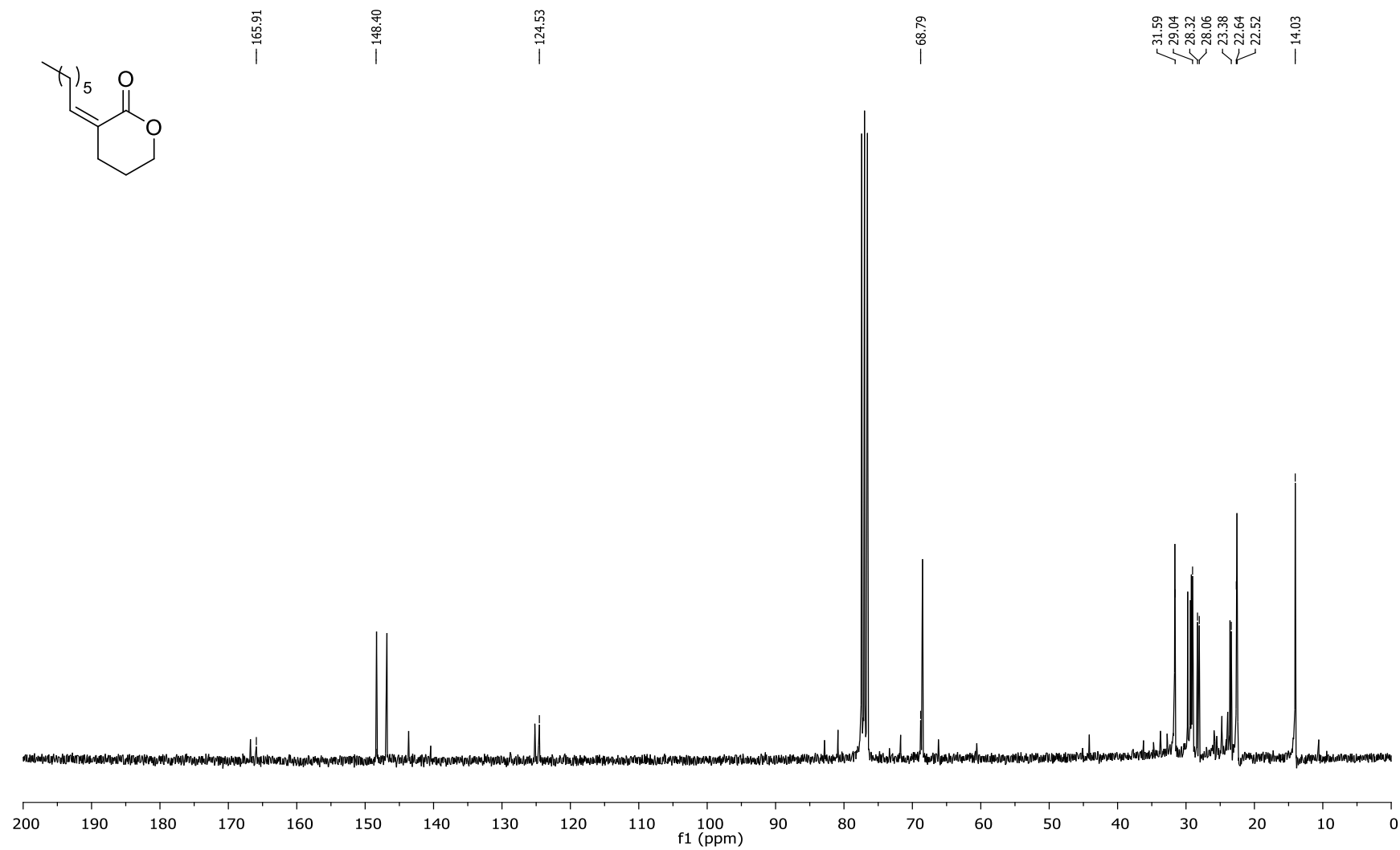
S2.30. ^{13}C NMR (75 MHz) spectrum of **12E** in CDCl_3 .



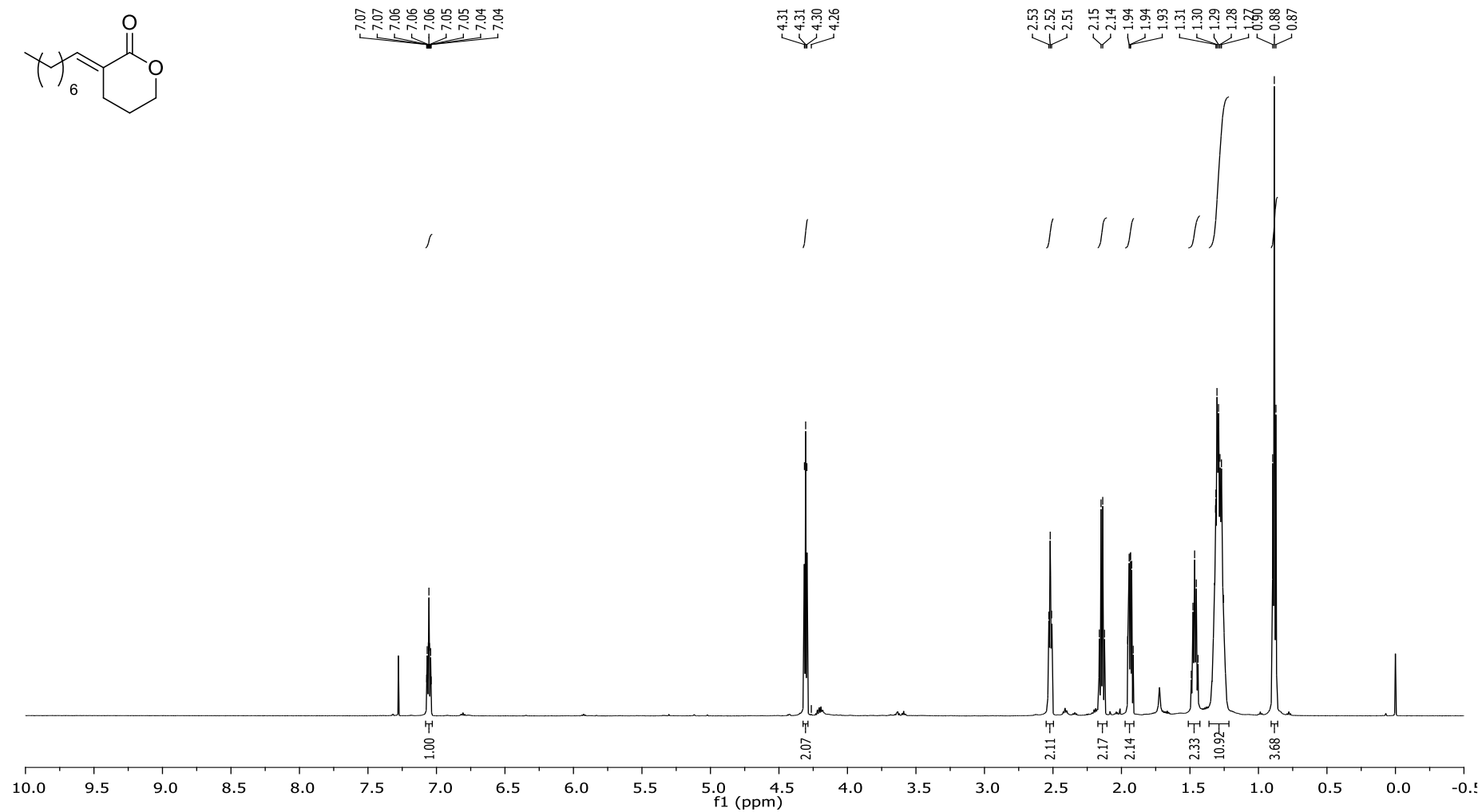
S2.31. ^1H NMR (600 MHz) spectrum of **12Z** in CDCl_3 .



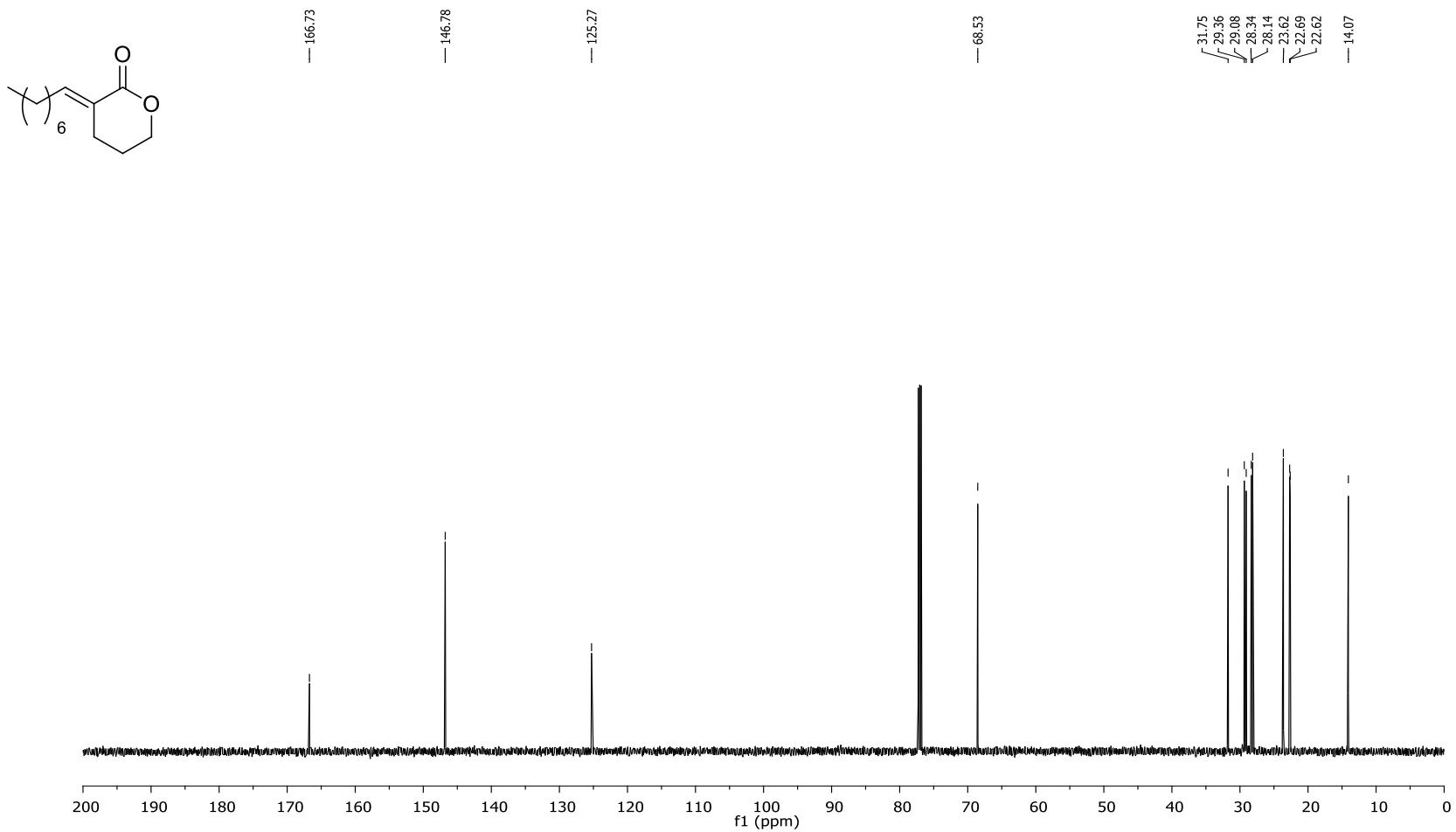
S2.32. ^{13}C NMR (75 MHz) spectrum of **12Z** in CDCl_3 .



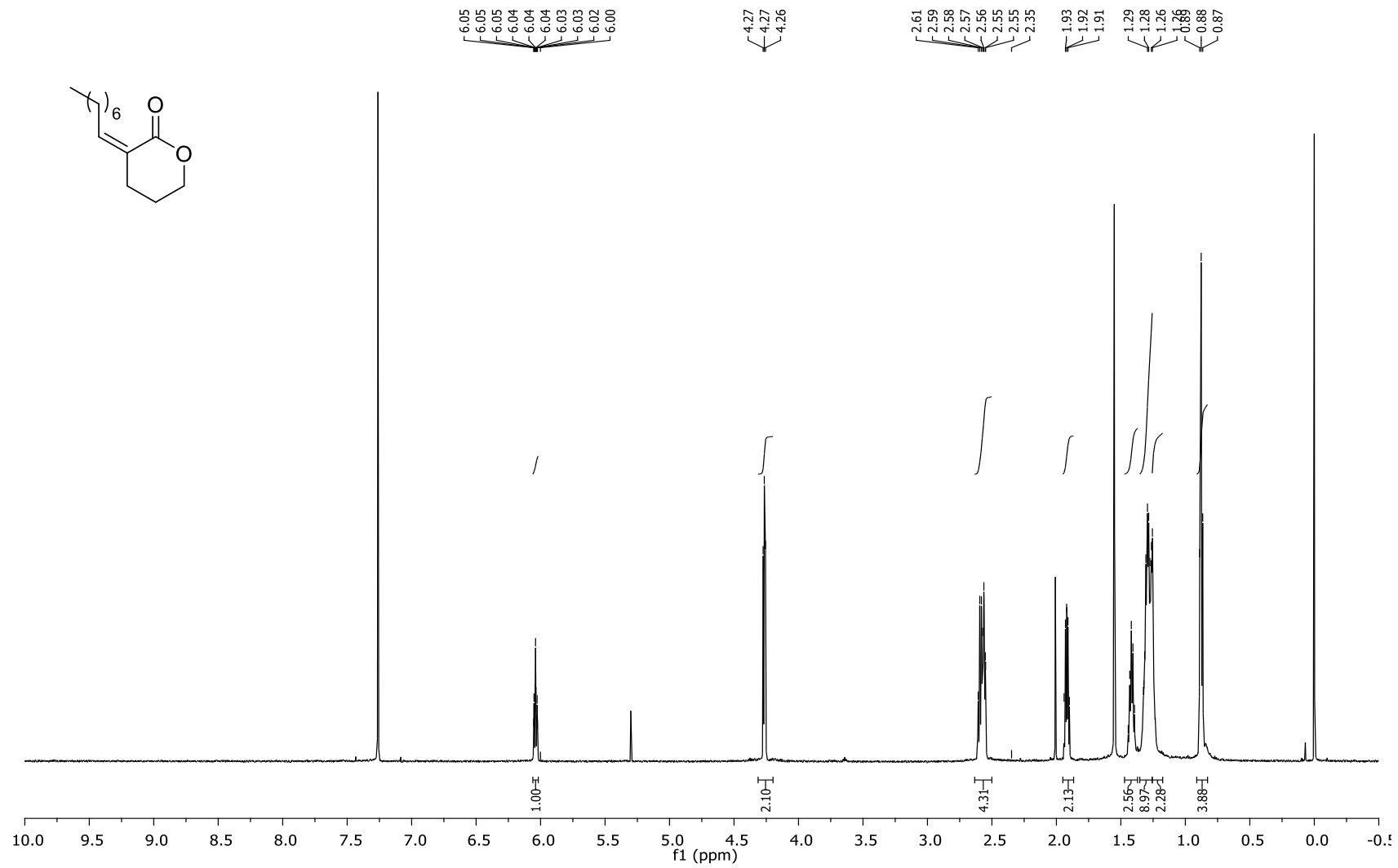
S2.33. ^1H NMR (600 MHz) spectrum of **13E** in CDCl_3 .



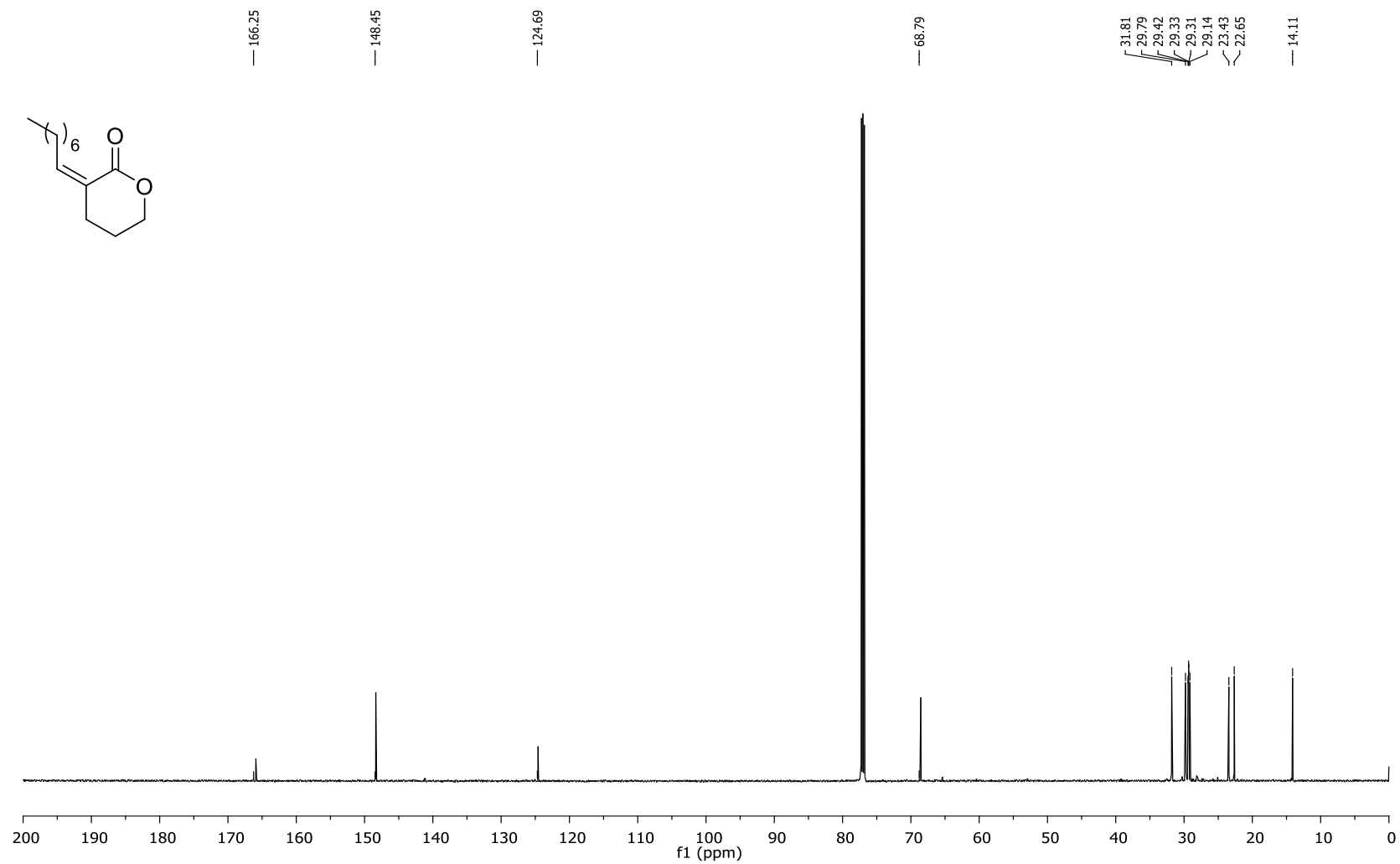
S2.34. ^{13}C NMR (151 MHz) spectrum of **13E** in CDCl_3 .



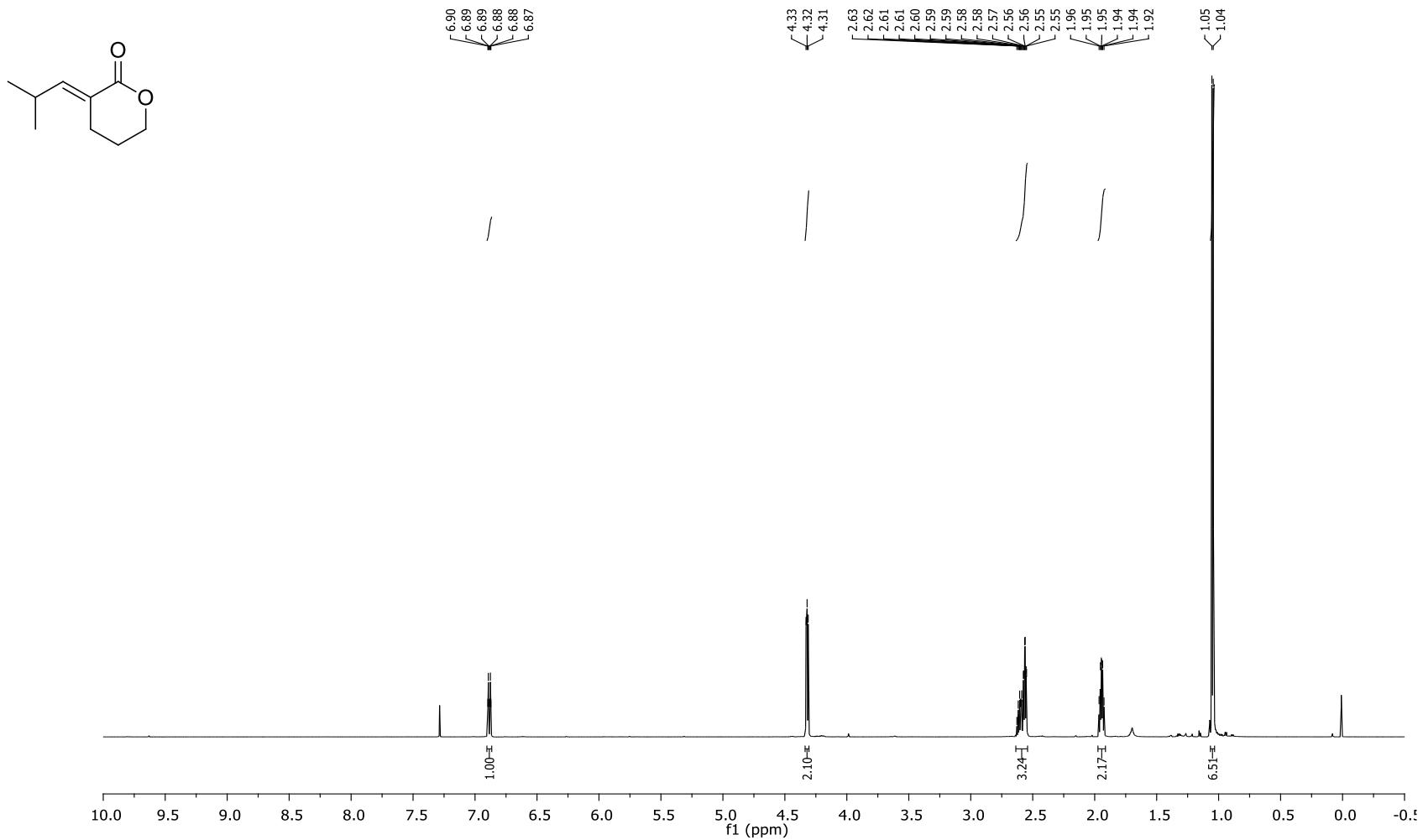
S2.35. ^1H NMR (600 MHz) spectrum of **13Z** in CDCl_3 .



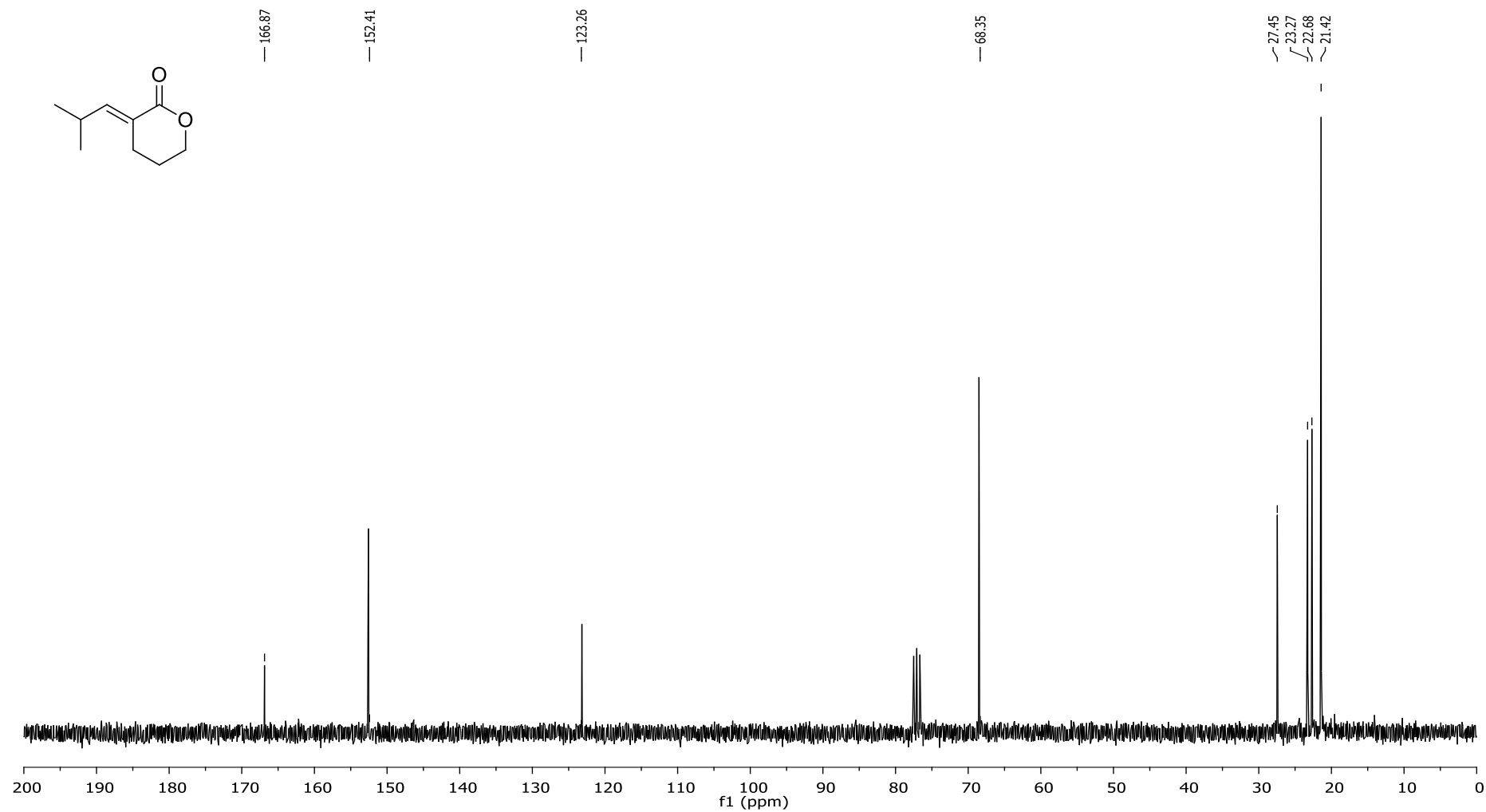
S2.36. ^{13}C NMR (151 MHz) spectrum of **13Z** in CDCl_3 .



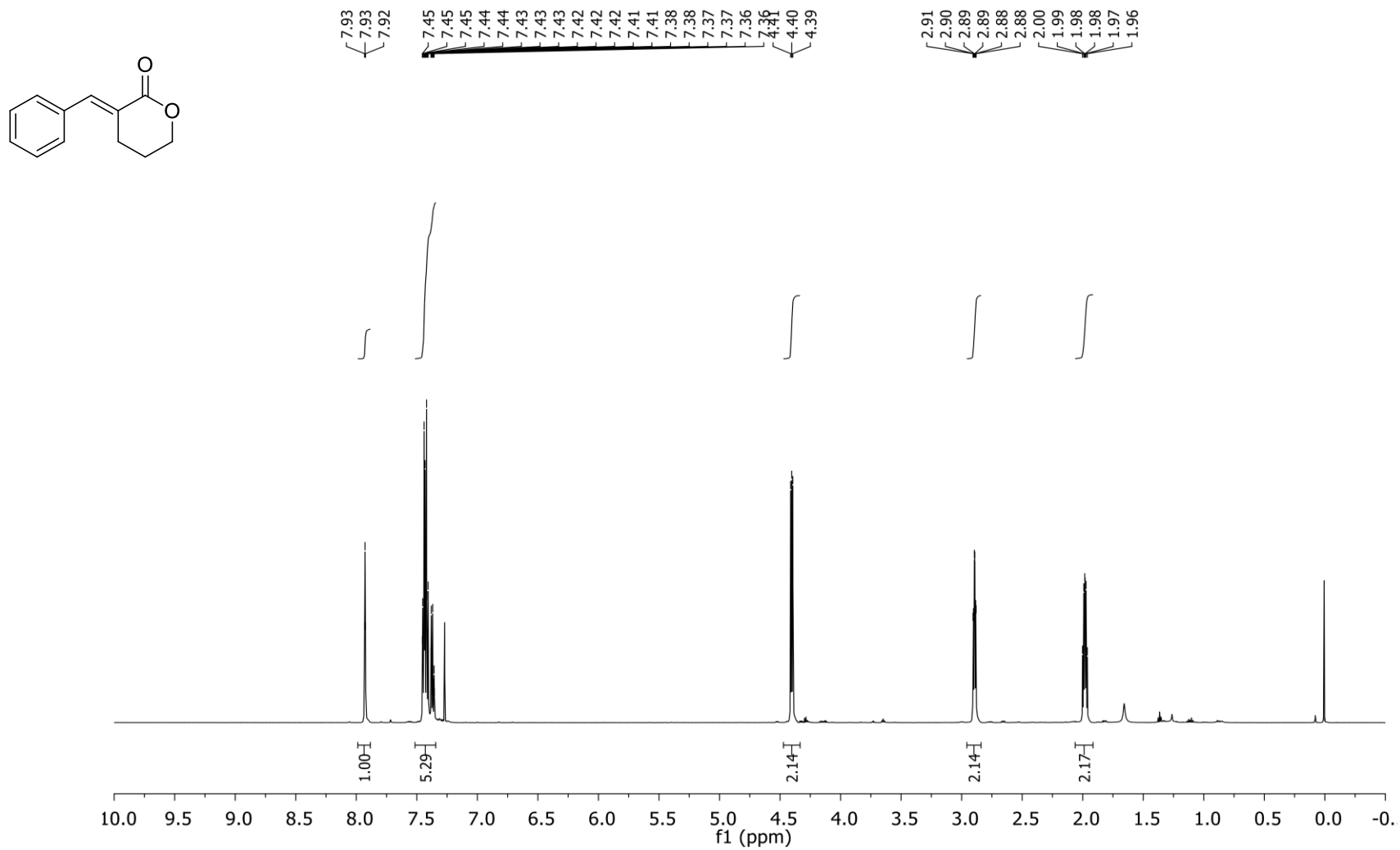
S2.37. ^1H NMR (600 MHz) spectrum of **14E** in CDCl_3 .



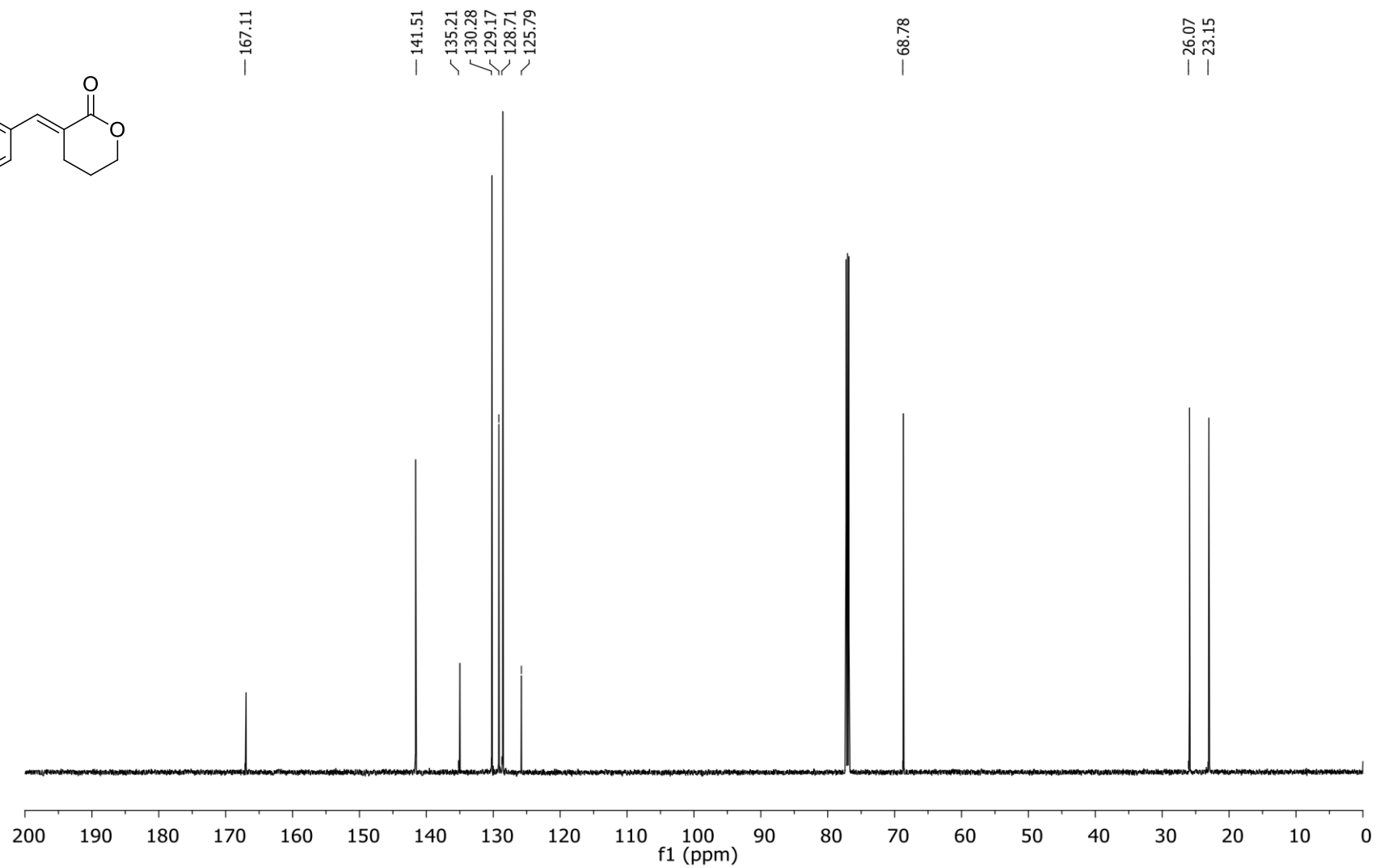
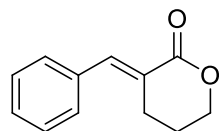
S2.38. ^{13}C NMR (75 MHz) spectrum of **14E** in CDCl_3 .



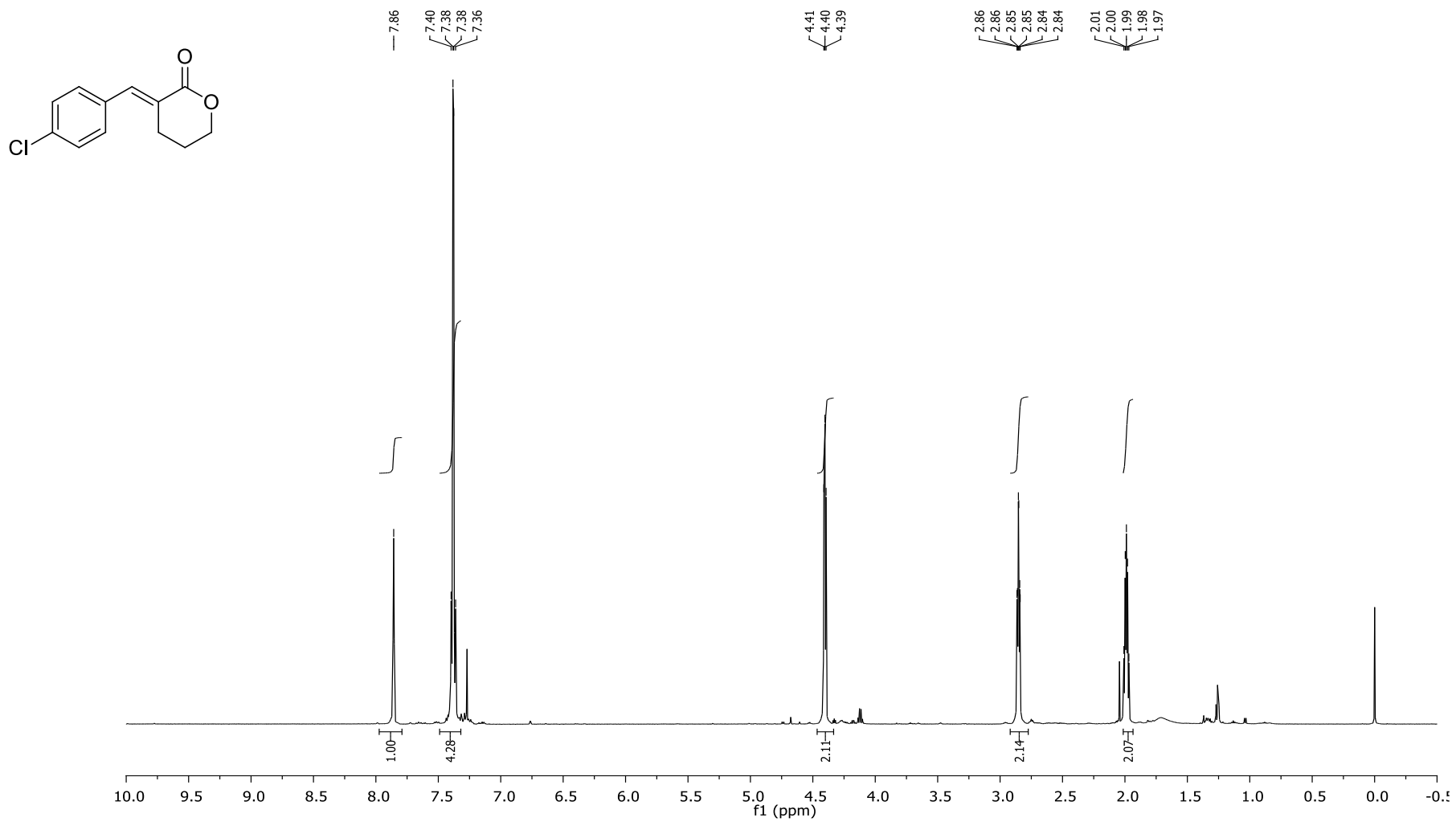
S2.39. ^1H NMR (600 MHz) spectrum of **15E** in CDCl_3 .



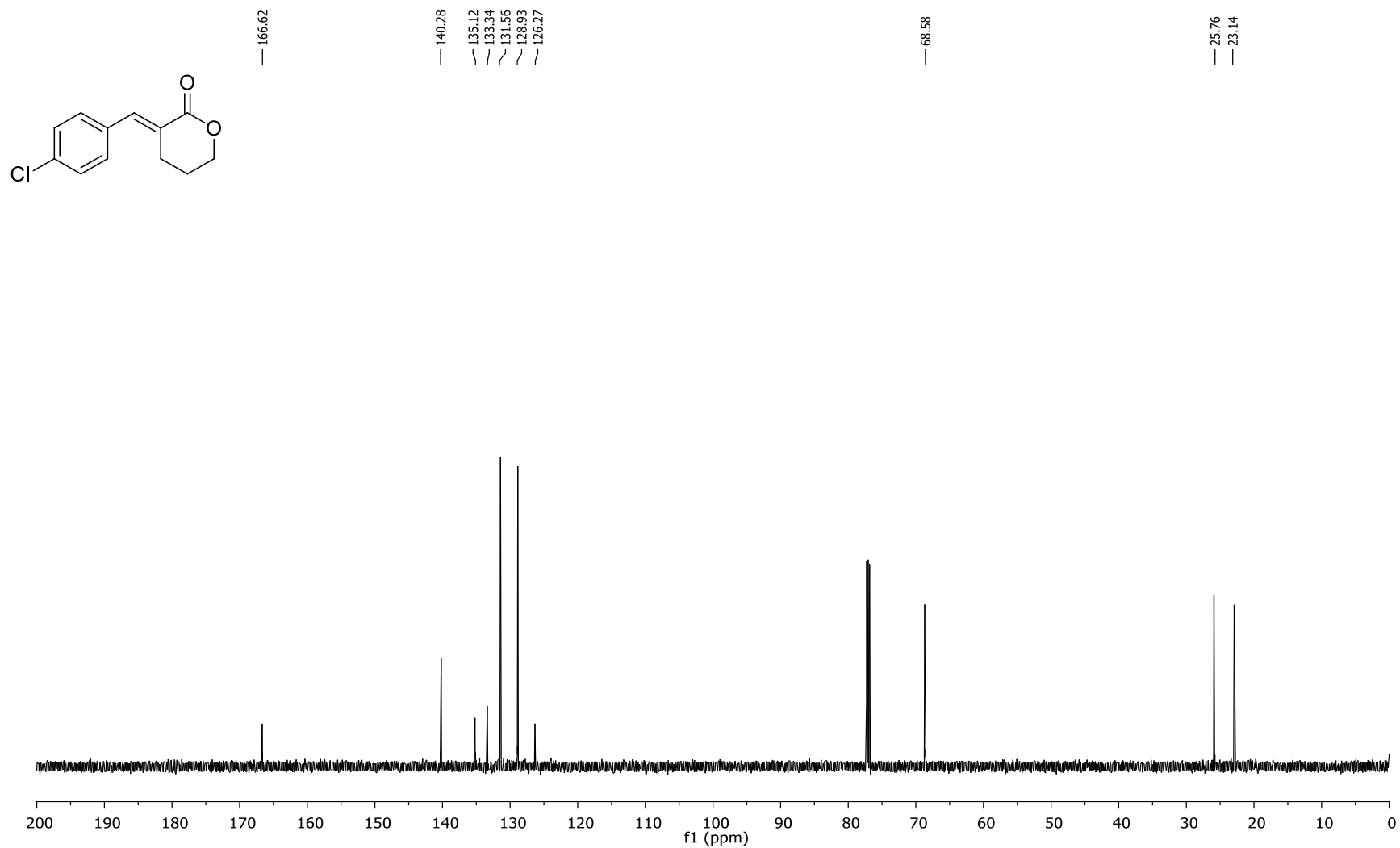
S2.40. ^{13}C NMR (151 MHz) spectrum of **15E** in CDCl_3 .



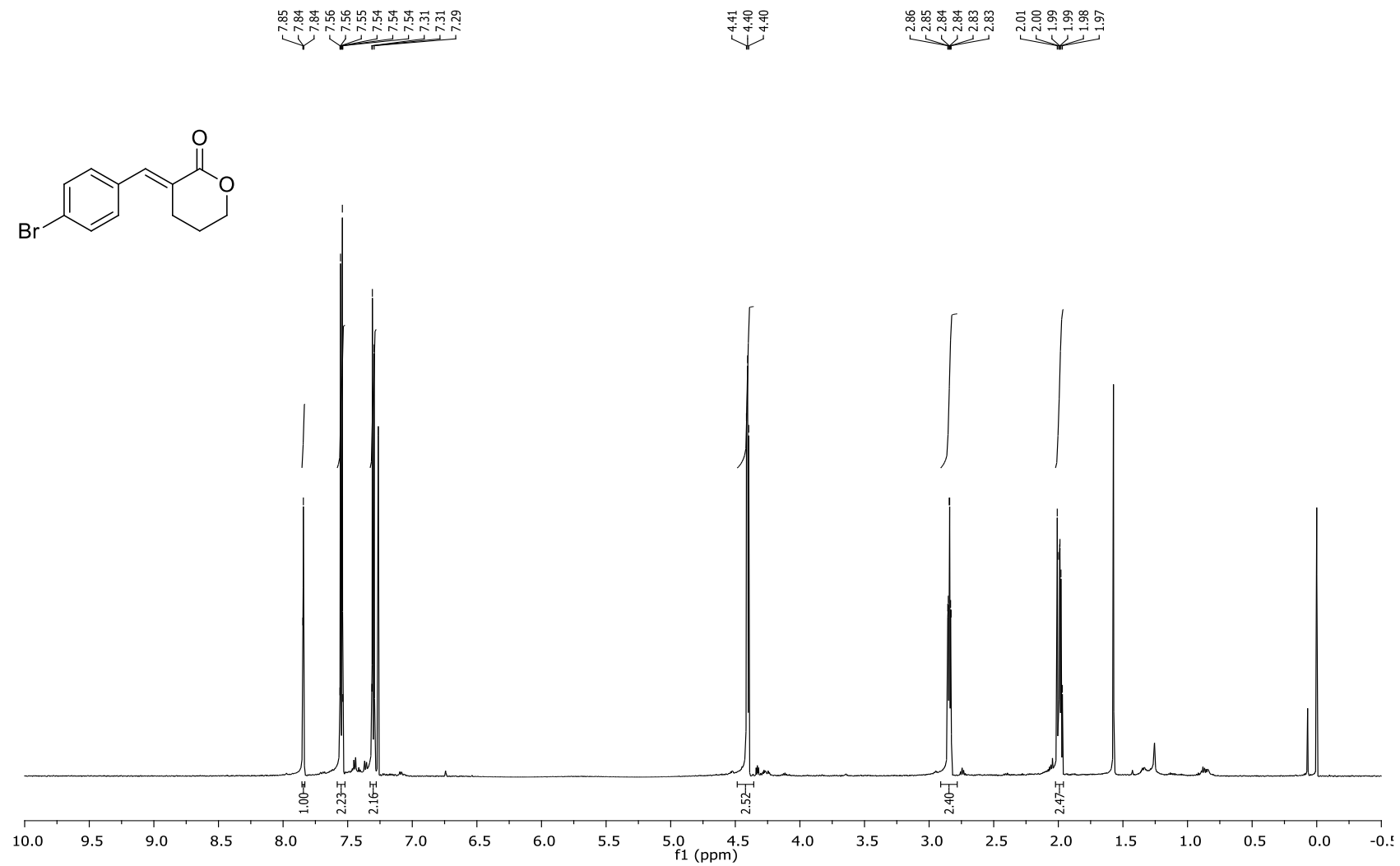
S2.41. ^1H NMR (600 MHz) spectrum of **16E** in CDCl_3 in CDCl_3 .



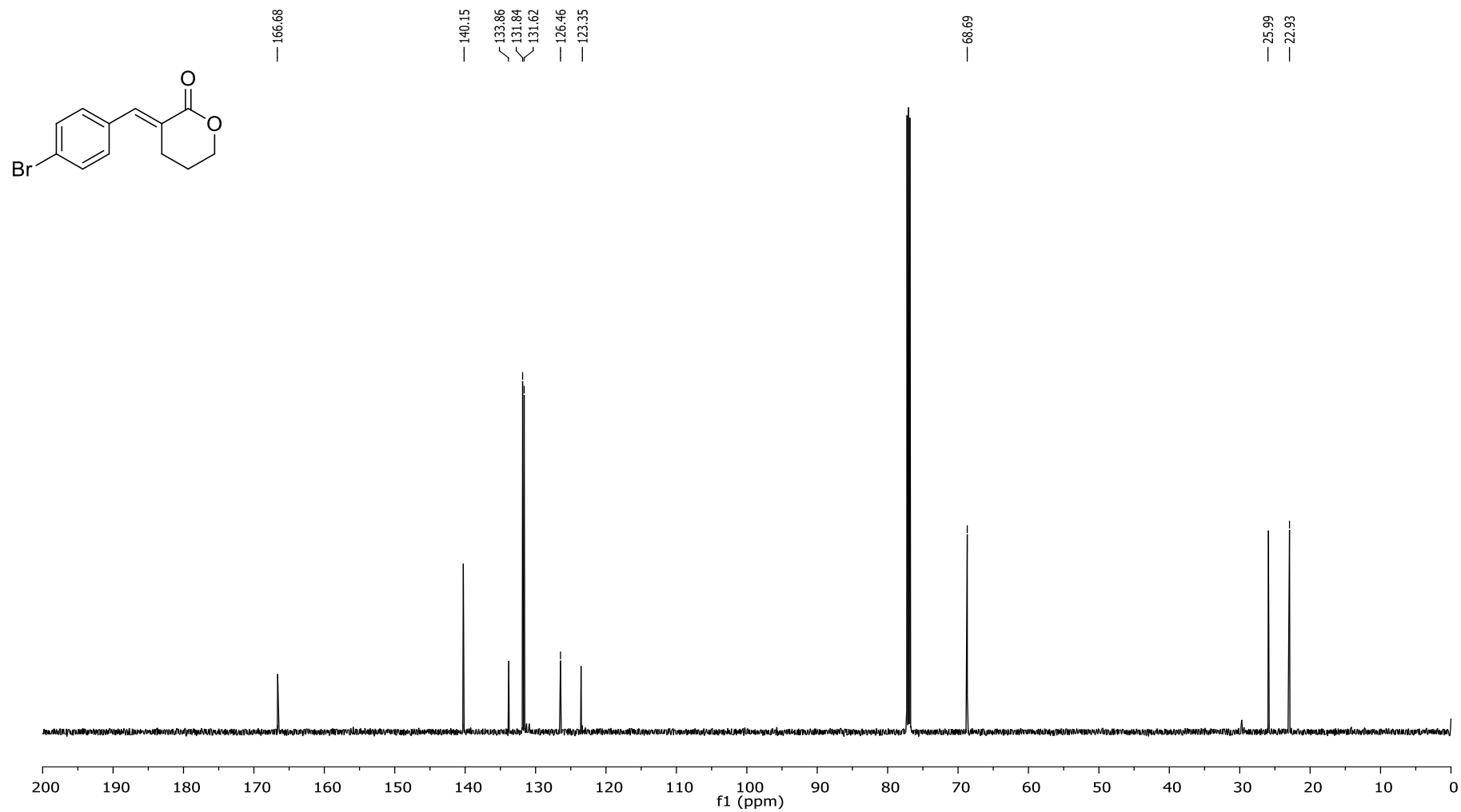
S2.42. ^{13}C NMR (151 MHz) spectrum of **16E** in CDCl_3 .



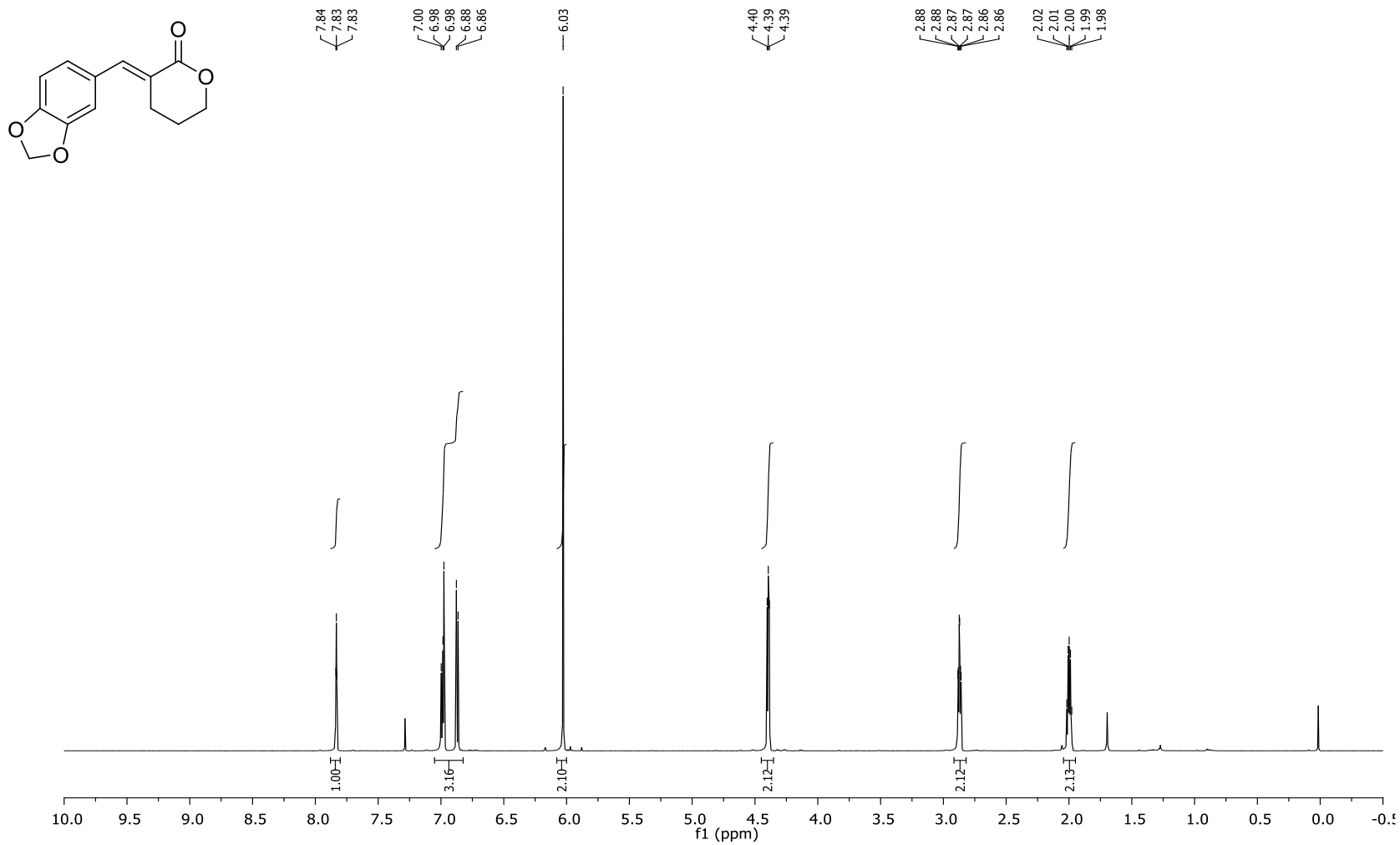
S2.43. ^1H NMR (600 MHz) spectrum of **17E** in CDCl_3 in CDCl_3 .



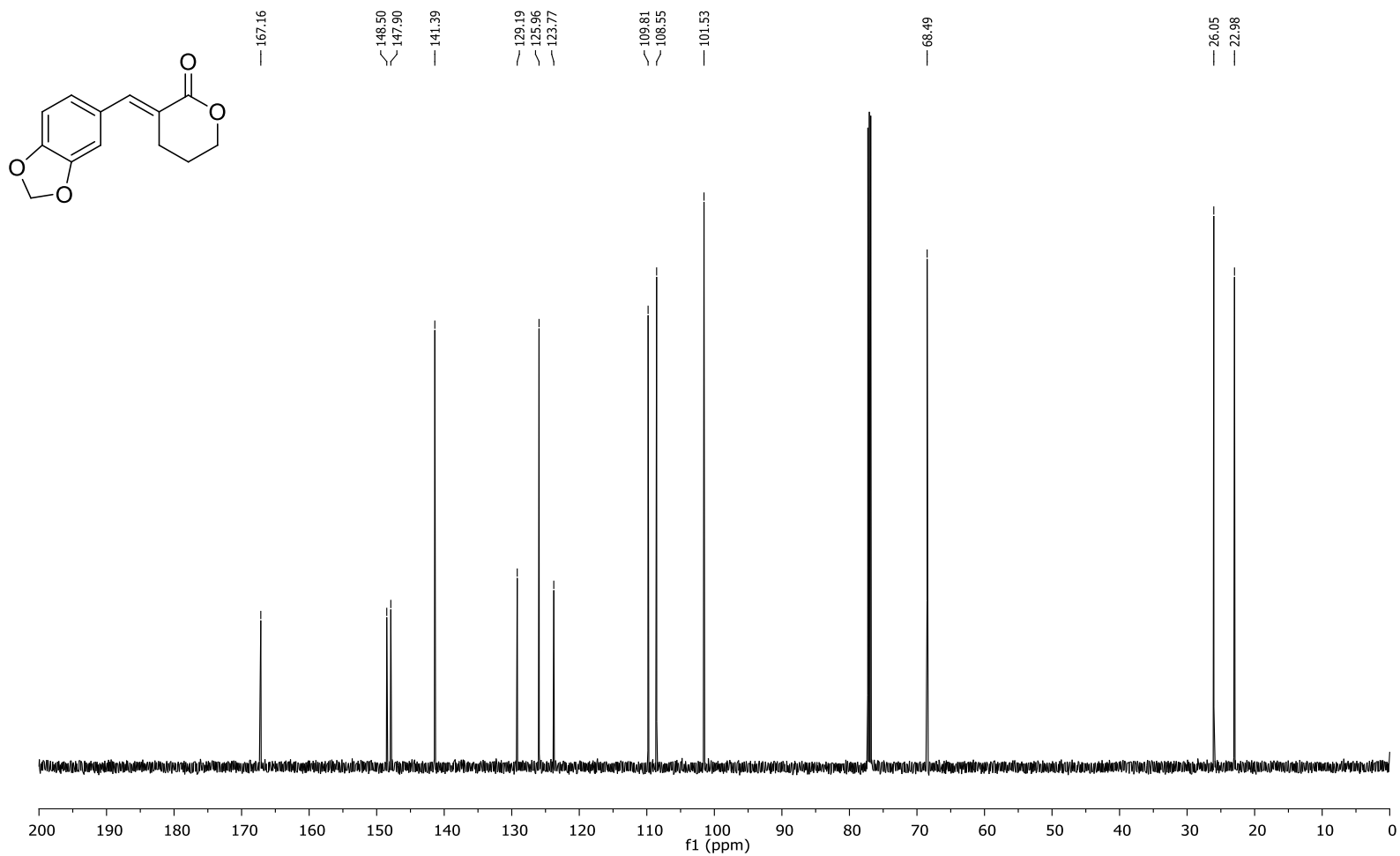
S2.44. ^{13}C NMR (151 MHz) spectrum of **17E** in CDCl_3 .



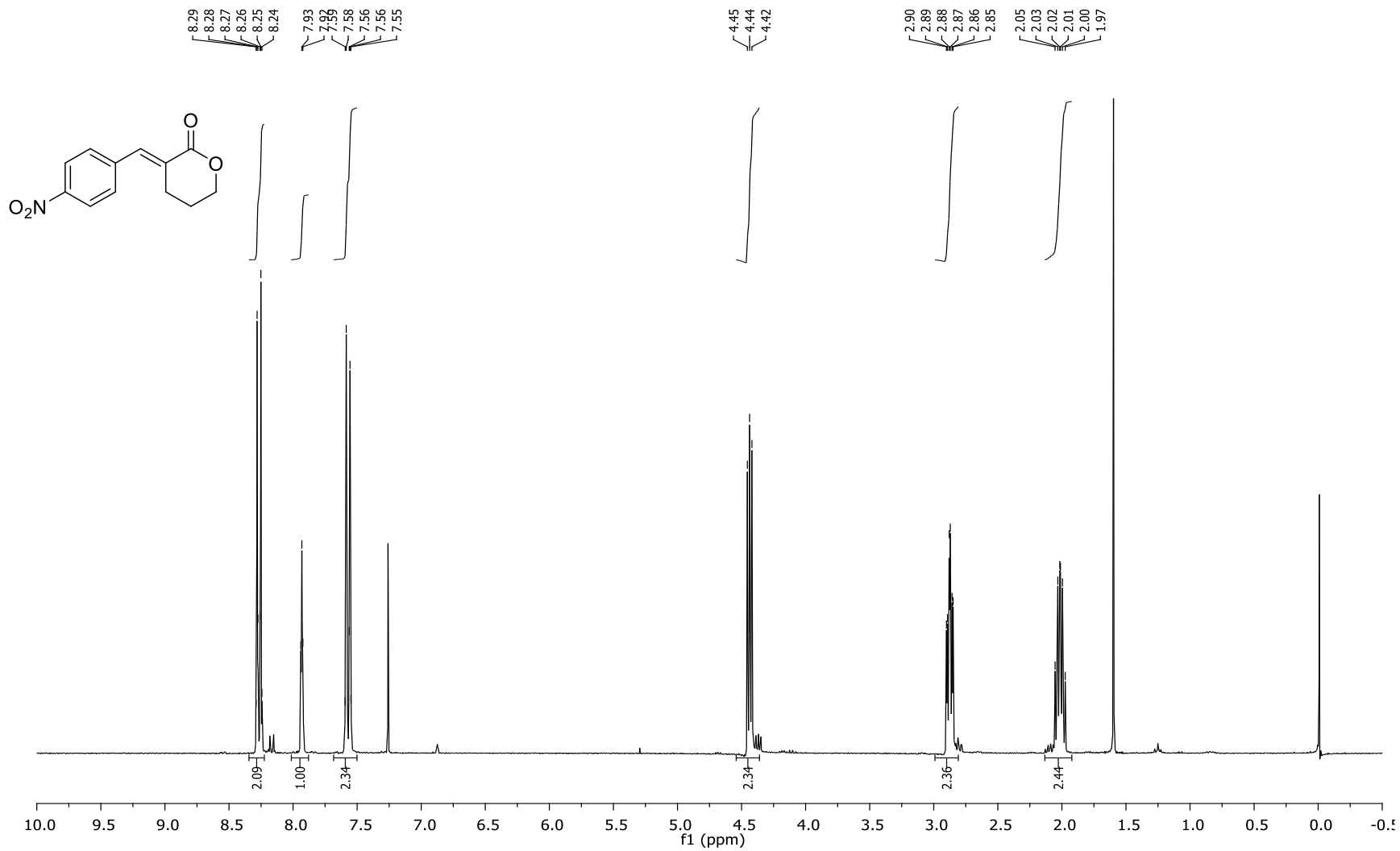
S2.45. ^1H NMR (600 MHz) spectrum of **18E** in CDCl_3 .



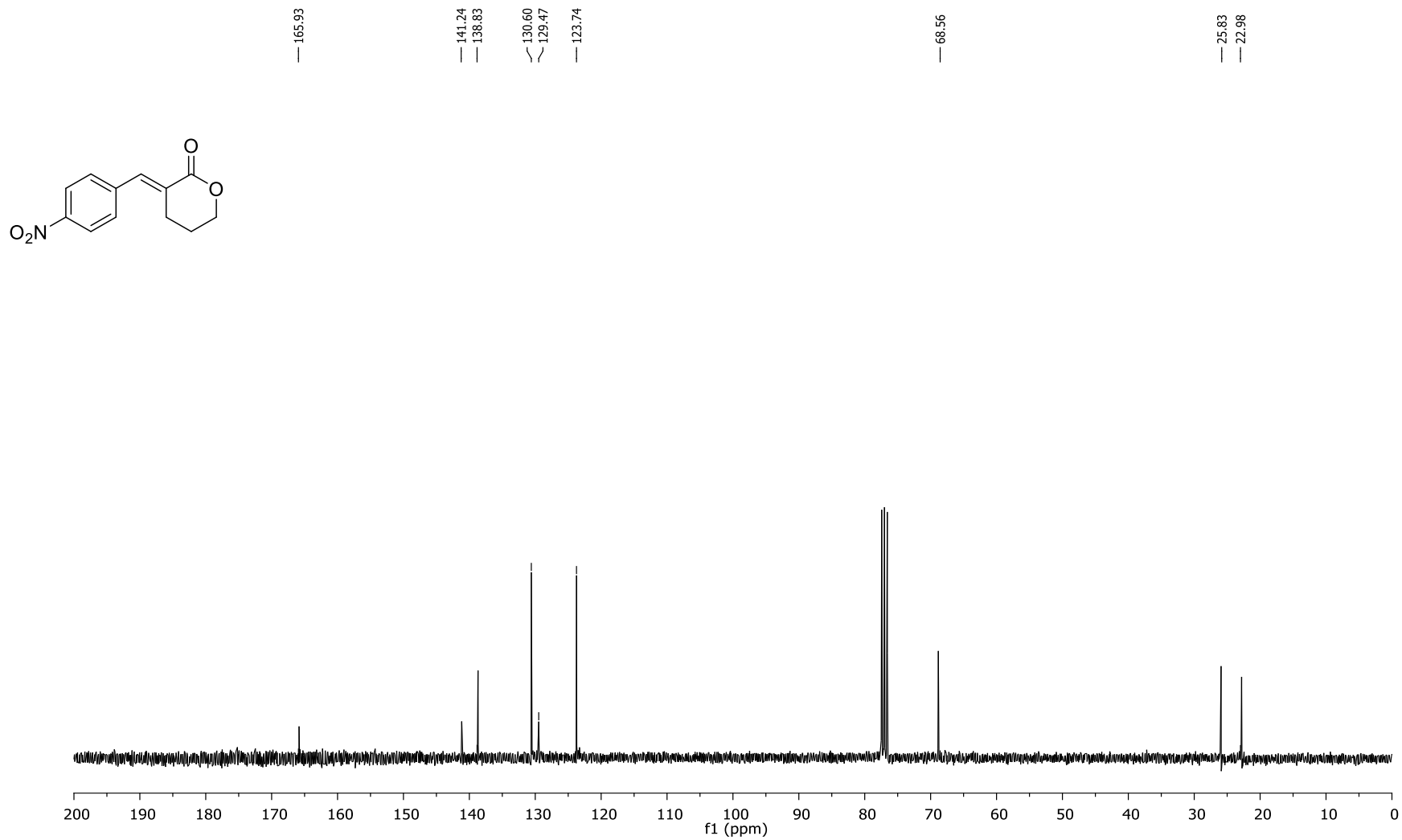
S2.46. ^{13}C NMR (151 MHz) spectrum of **18E** in CDCl_3 .



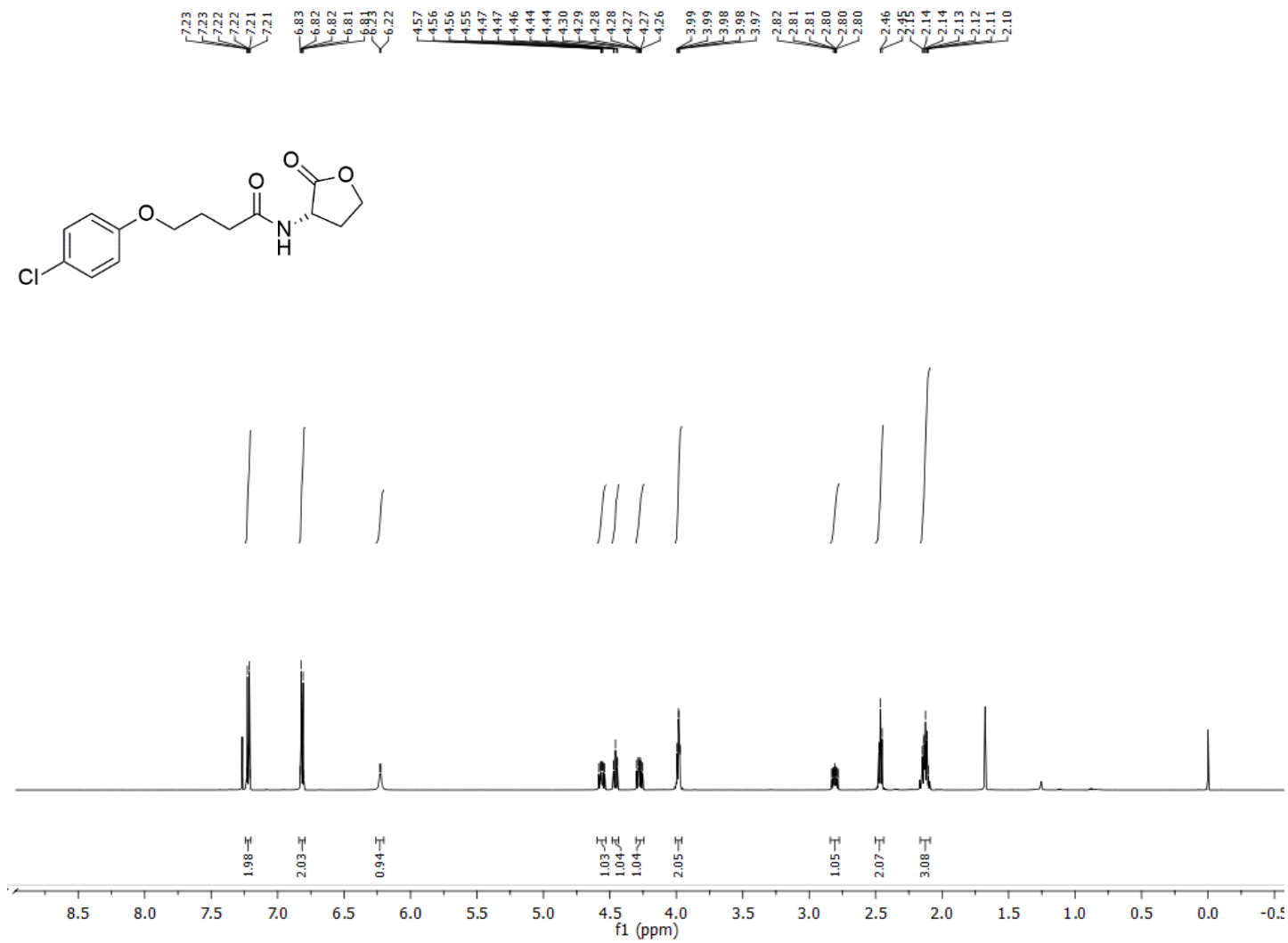
S2.47. ^1H NMR (300 MHz) spectrum of **19E** in CDCl_3 .



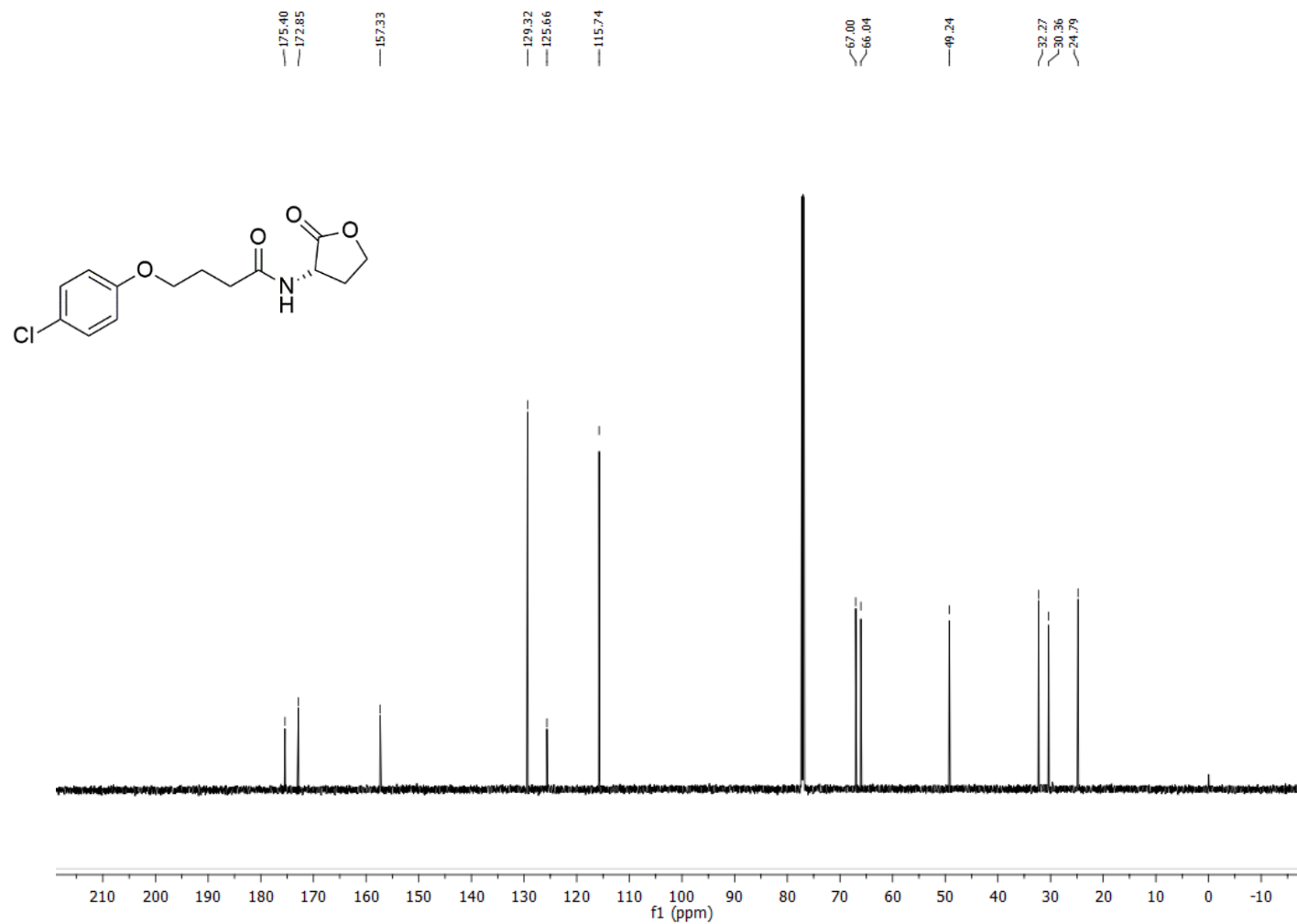
S2.48. ^{13}C NMR (75 MHz) spectrum of **19E** in CDCl_3 .



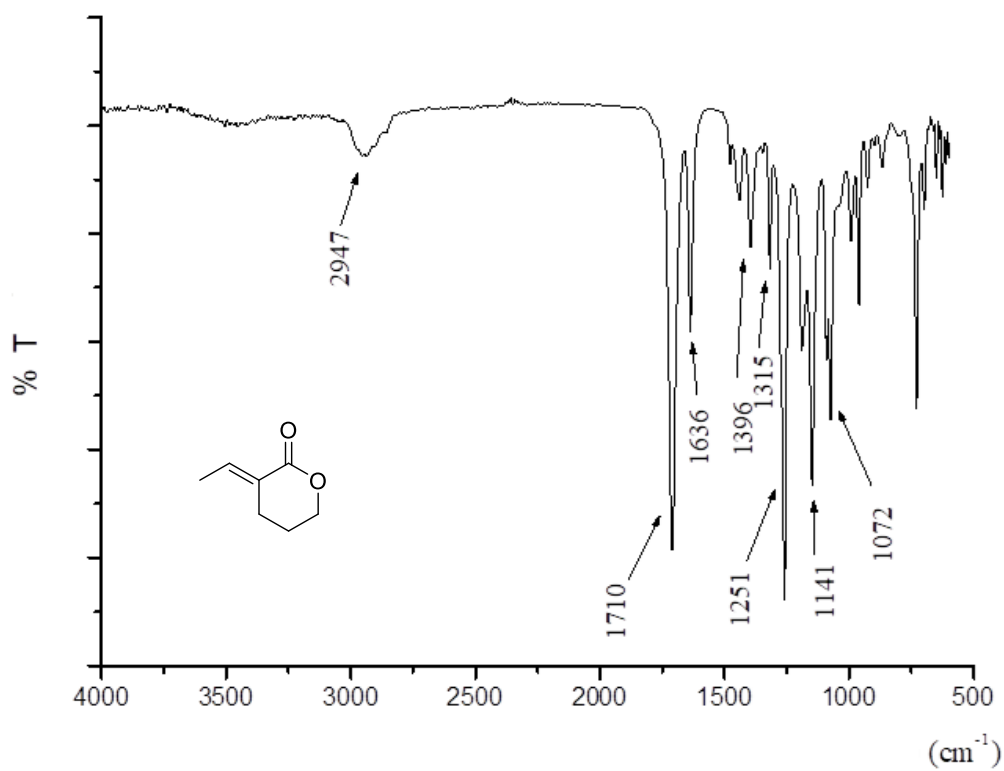
S2.49. ^1H NMR spectrum of **20** in CDCl_3 .



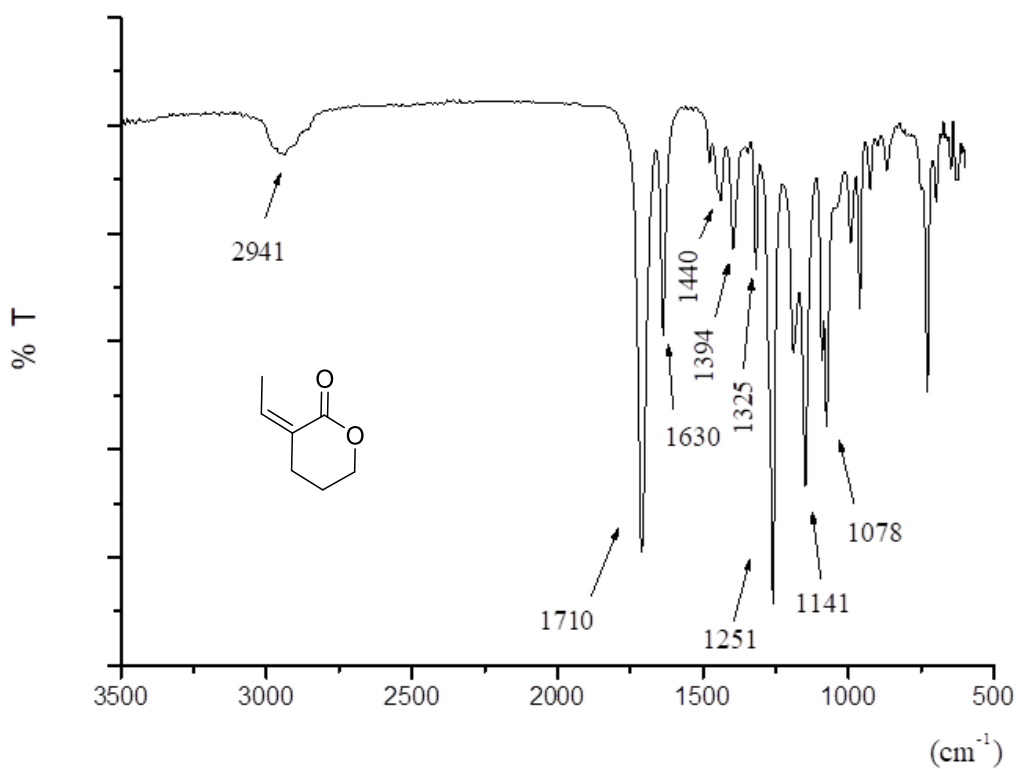
S2.50. ^{13}C NMR spectrum of **20** in CDCl_3 .



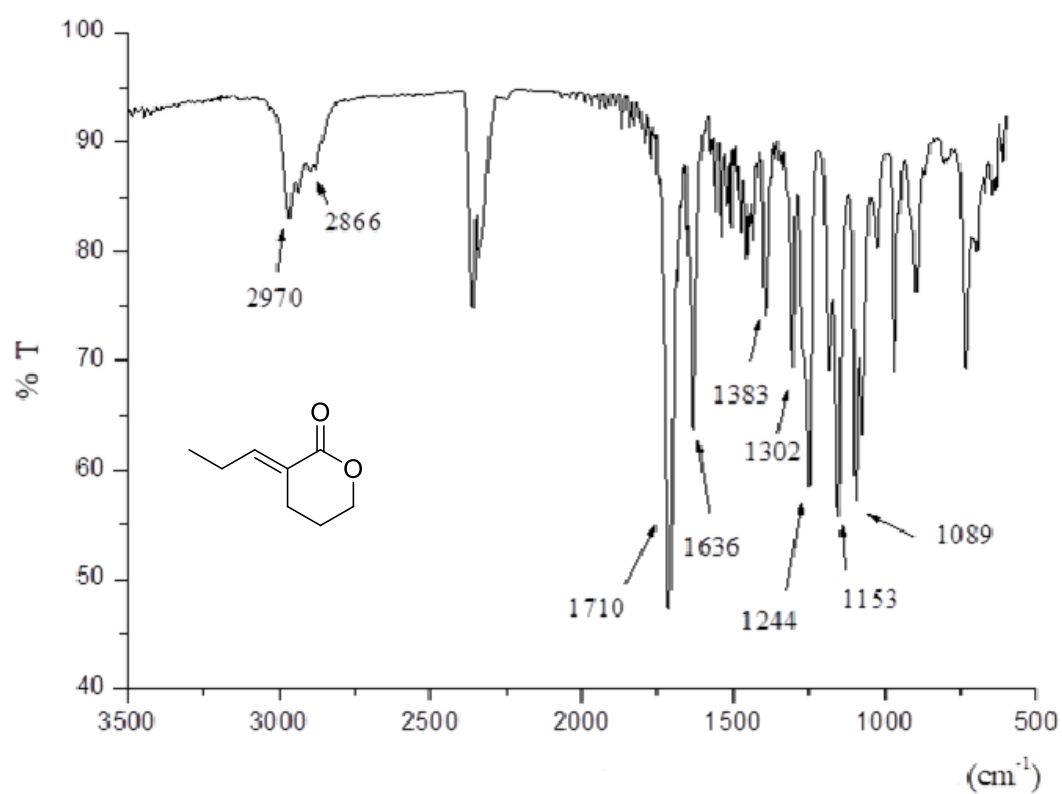
S3.1. IR (ATR) spectrum of 10E.



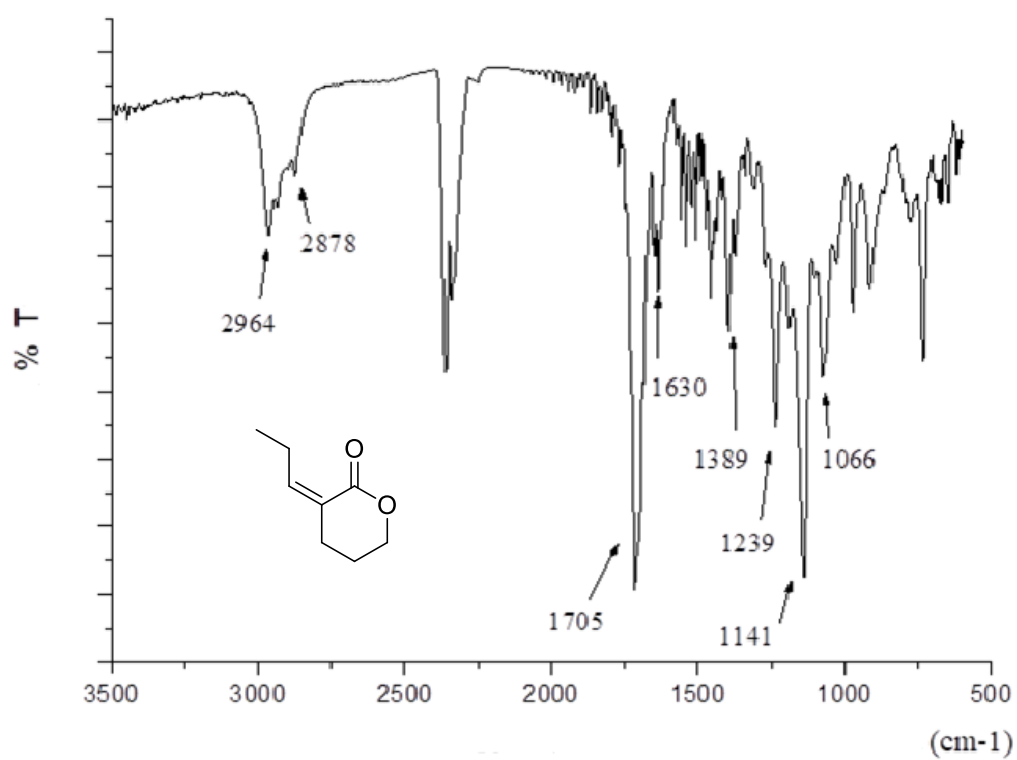
S3.2. IR (ATR) spectrum of 10Z.



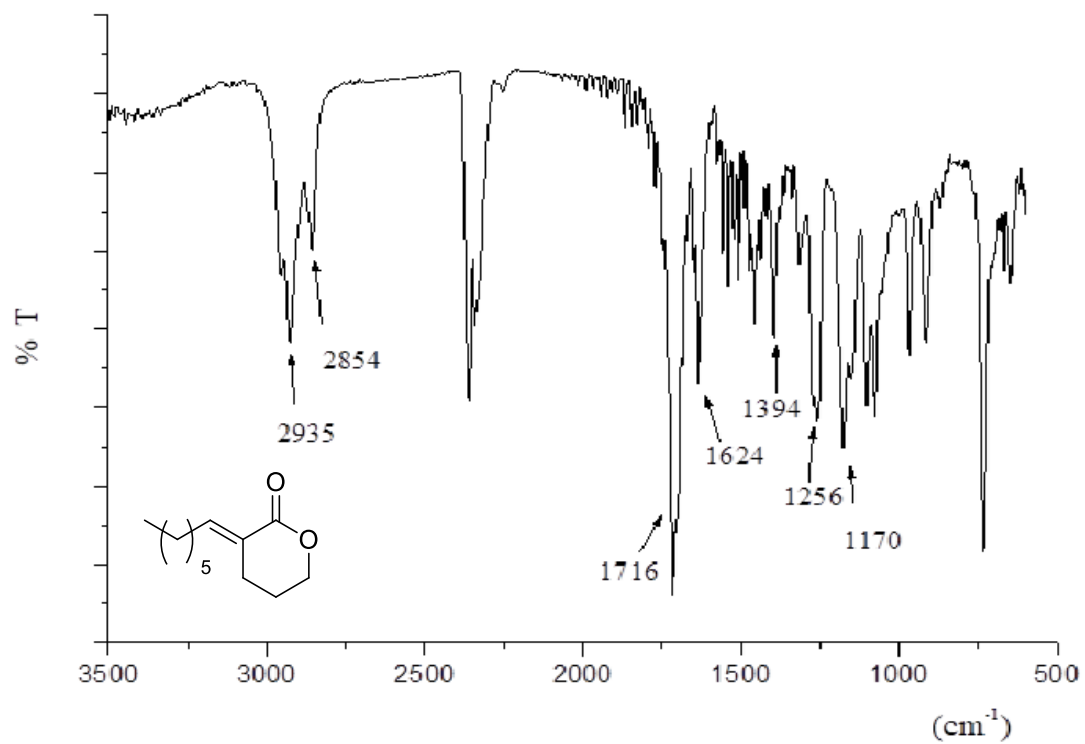
S3.3. IR (ATR) spectrum of 11E.



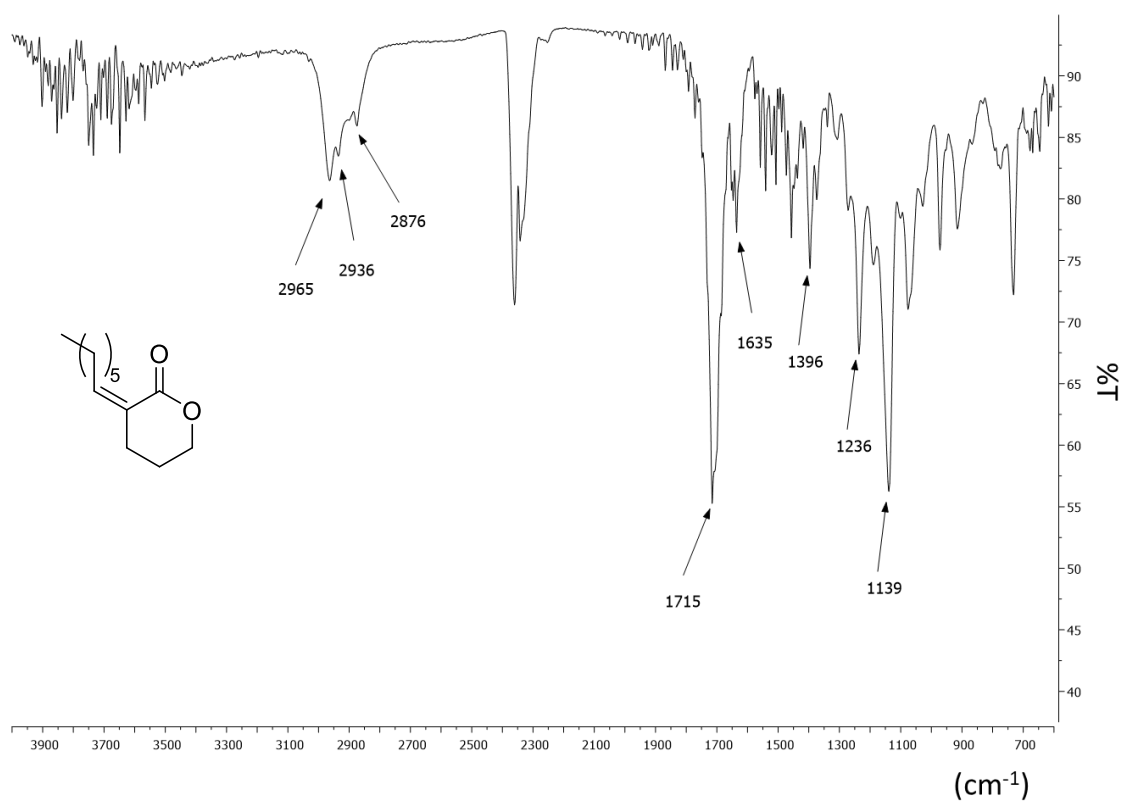
S3.4. IR (ATR) spectrum of 11Z



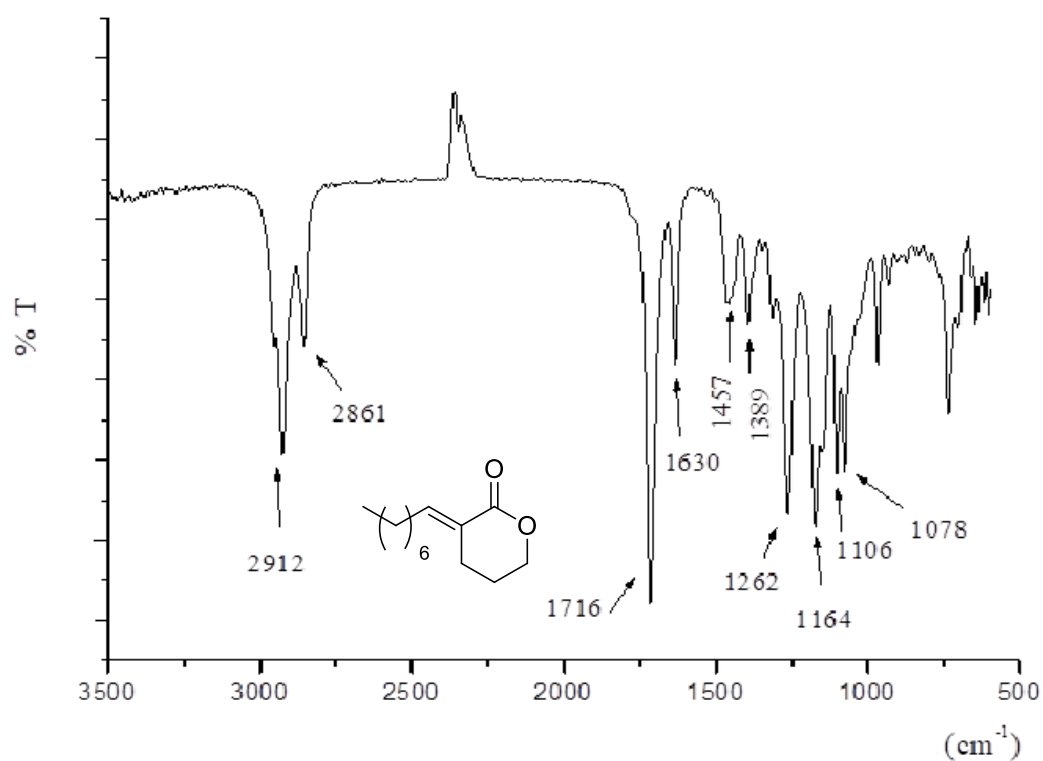
S3.5. IR (ATR) spectrum of 12E.



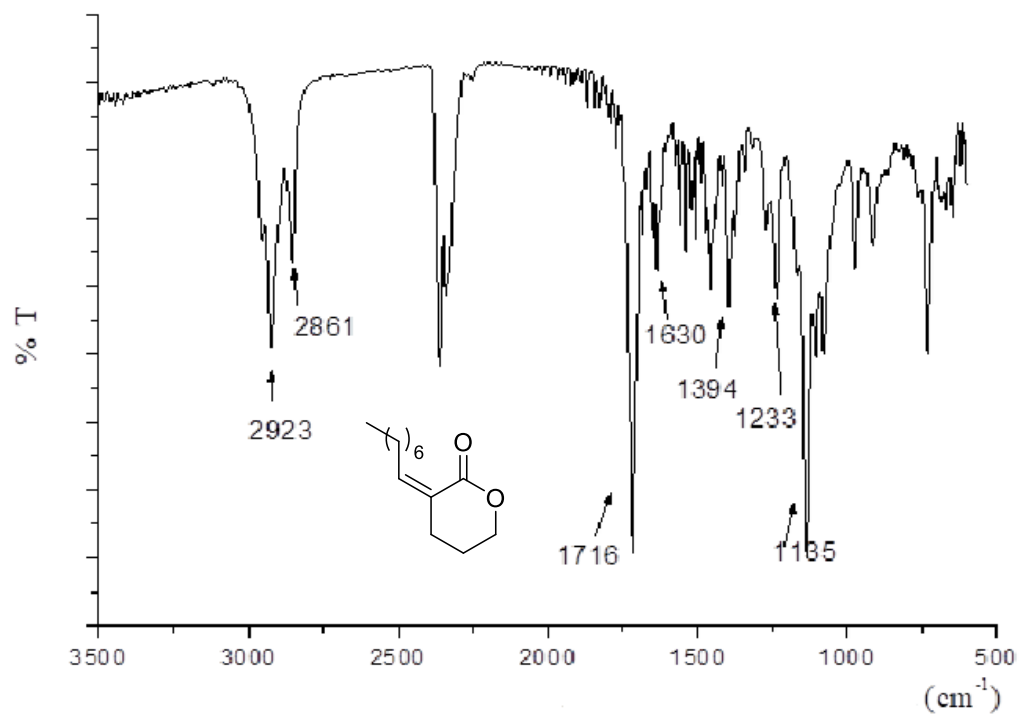
S3.6. IR (ATR) spectrum of 12Z.



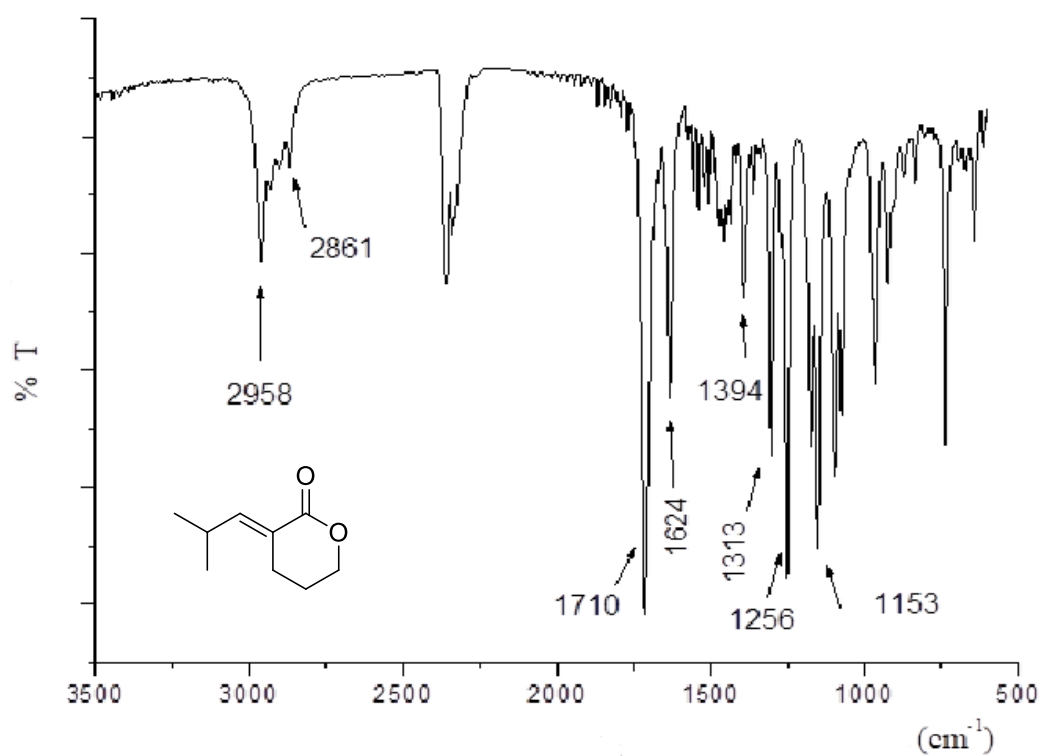
S3.7. IR (ATR) spectrum of 13E.



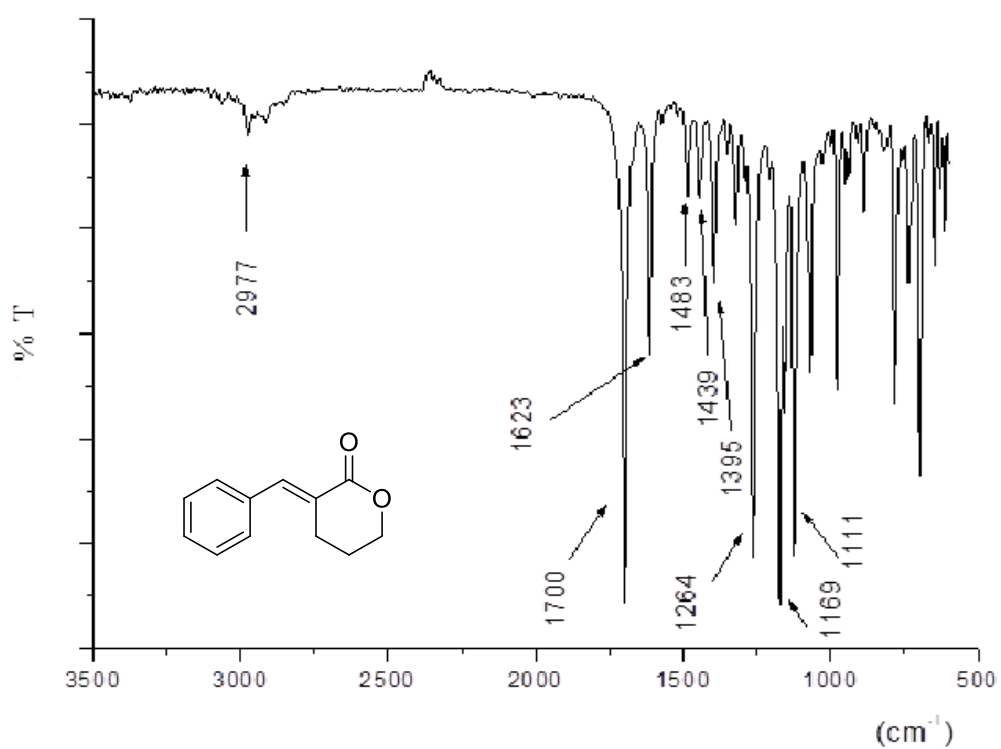
S3.8. IR (ATR) spectrum of 13Z.



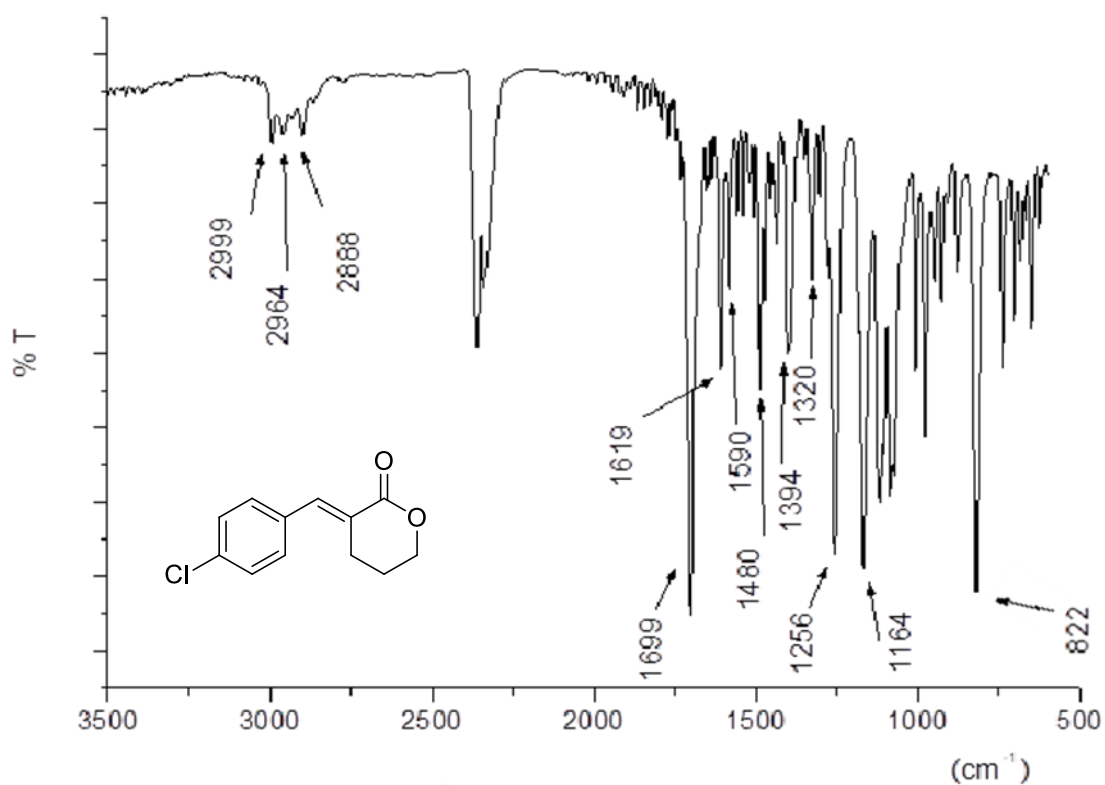
S3.9. IR (ATR) spectrum of 14E.



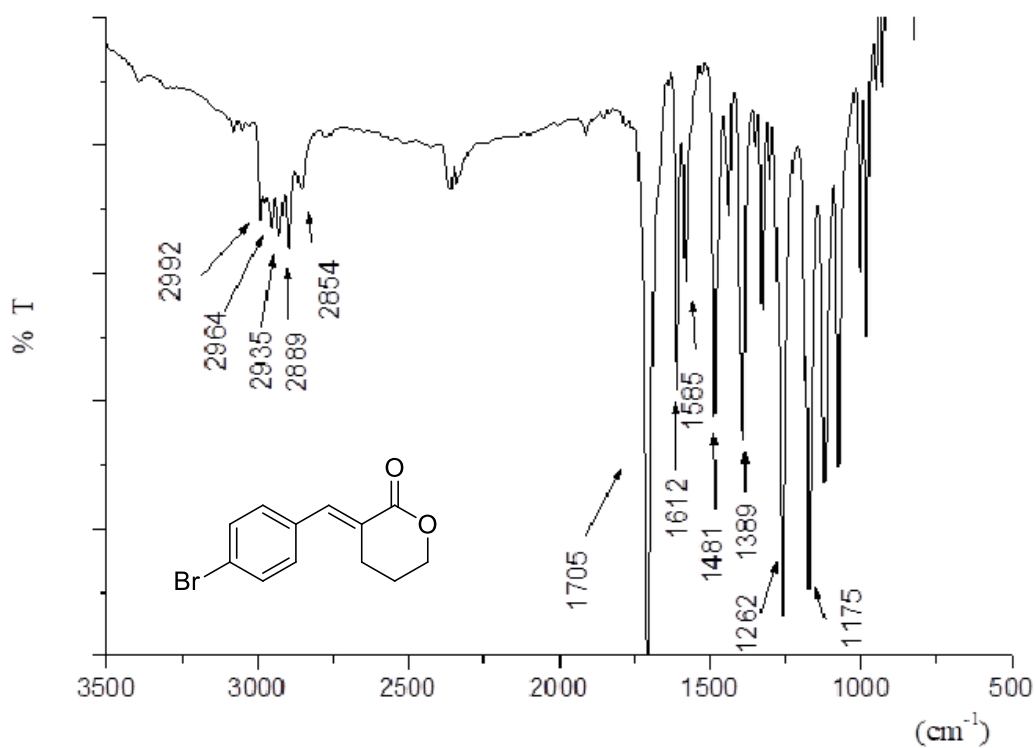
S3.10. IR (ATR) spectrum of 15E.



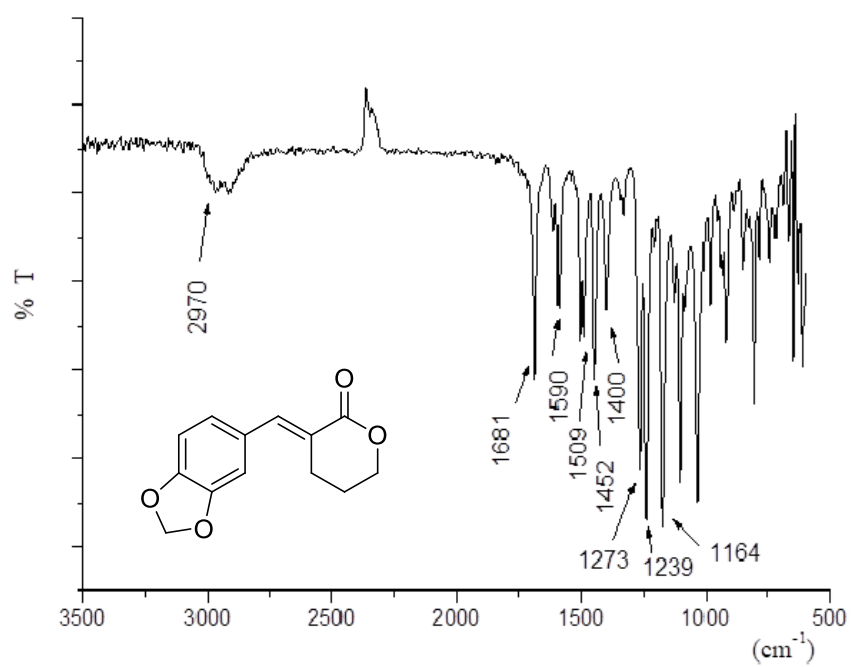
S3.11. IR (ATR) spectrum of 16E.



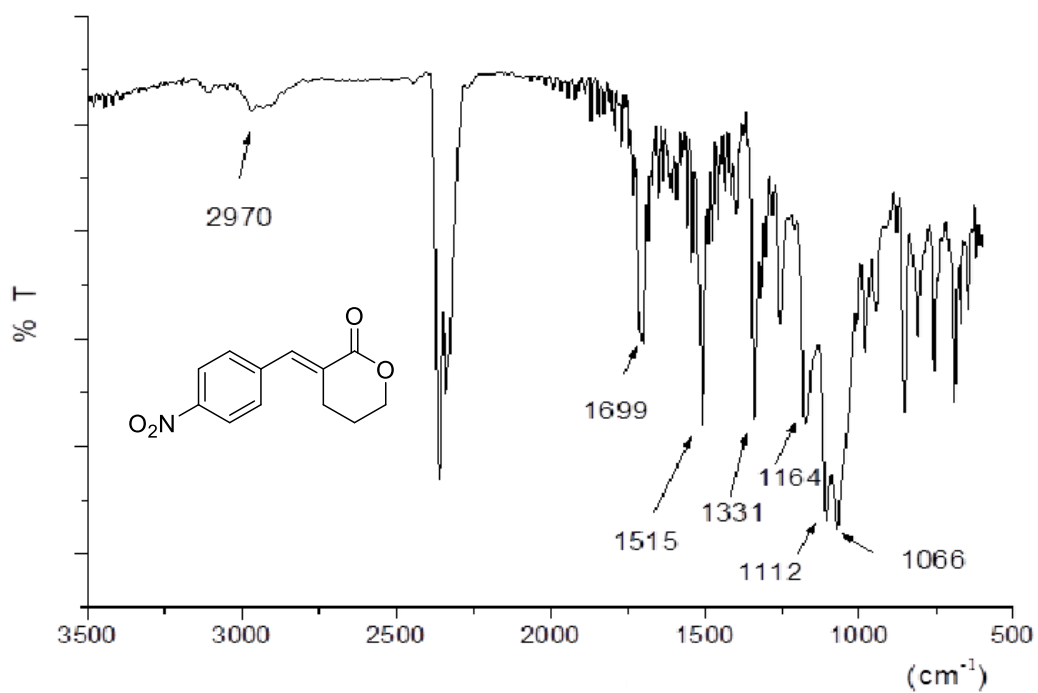
S3.12. IR (ATR) spectrum of 17E.



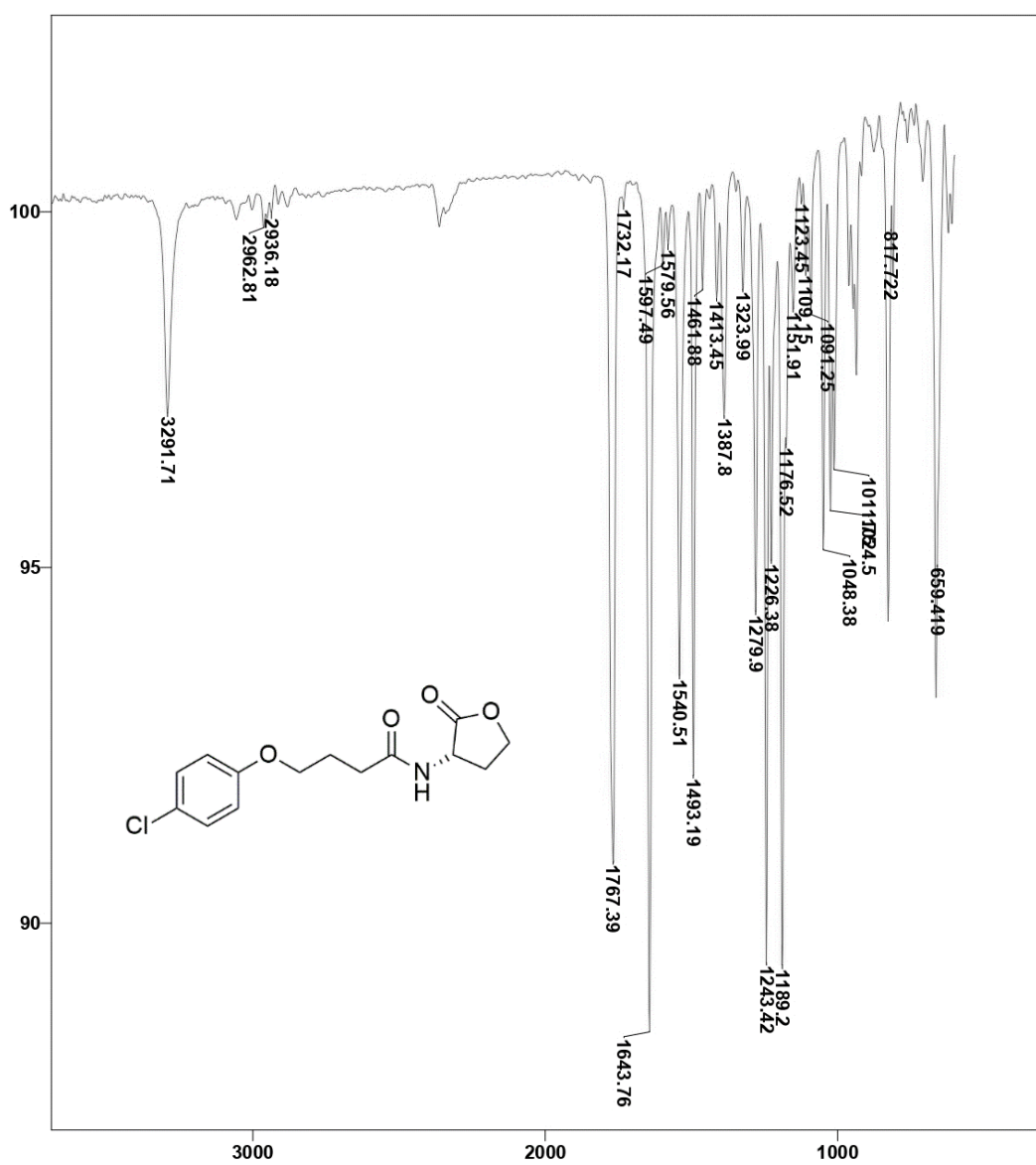
S3.13. IR (ATR) spectrum of 18E.



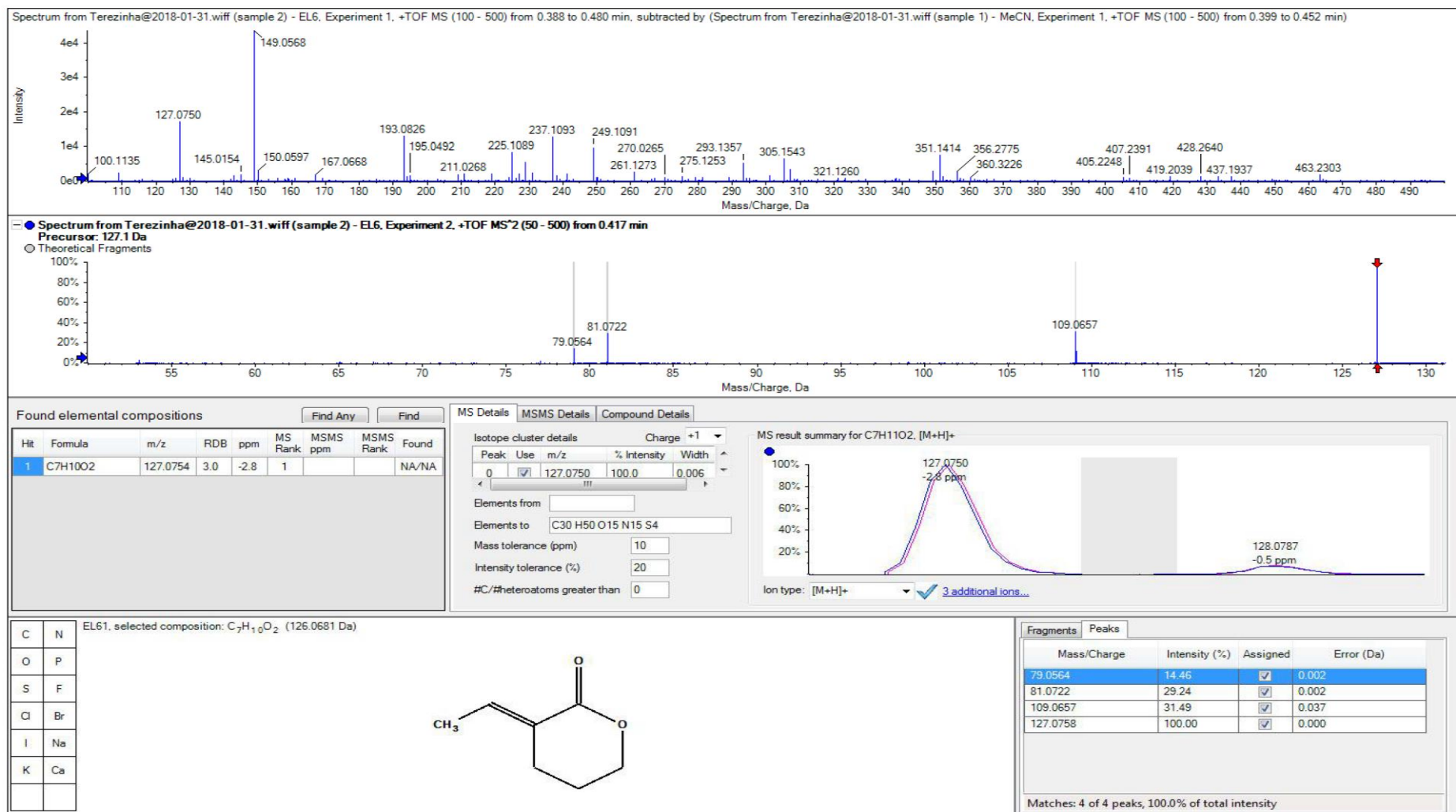
S3.14. IR (ATR) spectrum of 19E.



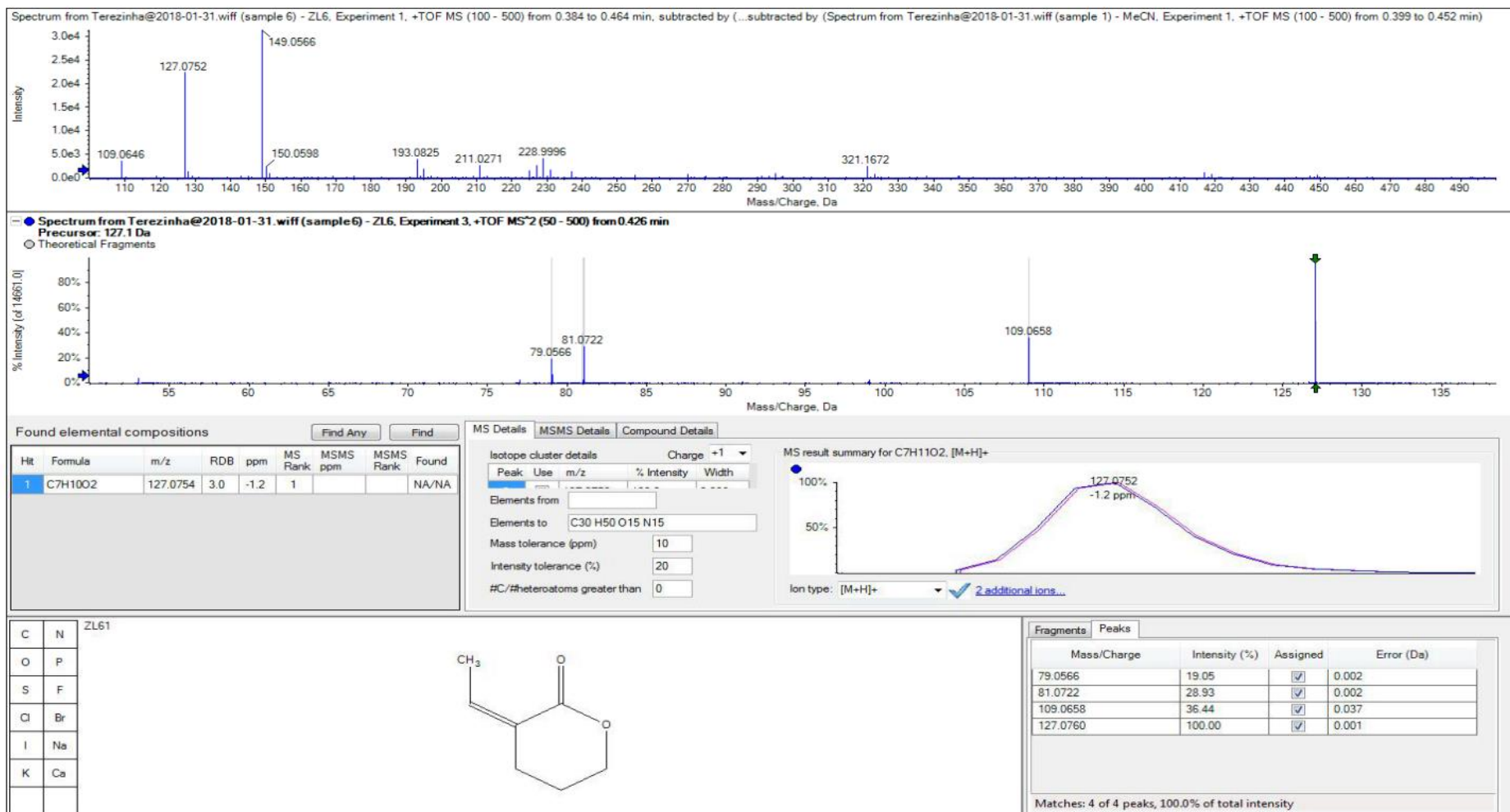
S3.15. IR (ATR) spectrum of 20.



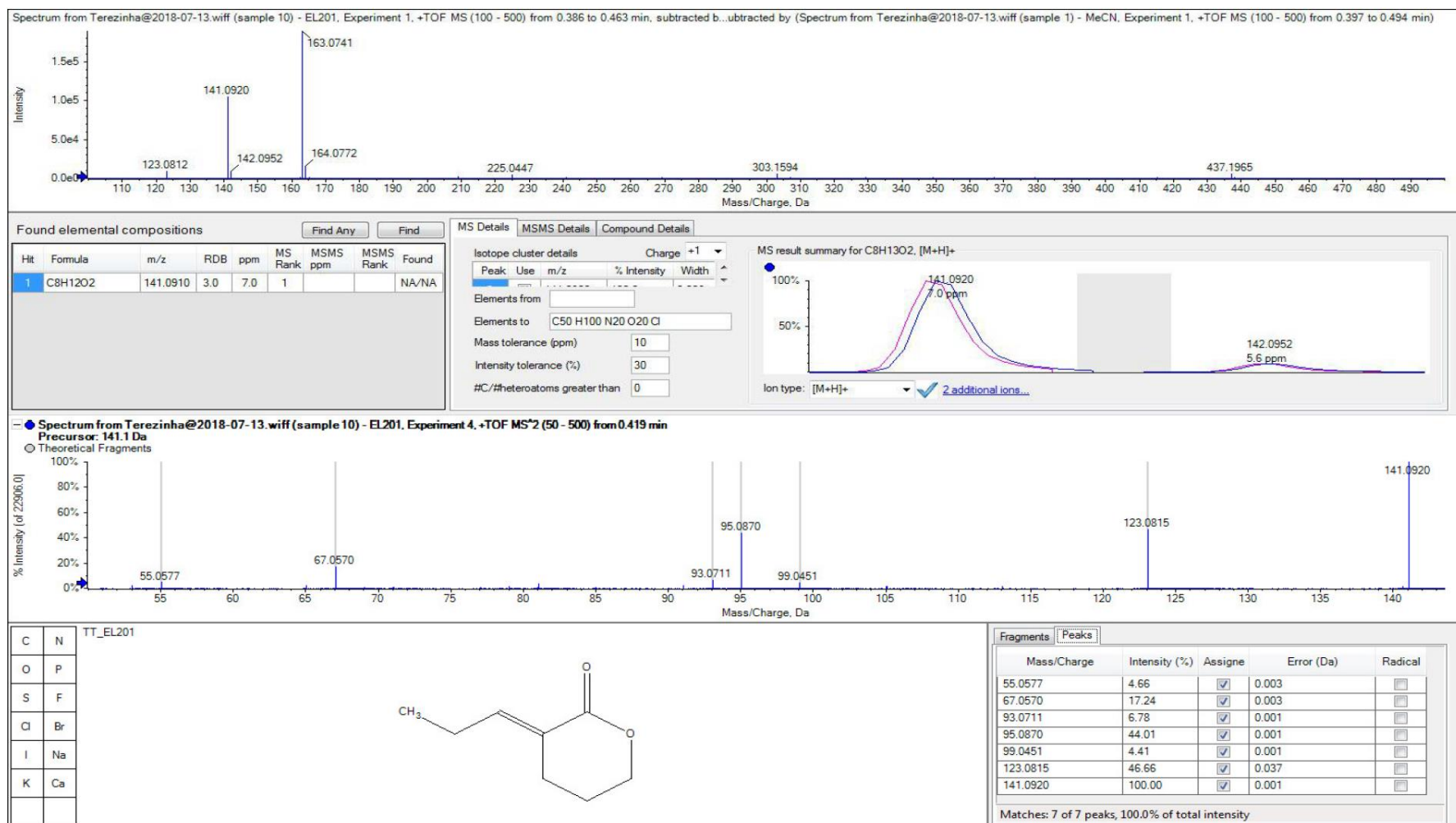
S4.1. HRMS data of 10E.



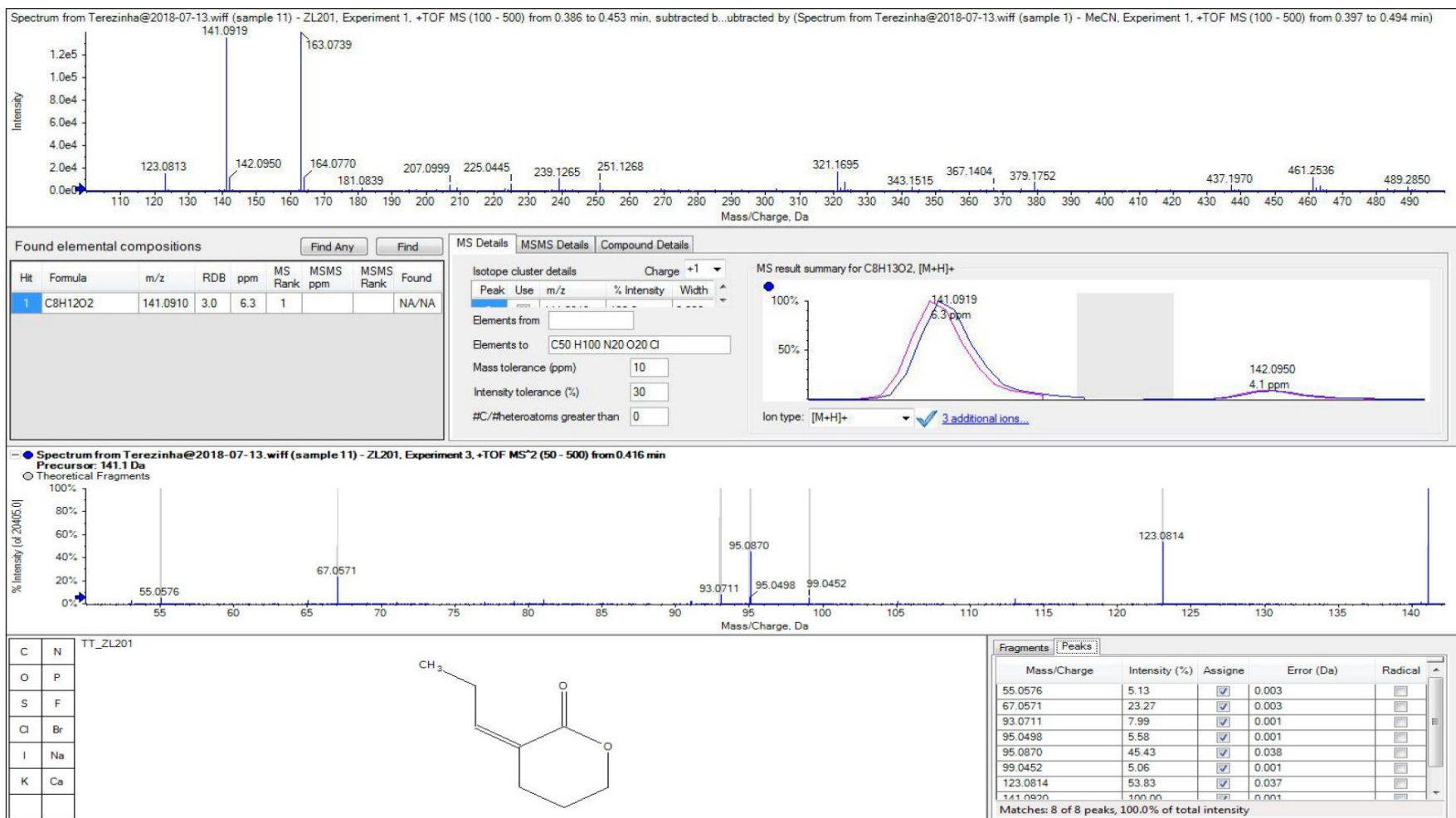
S4.2. HRMS data of 10Z.



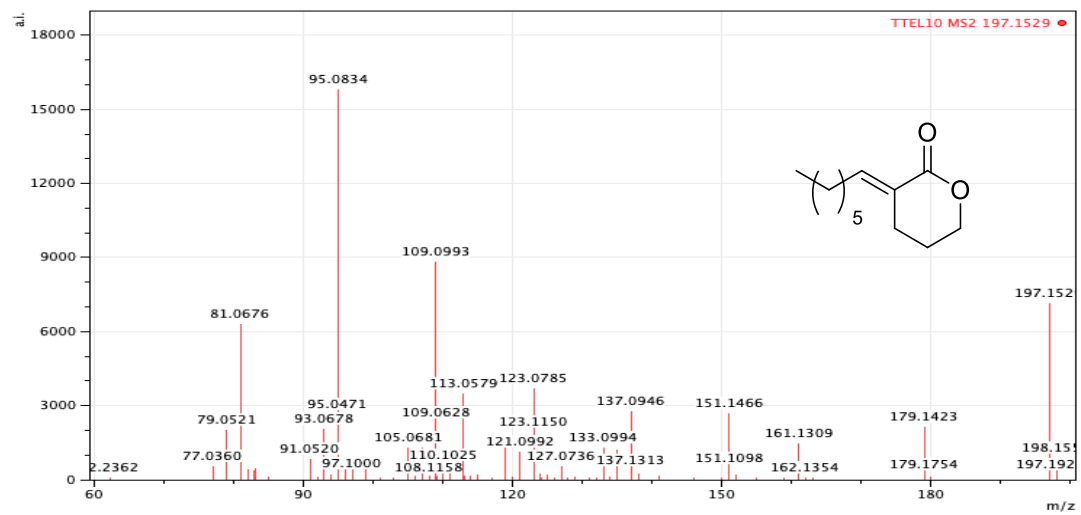
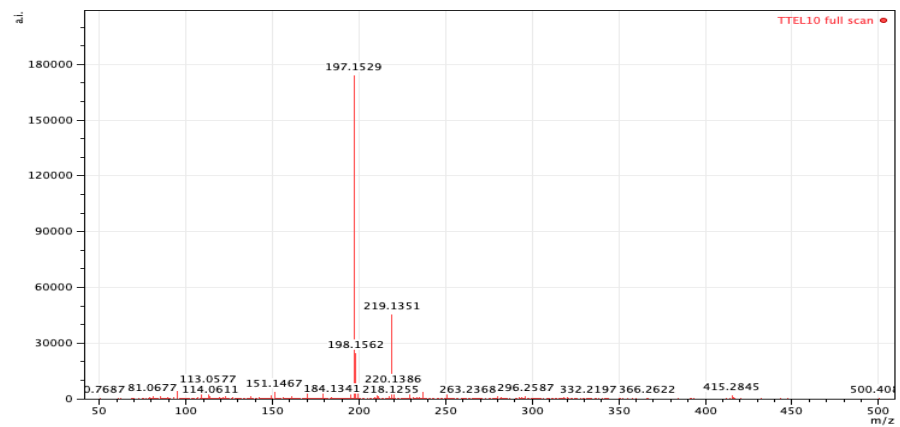
S4.3. HRMS data of 11E.



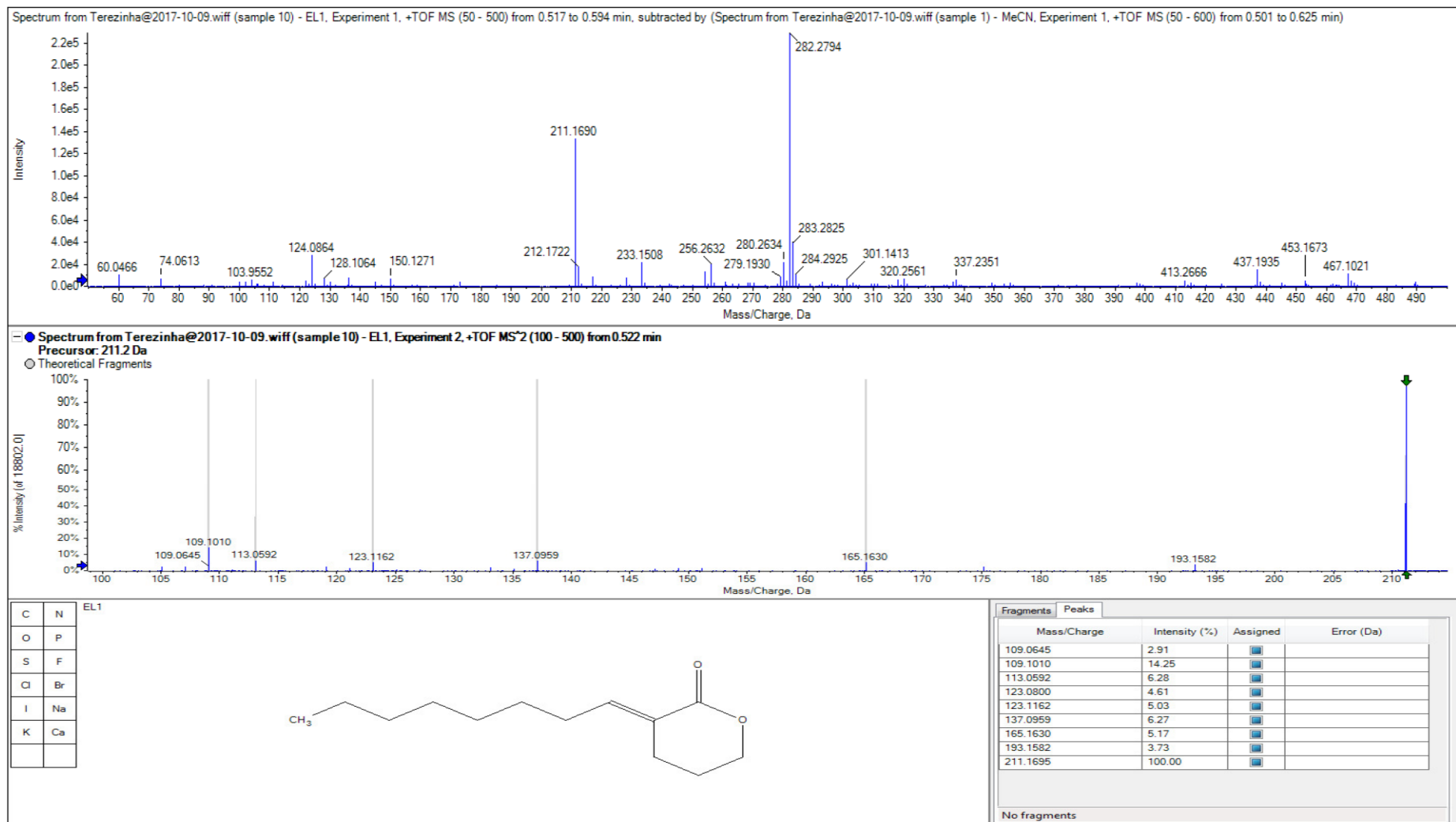
S4.4. HRMS data of 11Z.



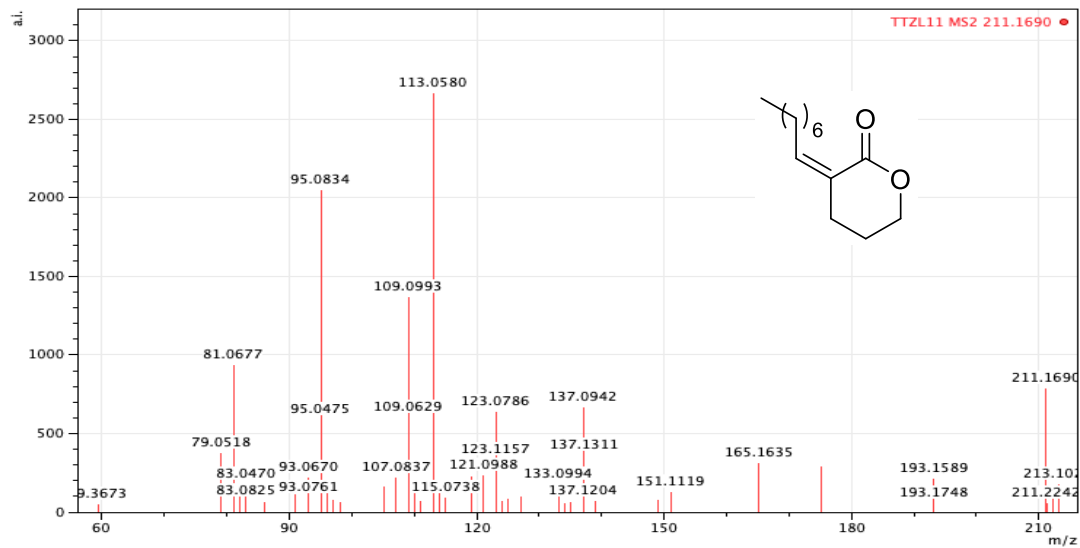
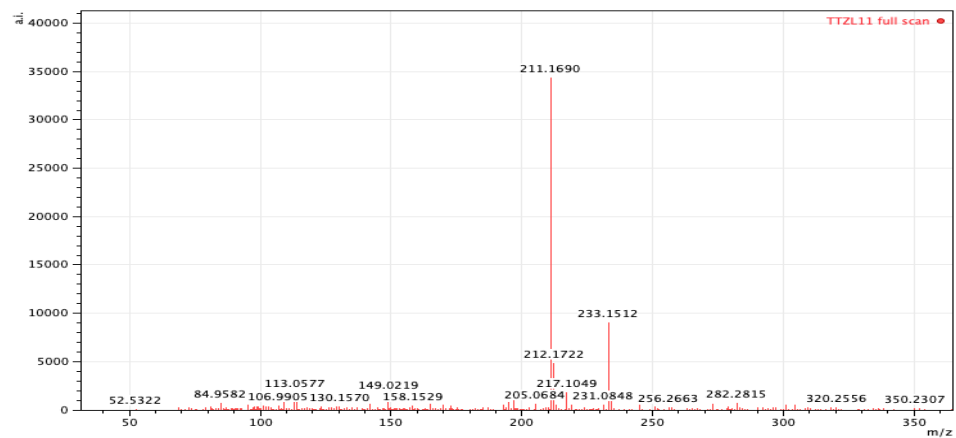
S4.5. HRMS data of 12E.



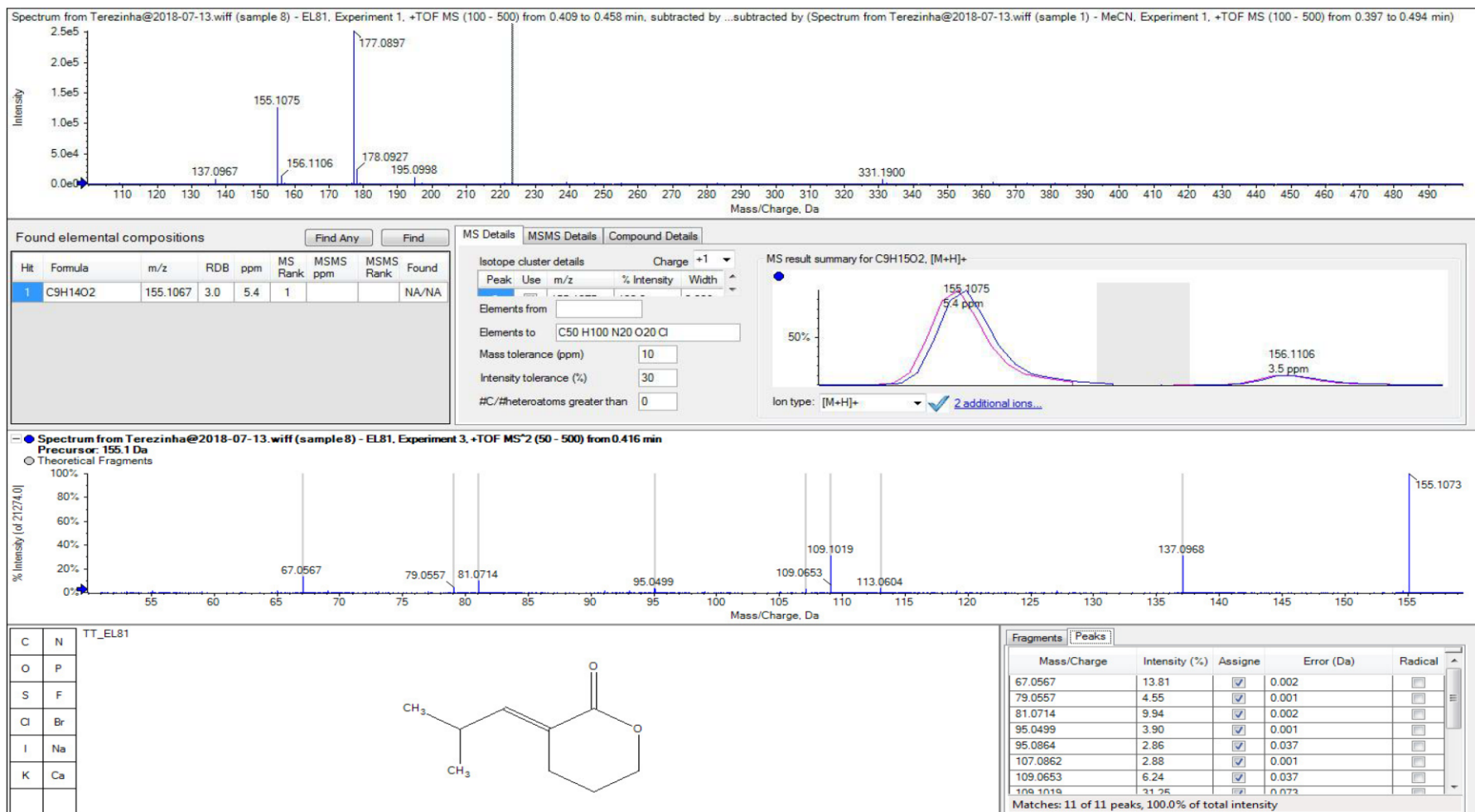
S4.7. HRMS data of 13E.



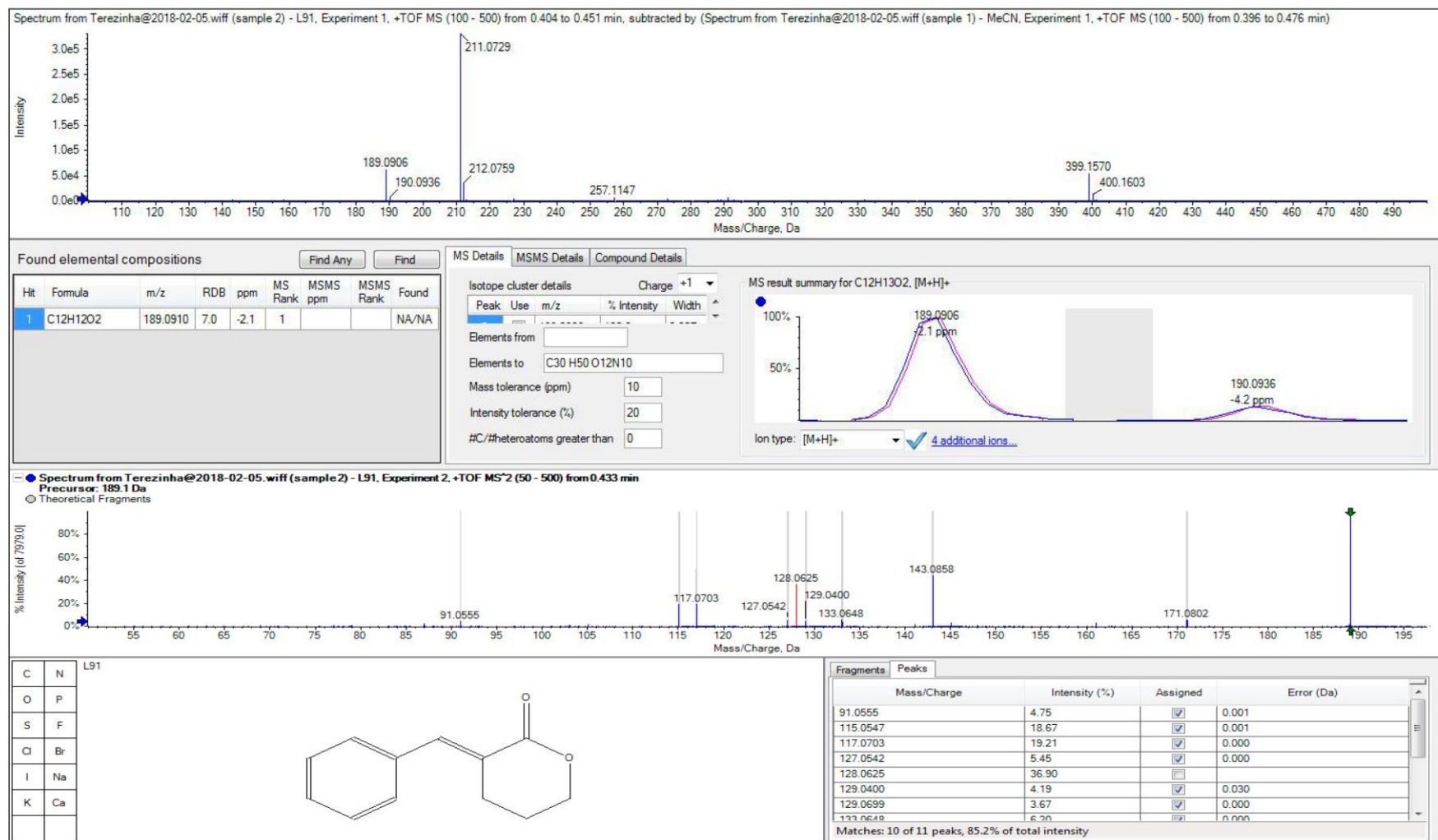
S4.8. HRMS data of 13Z.



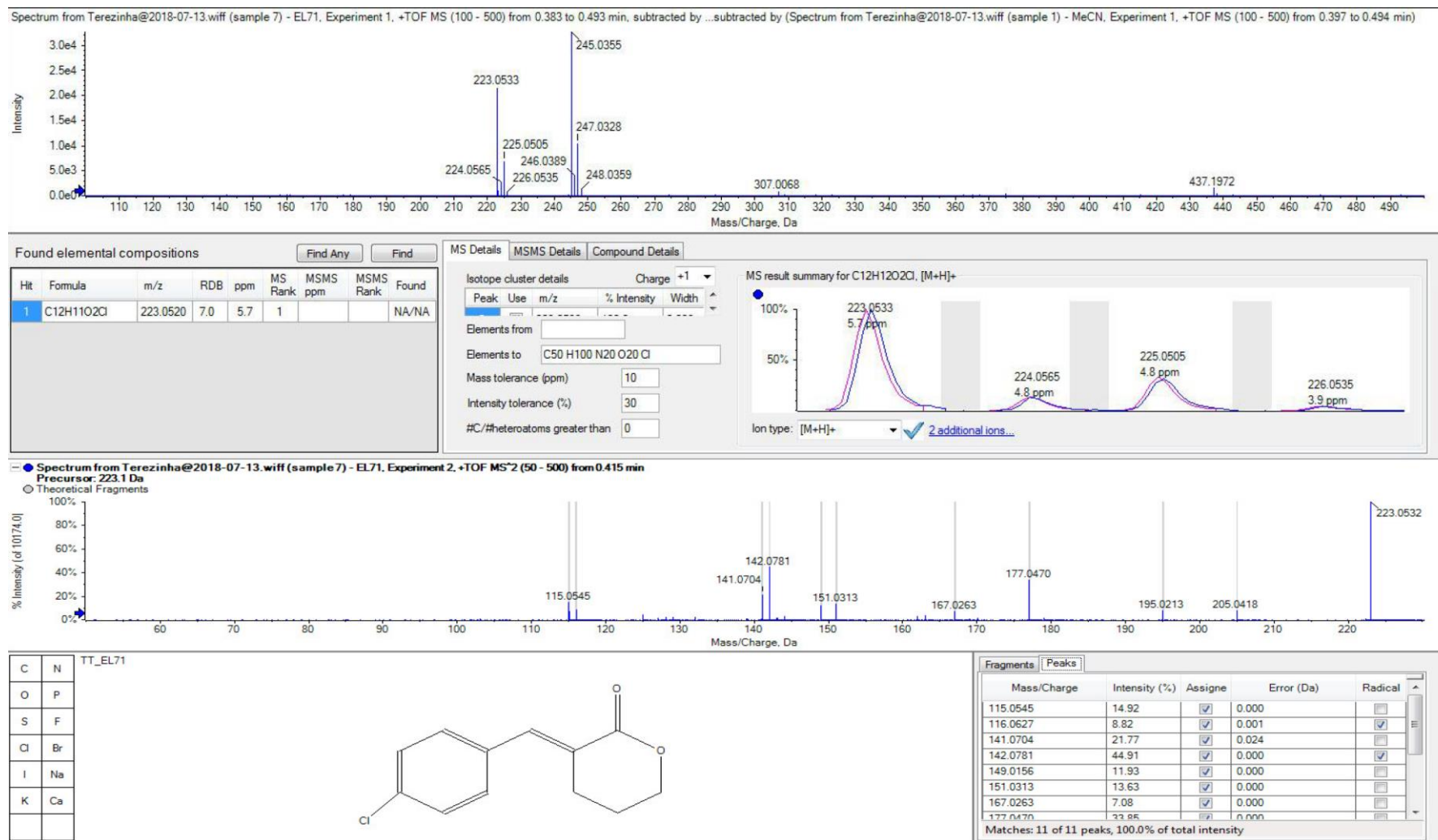
S4.9. HRMS data of 14E.



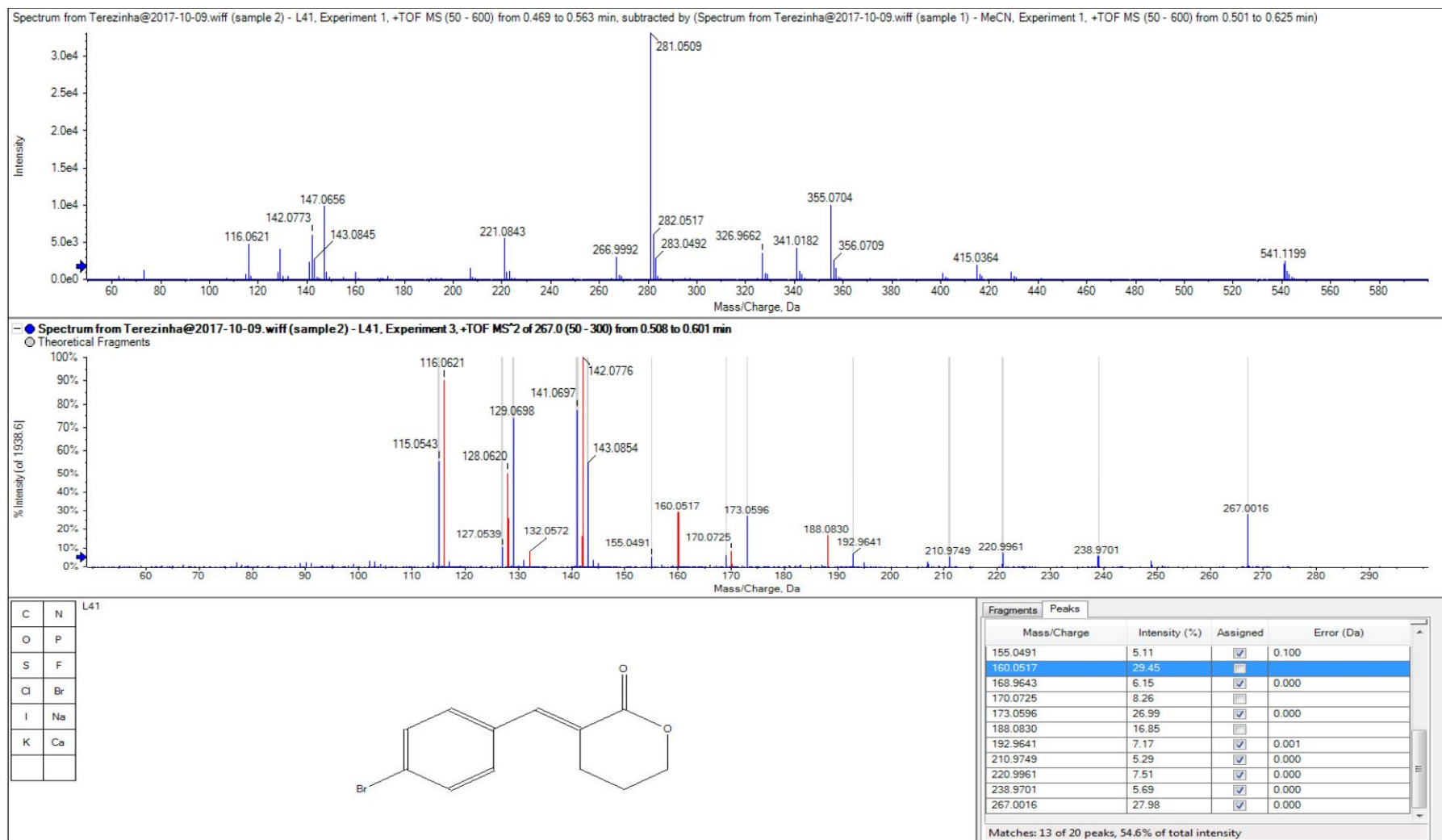
S4.10. HRMS data of 15E.



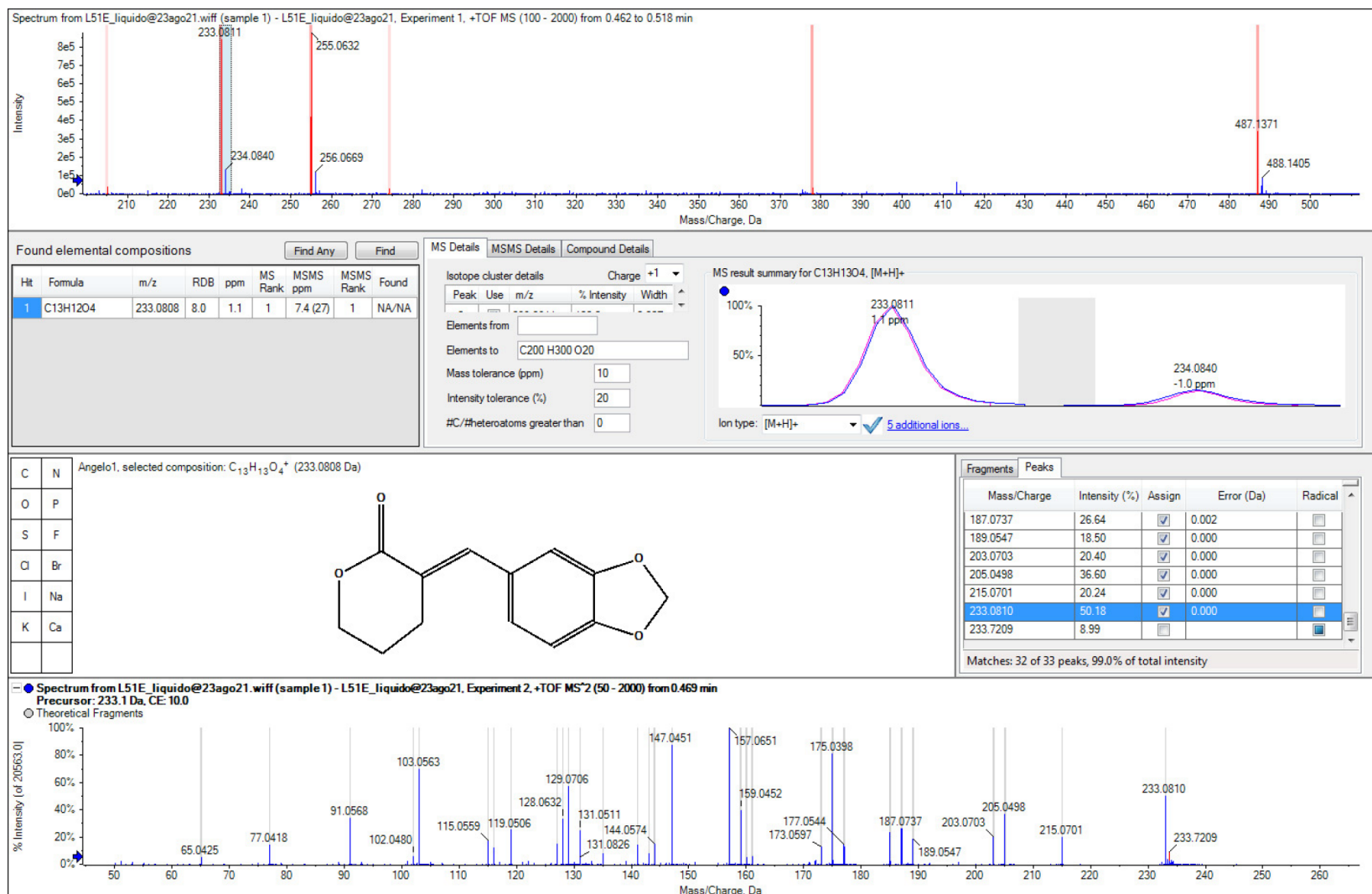
S4.11. HRMS data of 16E.



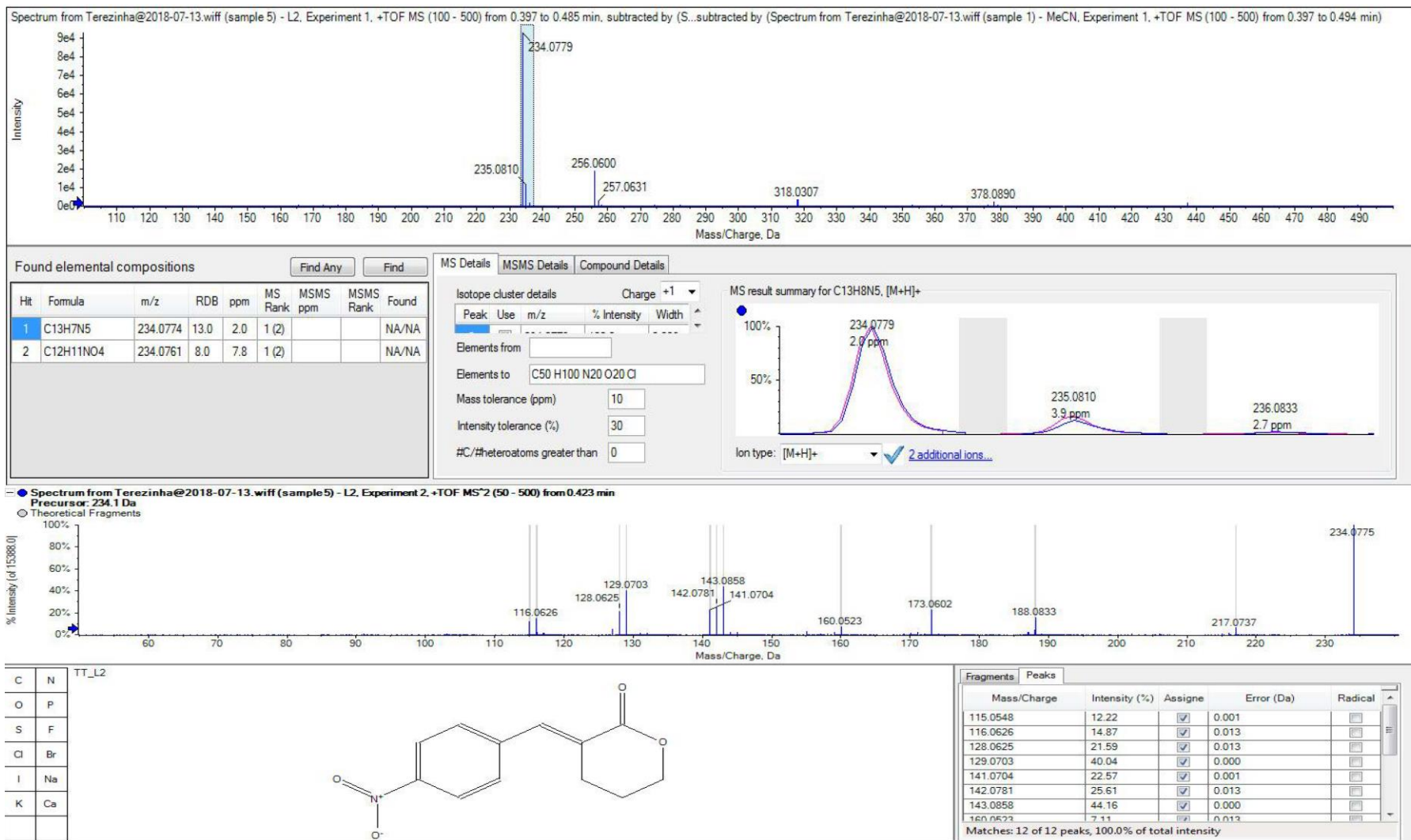
S4.12. HRMS data of 17E.



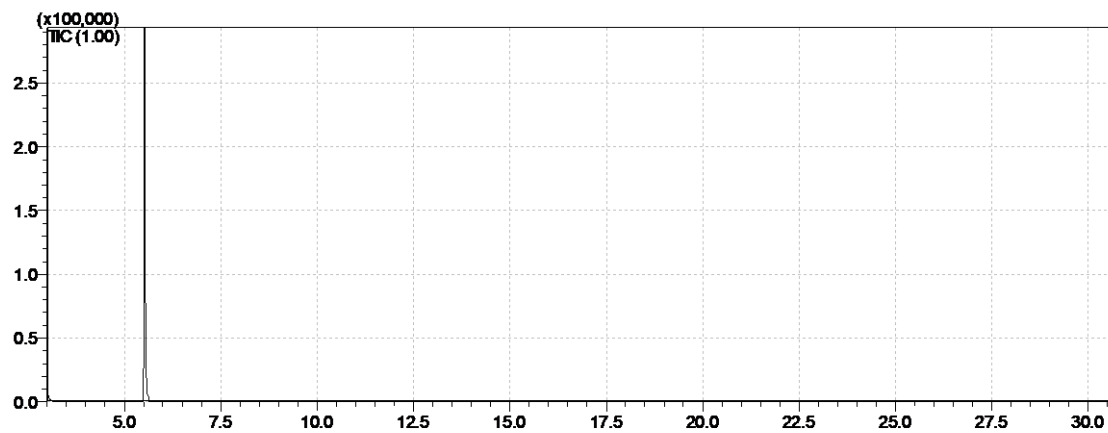
S4.13. HRMS data of 18E



S4.14. HRMS data of 19E.

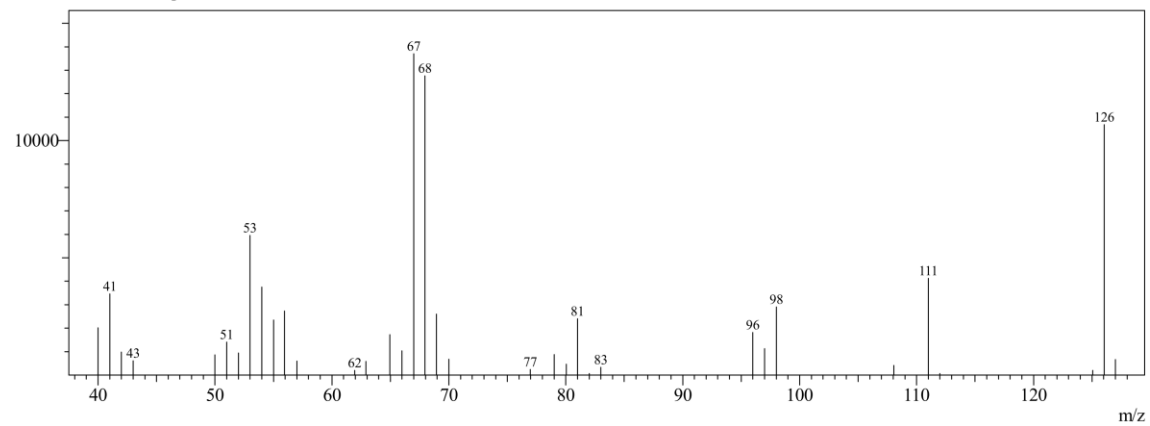


S5.1. GC-MS data of 10E.

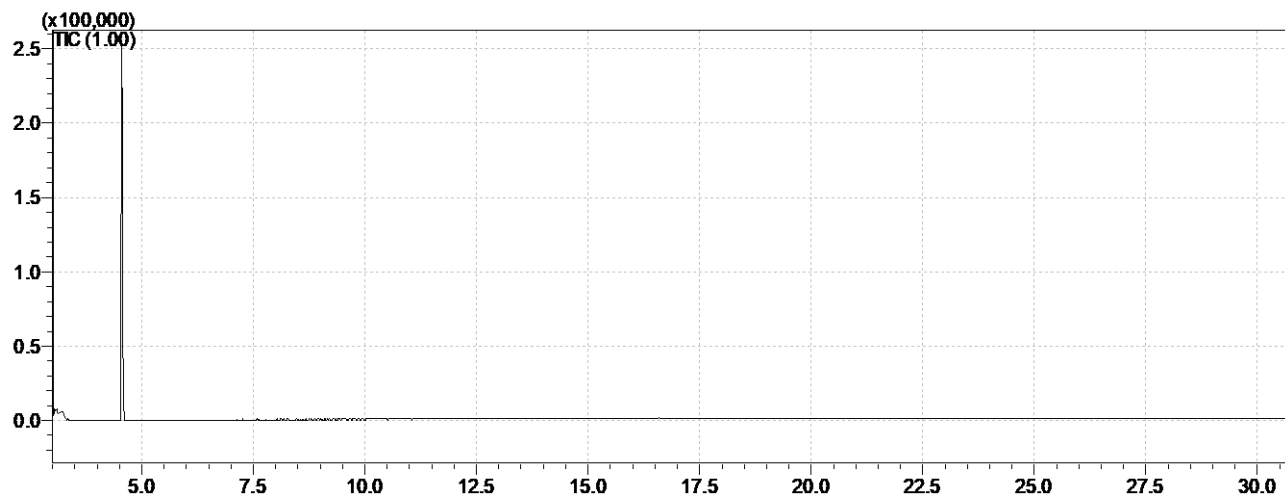


Purity: 98.1 %

Line#:1 R.Time:5.525(Scan#:304)
MassPeaks:35
RawMode:Averaged 5.492-5.625(300-316) BasePeak:67.00(13707)
BG Mode:None Group 1 - Event 1 Scan

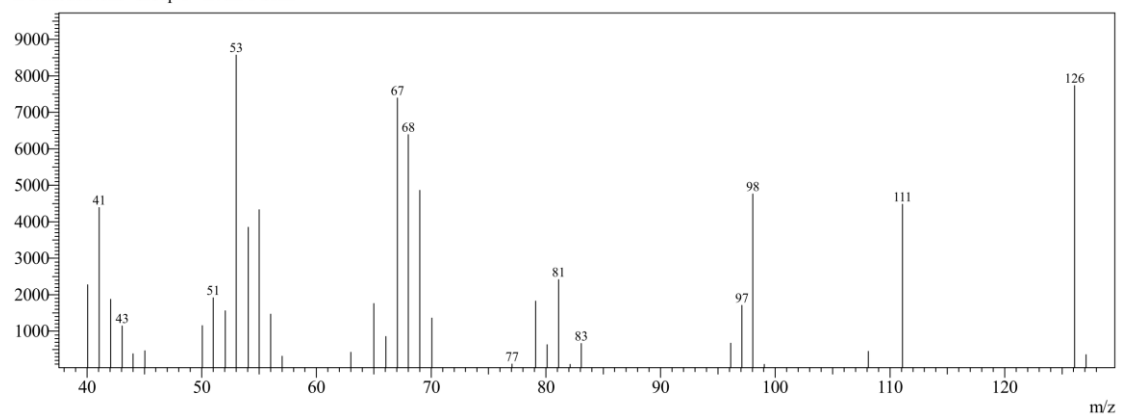


S5.2. GC-MS data of 10Z.

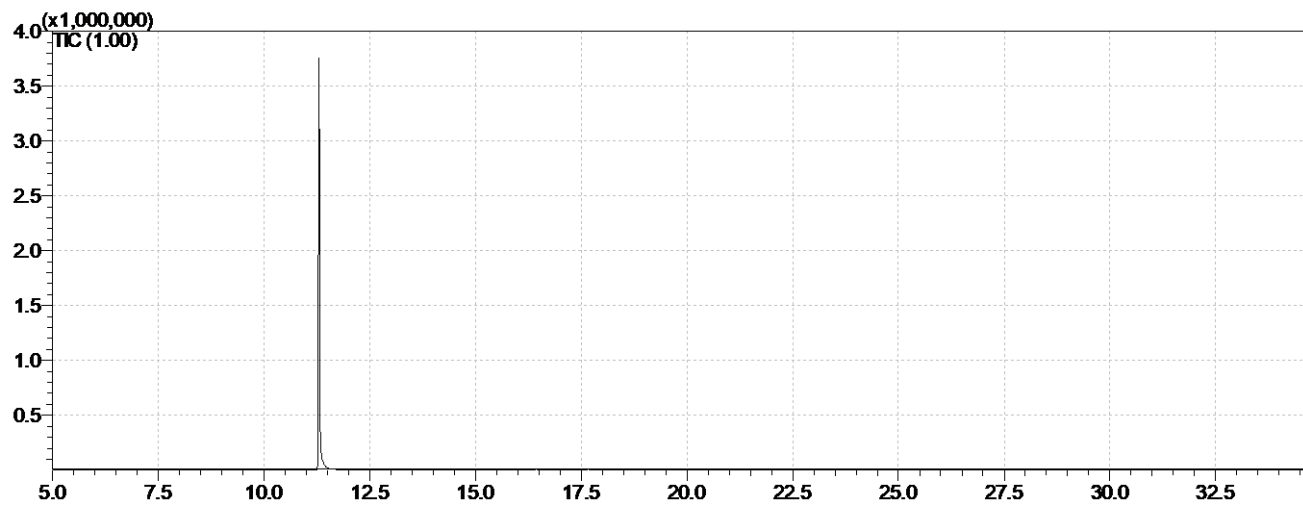


Purity: 96.9 %

Line#:1 R.Time:4.550(Scan#:187)
MassPeaks:35
RawMode:Averaged 4.517-4.608(183-194) BasePeak:53.00(8574)
BG Mode:None Group 1 - Event 1 Scan

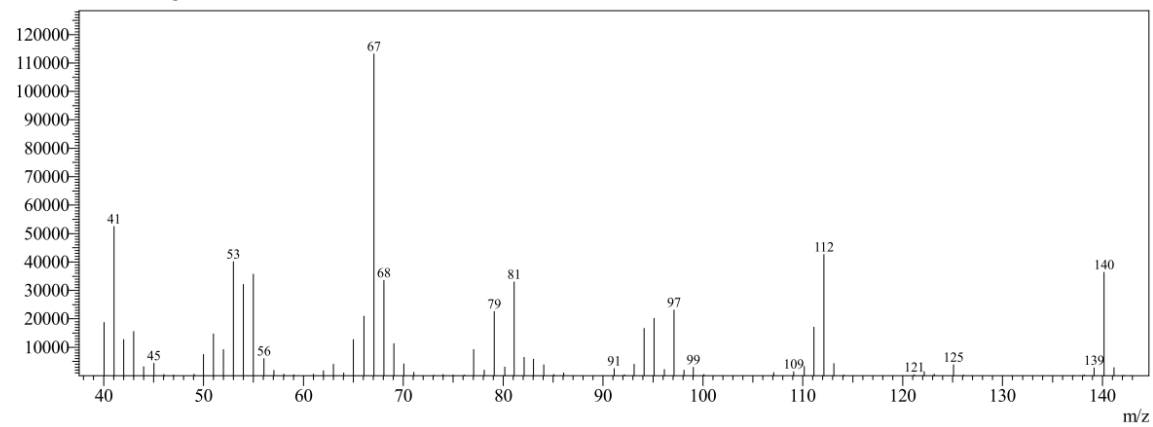


S5.3. GC-MS data of 11E.

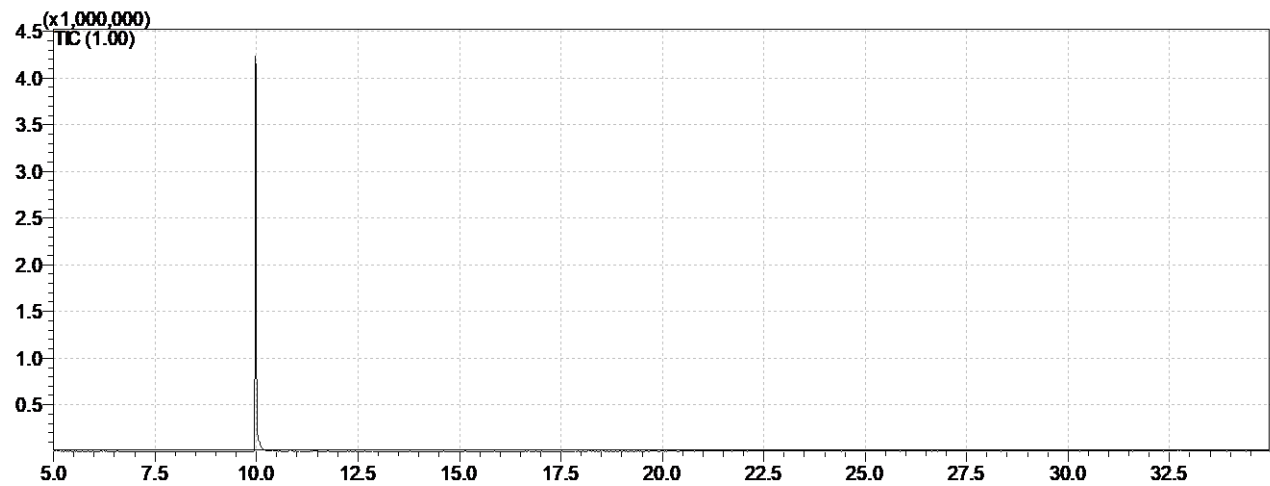


Purity: 99.6 %

Line#:1 R.Time:11.292(Scan#:756)
MassPeaks:72
RawMode:Averaged 11.258-11.433(752-773) BasePeak:67.05(113191)
BG Mode:None Group 1 - Event 1 Scan

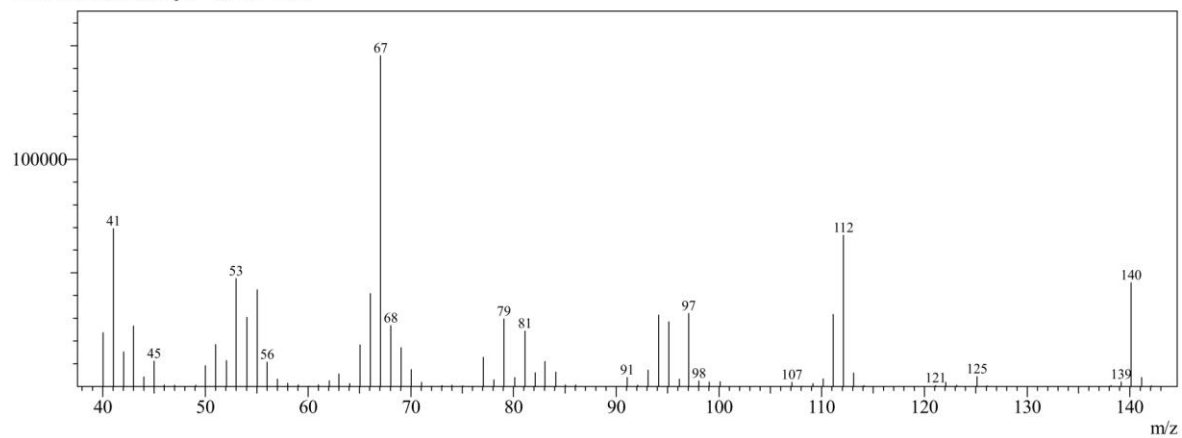


S5.4. GC-MS data of 11Z.

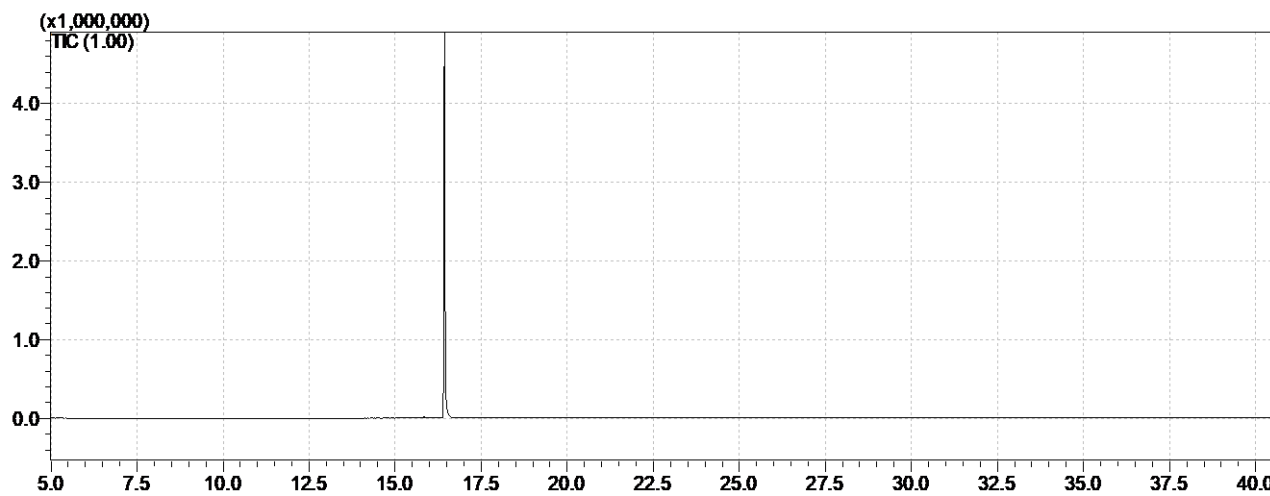


Purity: 98.9 %

Line#:1 R.Time:9.975(Scan#:598)
MassPeaks:74
RawMode:Averaged 9.942-10.083(594-611) BasePeak:67.05(145690)
BG Mode:None Group 1 - Event 1 Scan

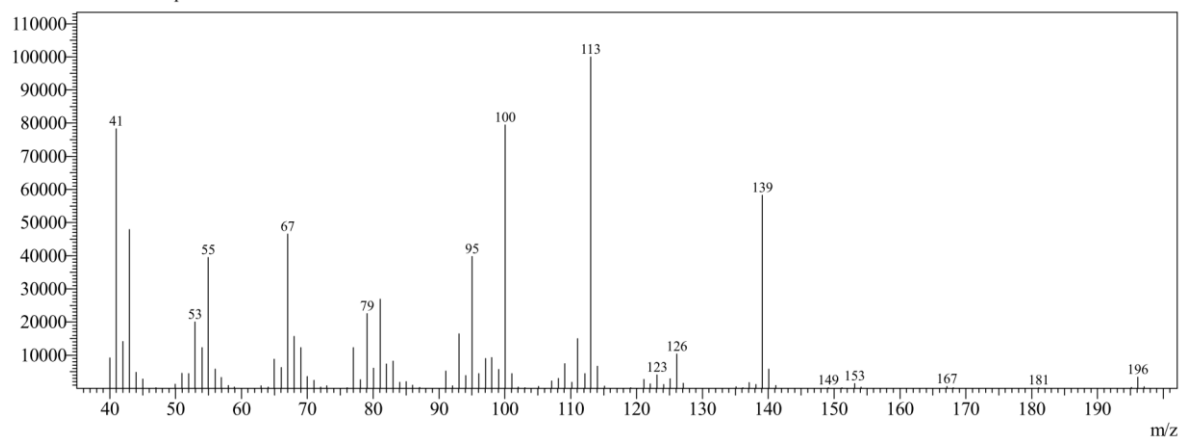


S5.5. GC-MS data of 12E.

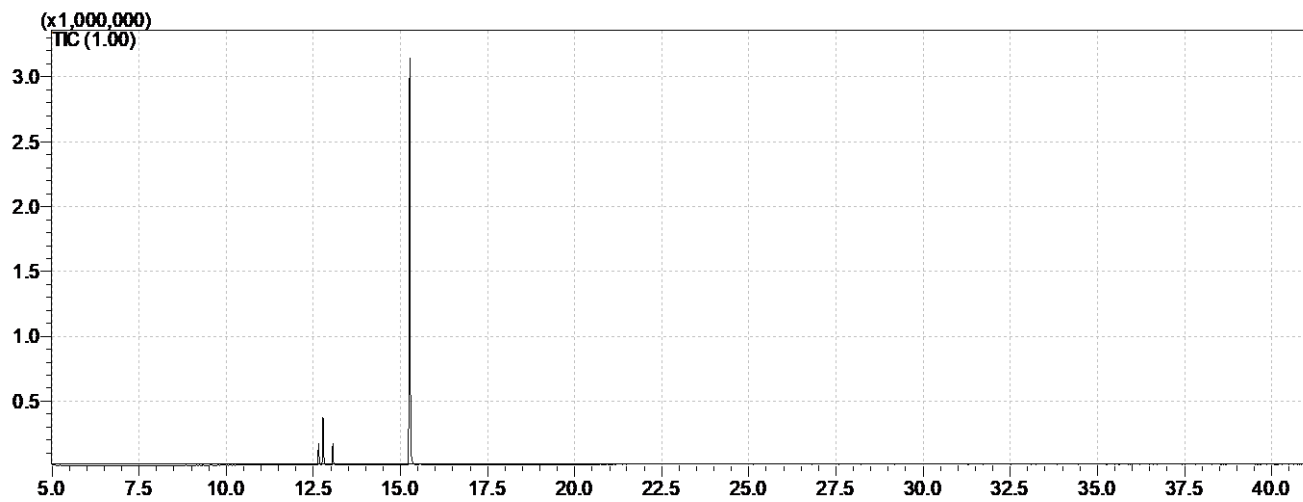


Purity: 98.8 %

Line#:1 R.Time:16.433(Scan#:1373)
MassPeaks:91
RawMode:Averaged 16.383-16.583(1367-1391) BasePeak:113.05(100004)
BG Mode:None Group 1 - Event 1 Scan

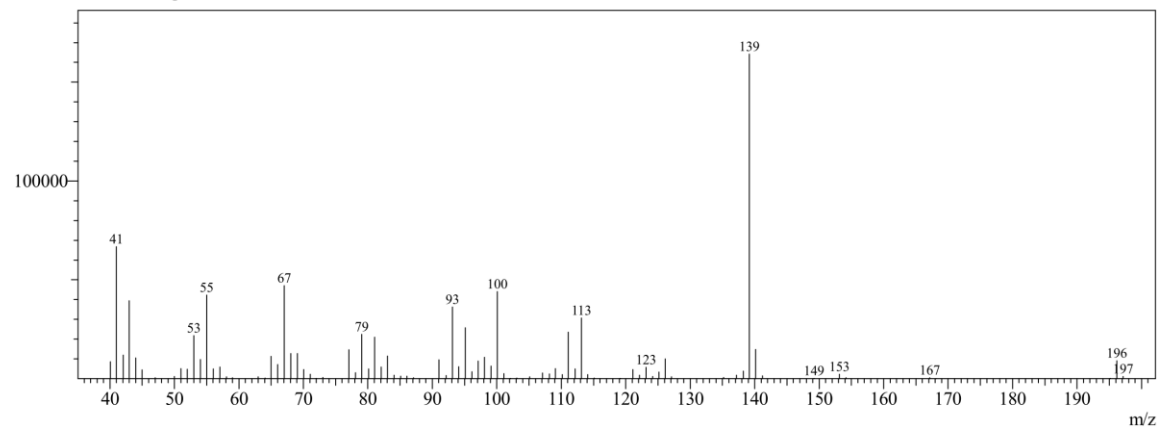


S5.6. GC-MS data of 12Z.

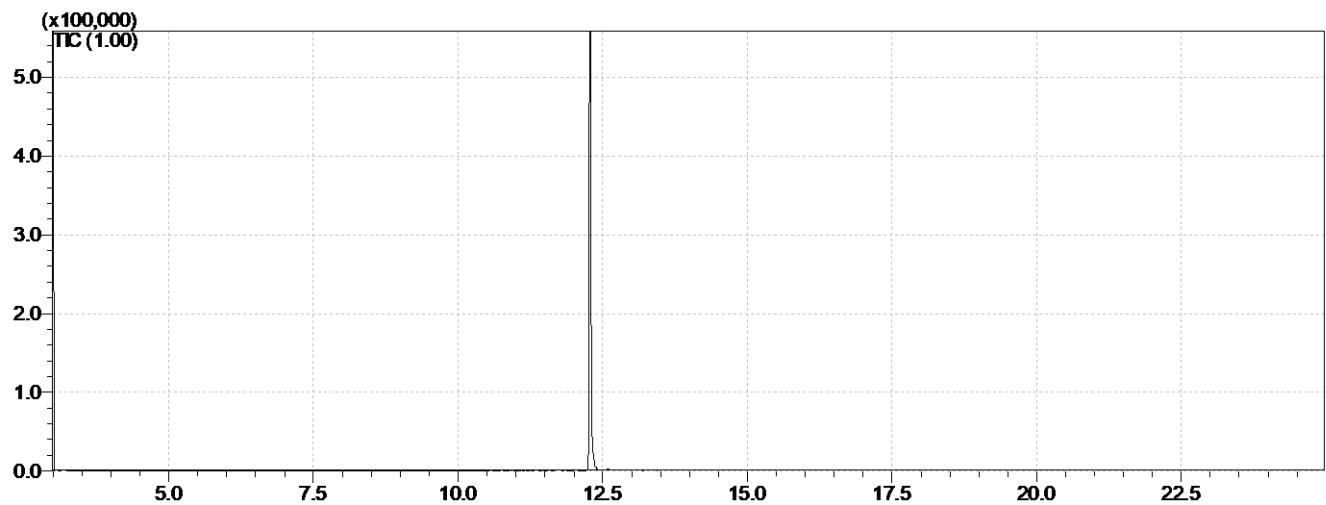


Purity: 82.3 %

Line#:1 R.Time:15.267(Scan#:1233)
MassPeaks:84
RawMode:Averaged 15.225-15.333(1228-1241) BasePeak:139.15(164241)
BG Mode:None Group 1 - Event 1 Scan

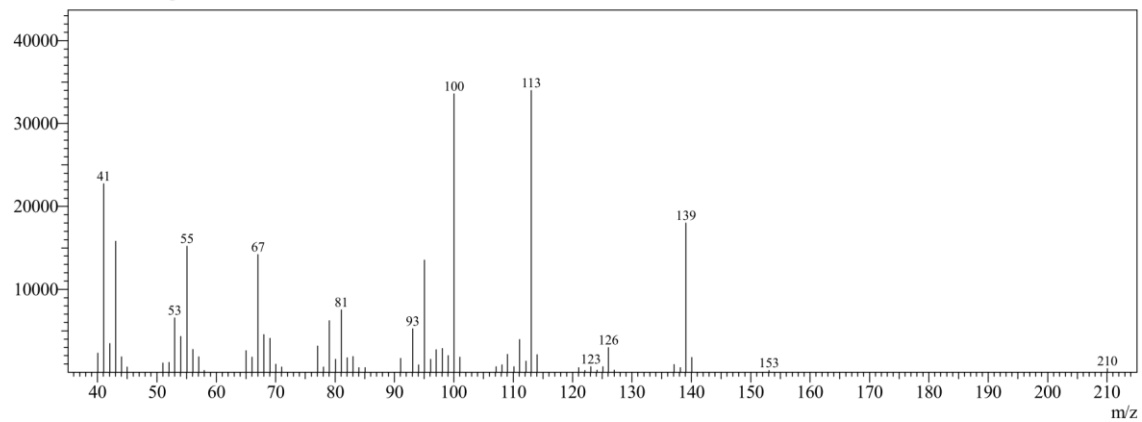


S5.7. GC-MS data of 13E.

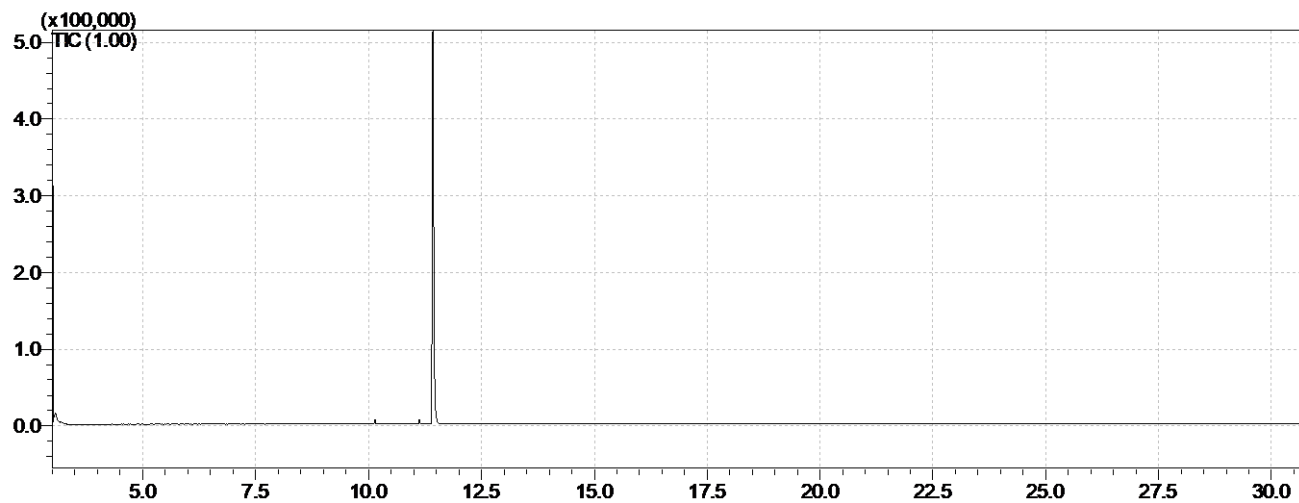


Purity: 99.7 %

Line#:1 R.Time:12.283(Scan#:1115)
MassPeaks:61
RawMode:Averaged 12.250-12.333(1111-1121) BasePeak:113.05(33980)
BG Mode:None Group 1 - Event 1 Scan

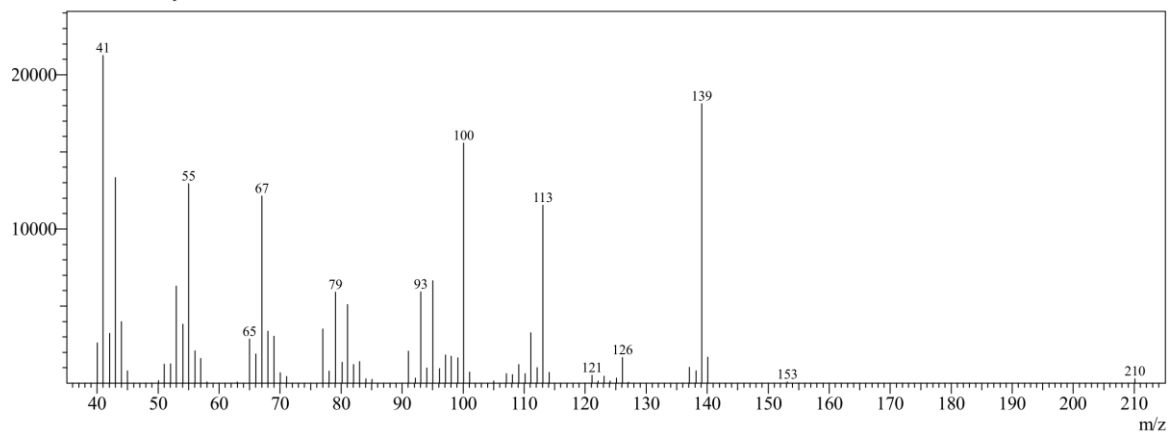


S5.8. GC-MS data of 13Z.

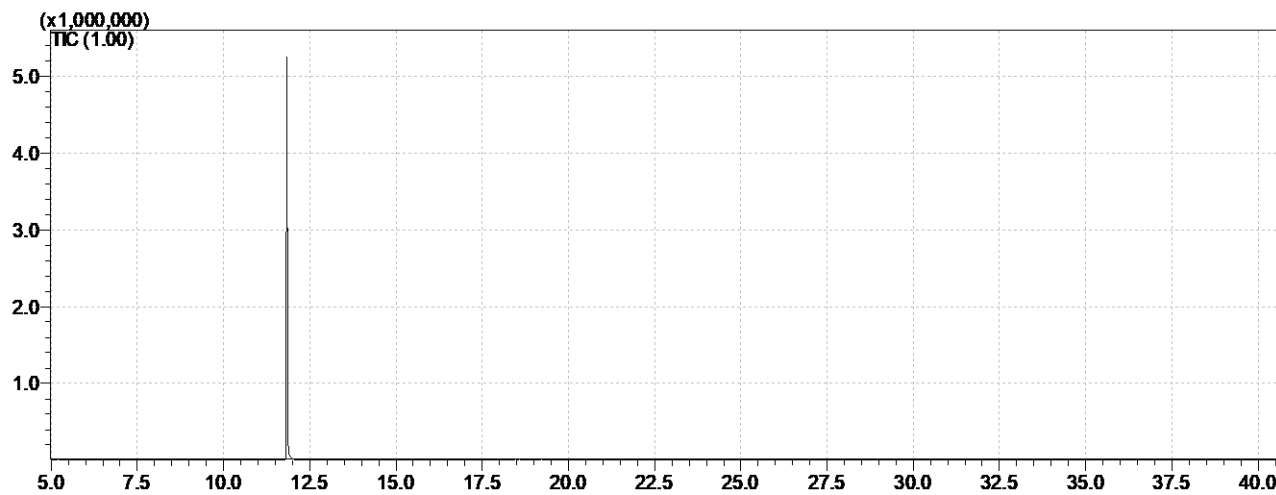


Purity: 98.8 %

Line#:1 R.Time:11.425(Scan#:1012)
MassPeaks:65
RawMode:Averaged 11.392-11.508(1008-1022) BasePeak:41.00(21255)
BG Mode:None Group 1 - Event 1 Scan

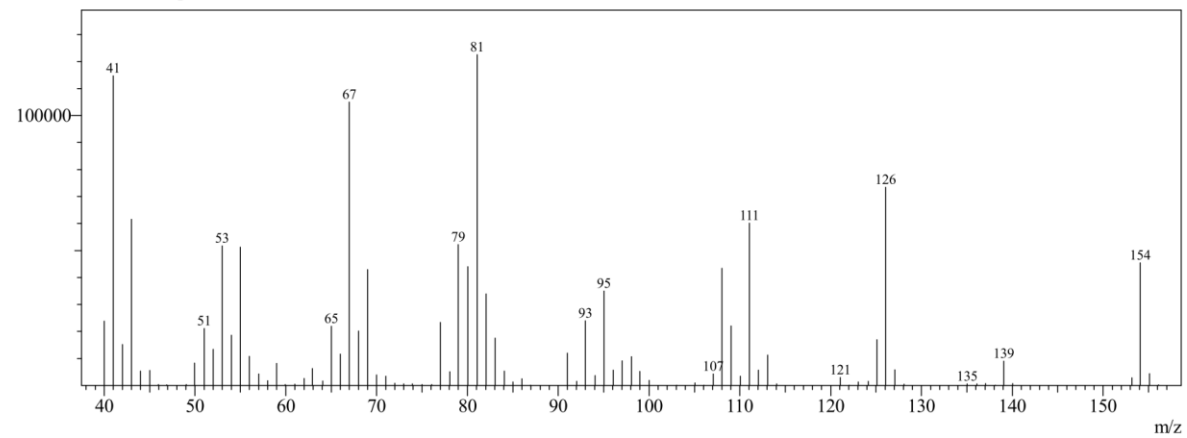


S5.9. GC-MS data of 14E.

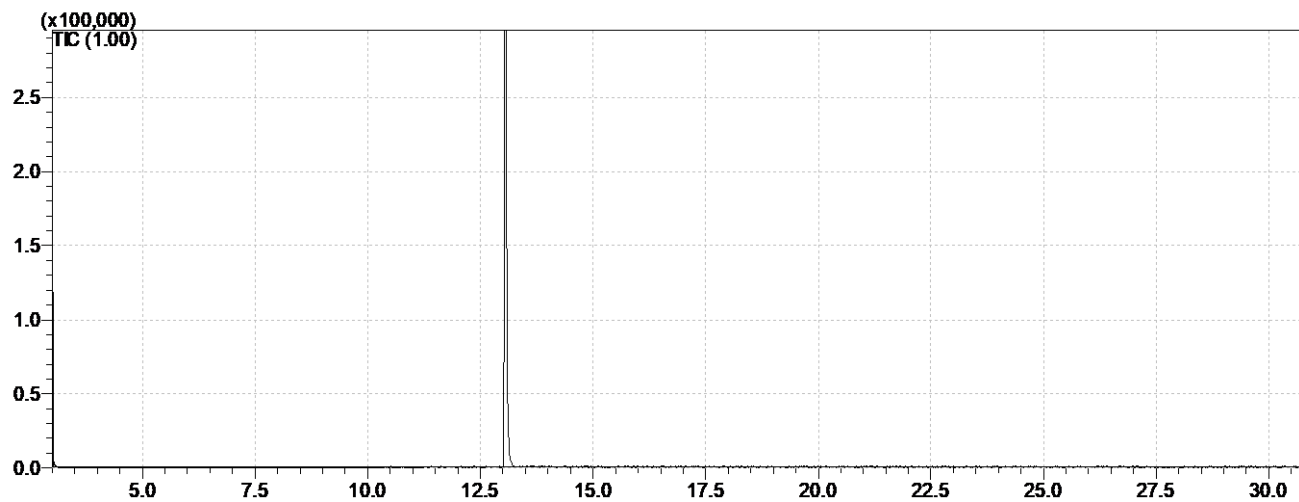


Purity: 99.8 %

Line#:1 R.Time:11.833(Scan#:821)
MassPeaks:86
RawMode:Averaged 11.792-11.908(816-830) BasePeak:81.05(122579)
BG Mode:None Group 1 - Event 1 Scan

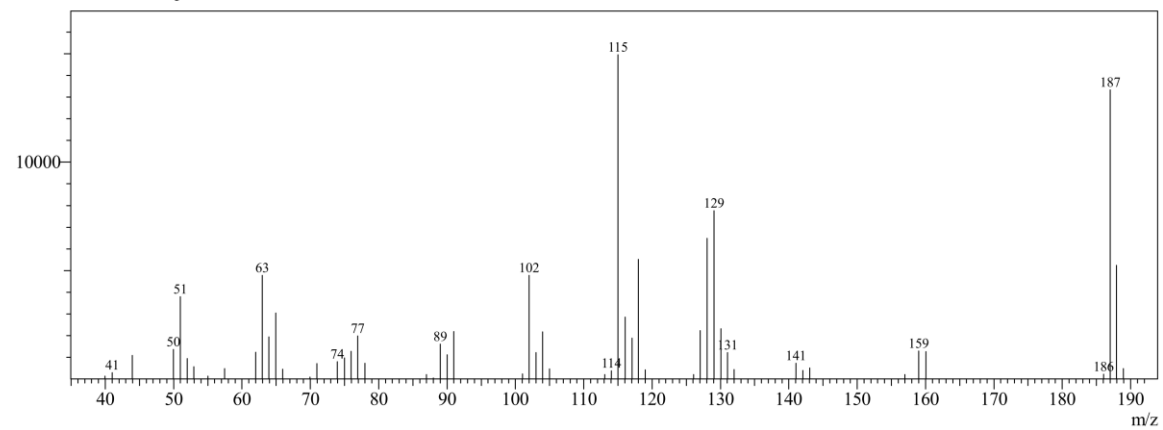


S5.10. GC-MS data of 15E.

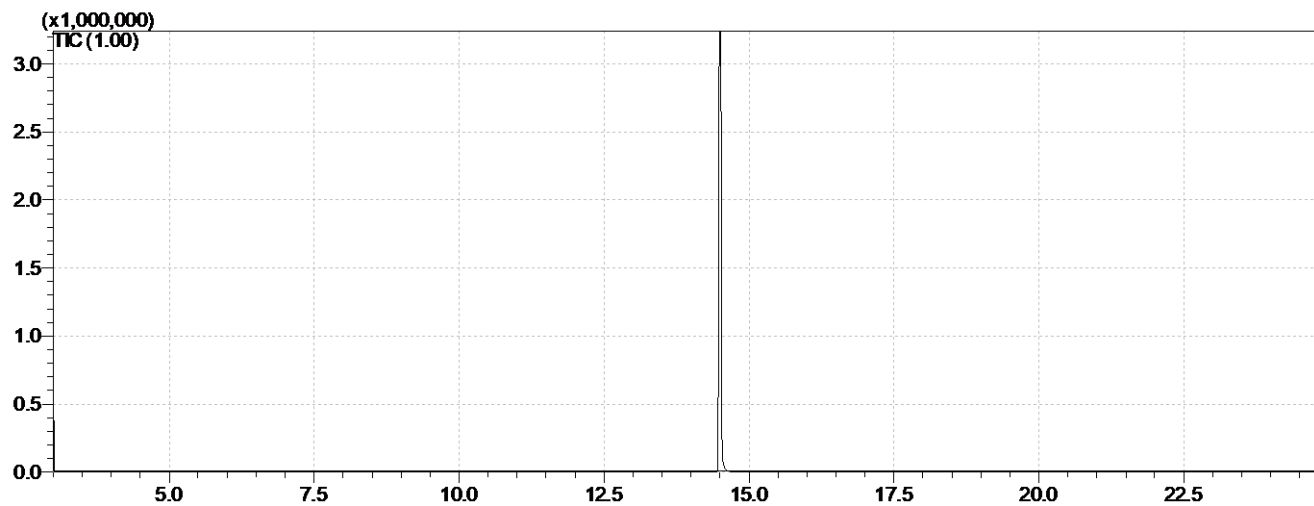


Purity: 99.9 %

Line#:1 R.Time:13.058(Scan#:1208)
MassPeaks:55
RawMode:Averaged 13.000-13.200(1201-1225) BasePeak:115.00(14962)
BG Mode:None Group 1 - Event 1 Scan

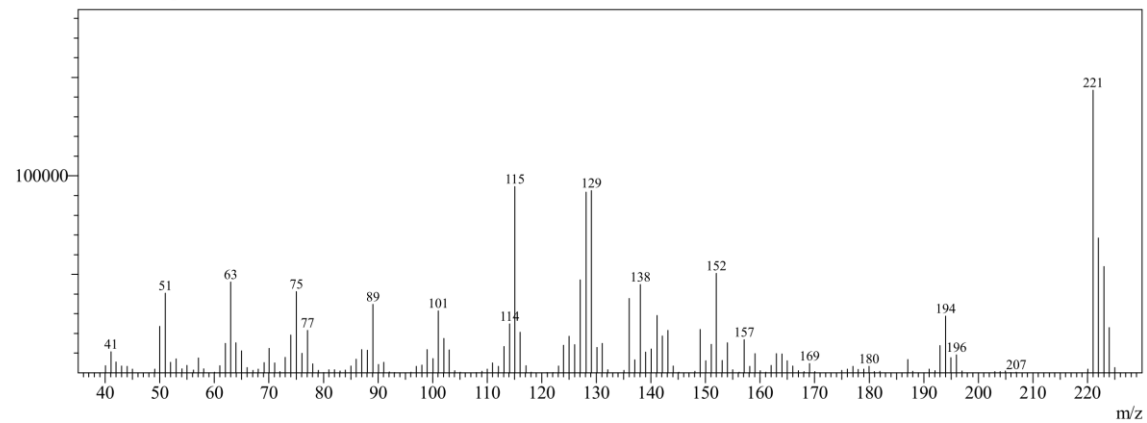


S5.11. GC-MS data of 16E.

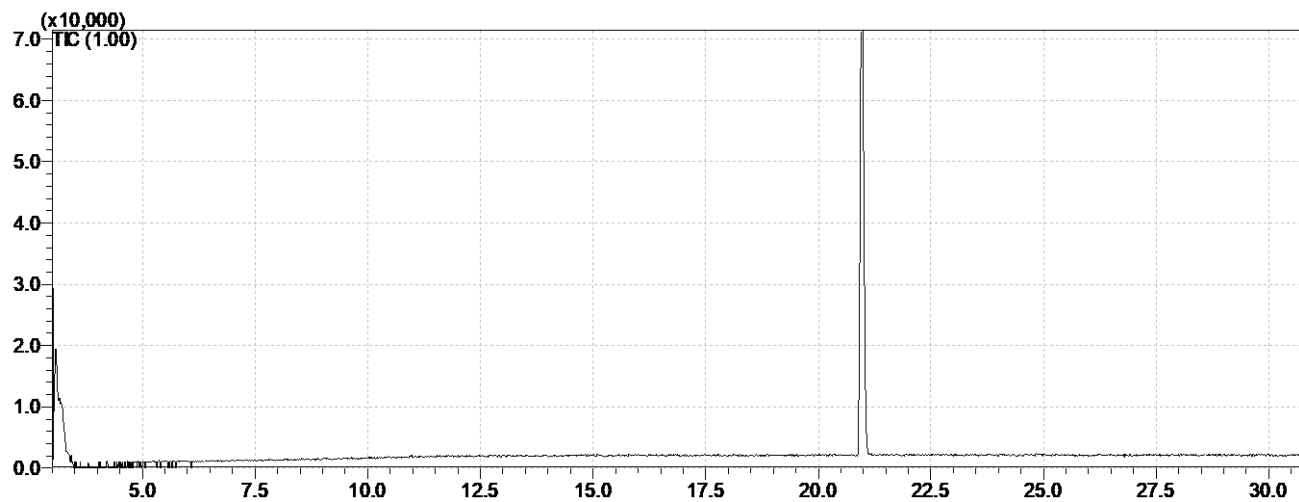


Purity: 99.9 %

Line#:1 R.Time:14.500(Scan#:1381)
MassPeaks:146
RawMode:Averaged 14.450-14.567(1375-1389) BasePeak:221.00(143438)
BG Mode:None Group 1 - Event 1 Scan

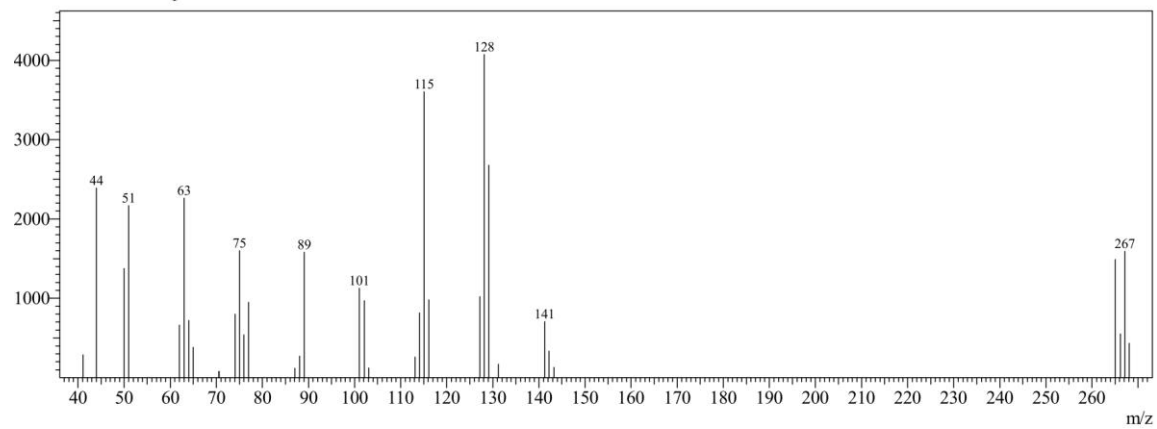


S5.12. GC-MS data of 17E.

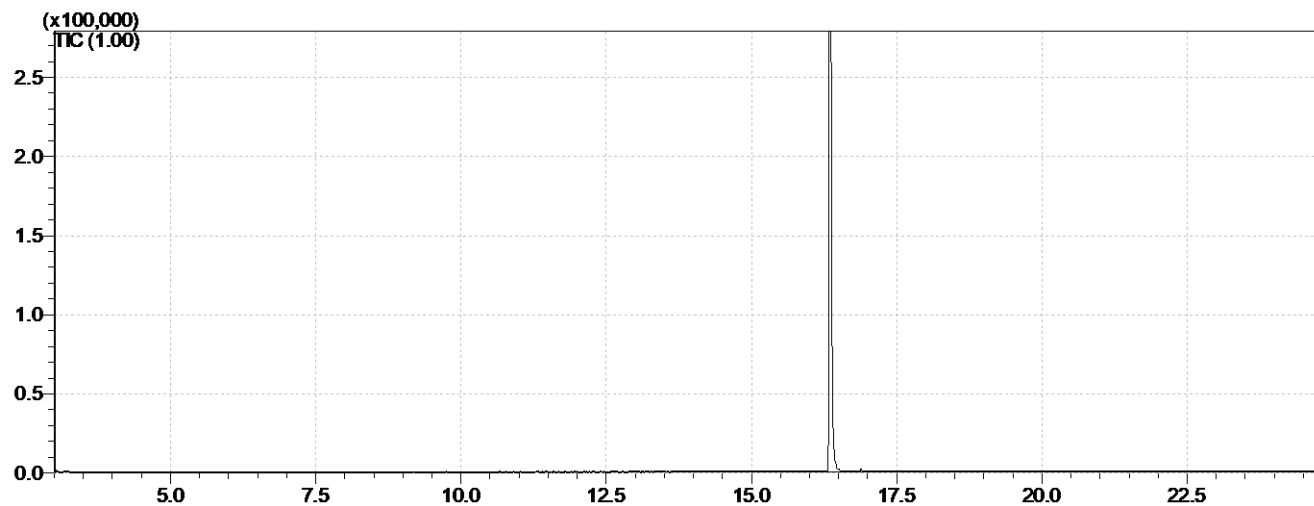


Purity: 99.9 %

Line#:1 R.Time:20.967(Scan#:2157)
MassPeaks:35
RawMode:Averaged 20.875-21.083(2146-2171) BasePeak:128.15(4074)
BG Mode:None Group 1 - Event 1 Scan

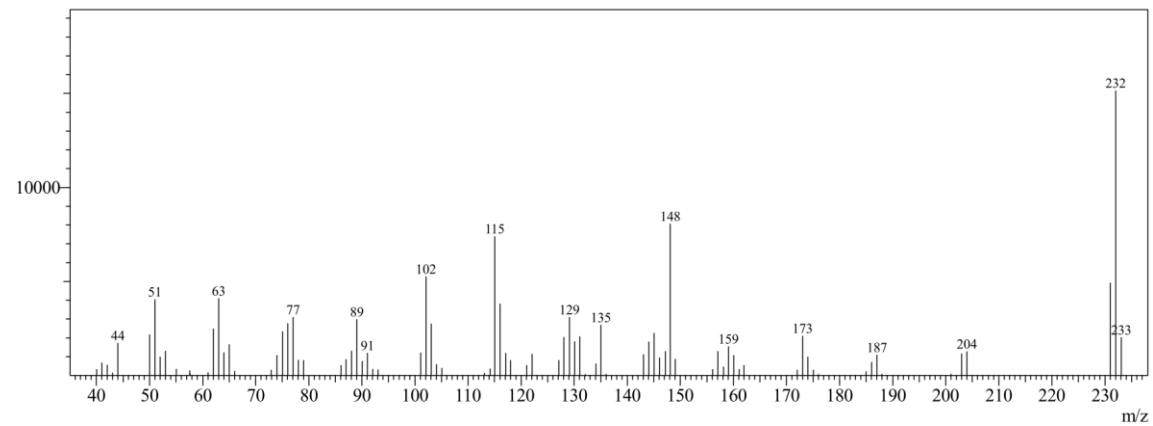


S5.13. GC-MS data of 18E.

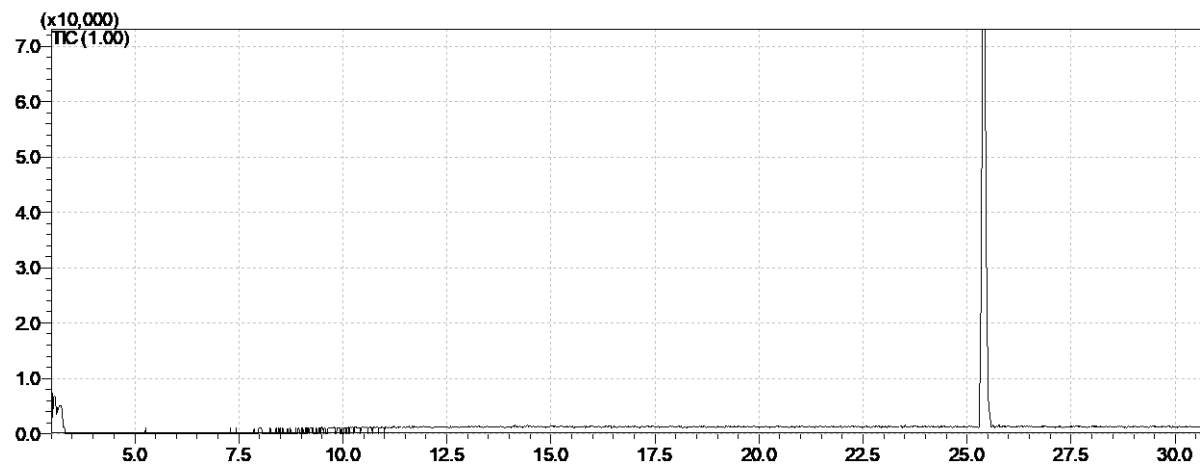


Purity: 99.9 %

Line#:1 R.Time:16.350(Scan#:1603)
MassPeaks:84
RawMode:Averaged 16.308-16.450(1598-1615) BasePeak:232.00(15131)
BG Mode:None Group 1 - Event 1 Scan

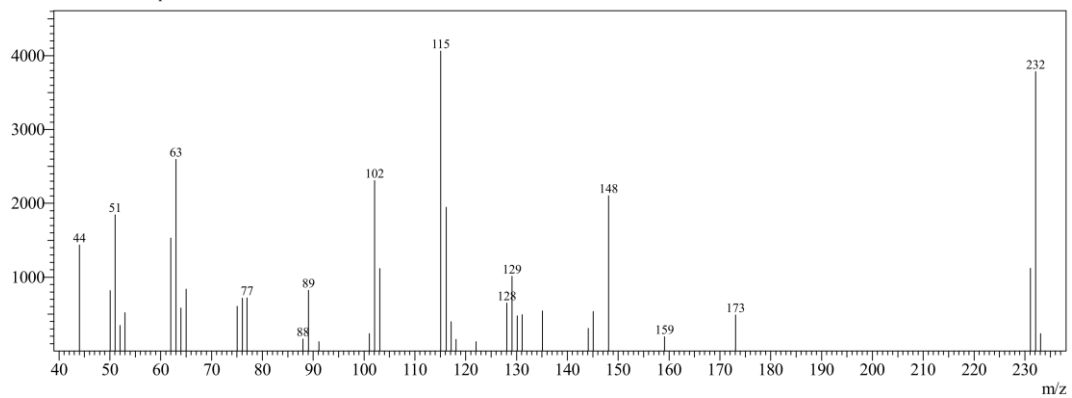


S5.14. GC-MS data of 19E.

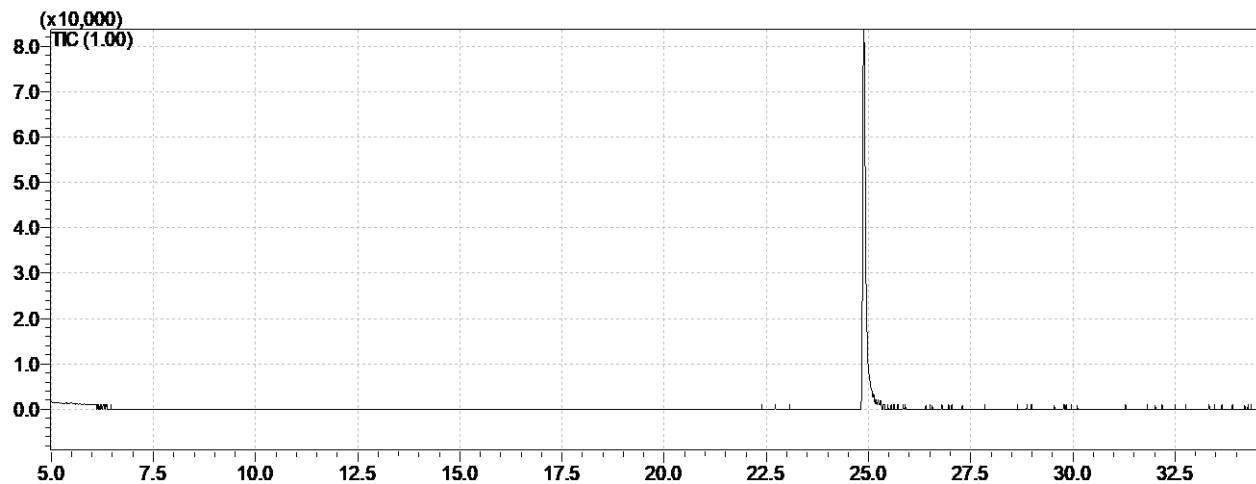


Purity: 99.9 %

Line#:1 R.Time:25.400(Scan#:2689)
MassPeaks:36
RawMode:Averaged 25.283-25.558(2675-2708) BasePeak:115.10(4064)
BG Mode:None Group 1 - Event 1 Scan



S5.14. GC-MS data of 20.



Purity: > 99.9 %

Line#:1 R.Time:24.883(Scan#:2387)
MassPeaks:25
RawMode:Averaged 24.692-25.417(2364-2451) BasePeak:170.10(2830)
BG Mode:None Group 1 - Event 1 Scan

