

# New Chemistry of Chiral 1,3-Dioxolan-4-ones

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## Supplementary Material

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR, IR and HRMS spectra of **14**

<sup>1</sup>H NMR and DEPTQ <sup>13</sup>C NMR spectra of **6a**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR, IR and HRMS spectra of **6b**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and IR spectra of **7a**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and IR spectra of **7b**

<sup>1</sup>H NMR and DEPTQ <sup>13</sup>C NMR spectra of **16**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and IR spectra of **17**

IR and HRMS spectra of **18**

<sup>1</sup>H NMR spectrum of **19**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and HRMS spectra of **20**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR, IR and HRMS spectra of **21**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and IR spectra of **22a**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and IR spectra of **24**

<sup>1</sup>H NMR and DEPTQ <sup>13</sup>C NMR spectra of **25**

<sup>1</sup>H NMR and DEPTQ <sup>13</sup>C NMR spectra of **27**

<sup>1</sup>H NMR, DEPTQ <sup>13</sup>C NMR and HRMS spectra of **28**

<sup>1</sup>H NMR, <sup>13</sup>C NMR and IR spectra of **29a**

<sup>1</sup>H NMR and IR spectra of **29b**

## Figure

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Figure S1. 300 MHz DEPTQ  $^1\text{H}$  NMR spectrum of **14**

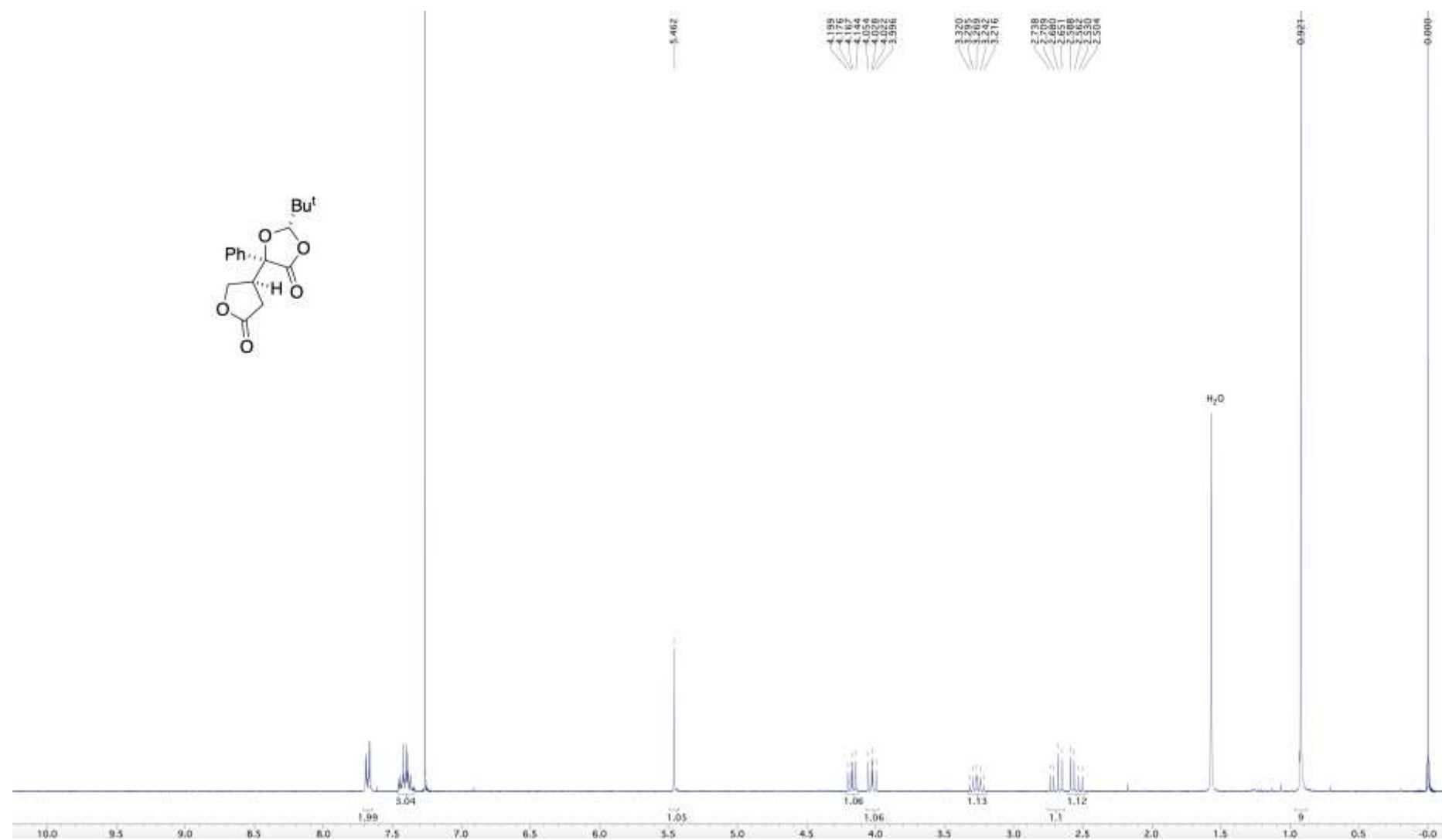


Figure S2. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **14**

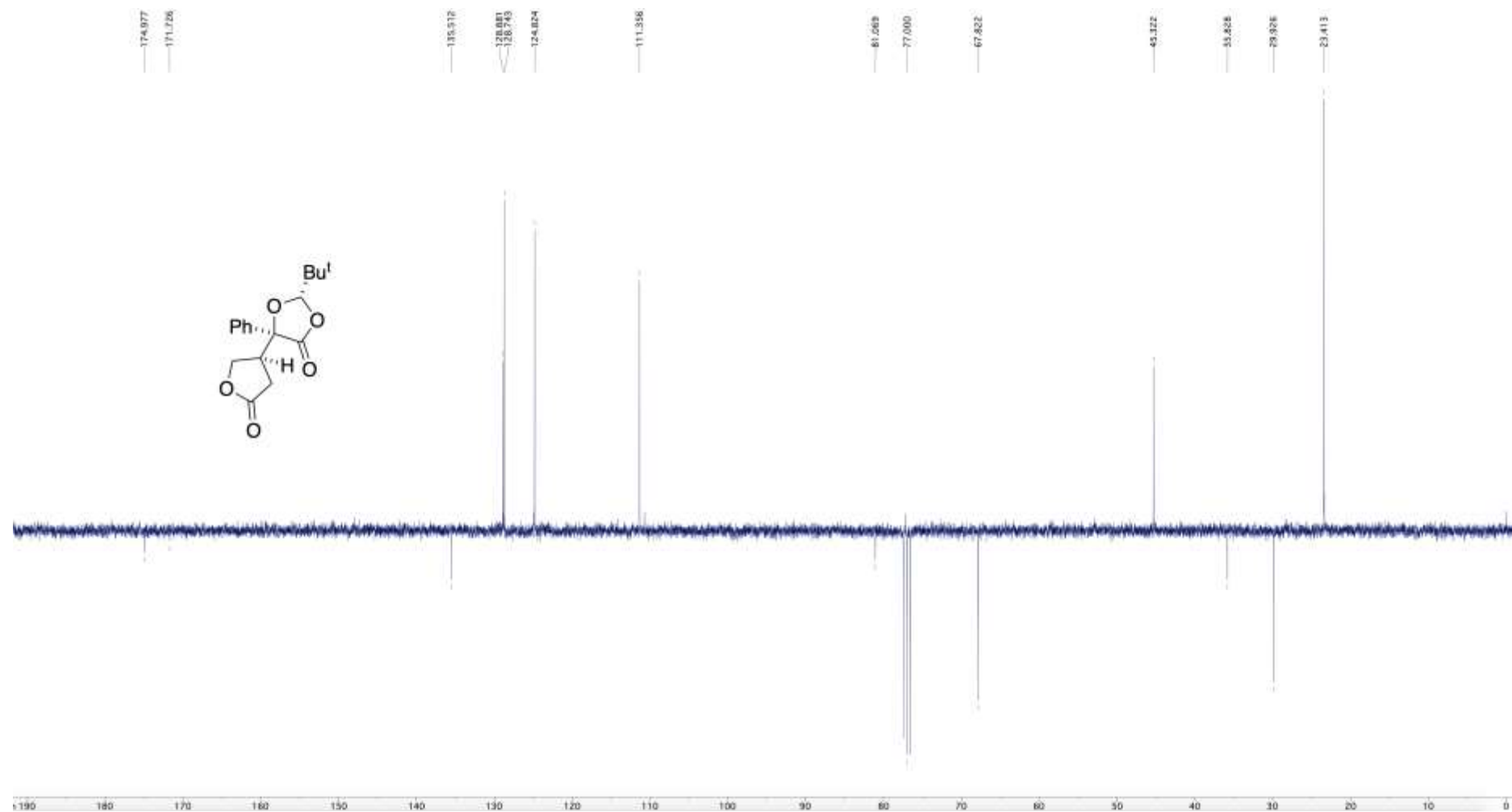


Figure S3. IR spectrum of **14**

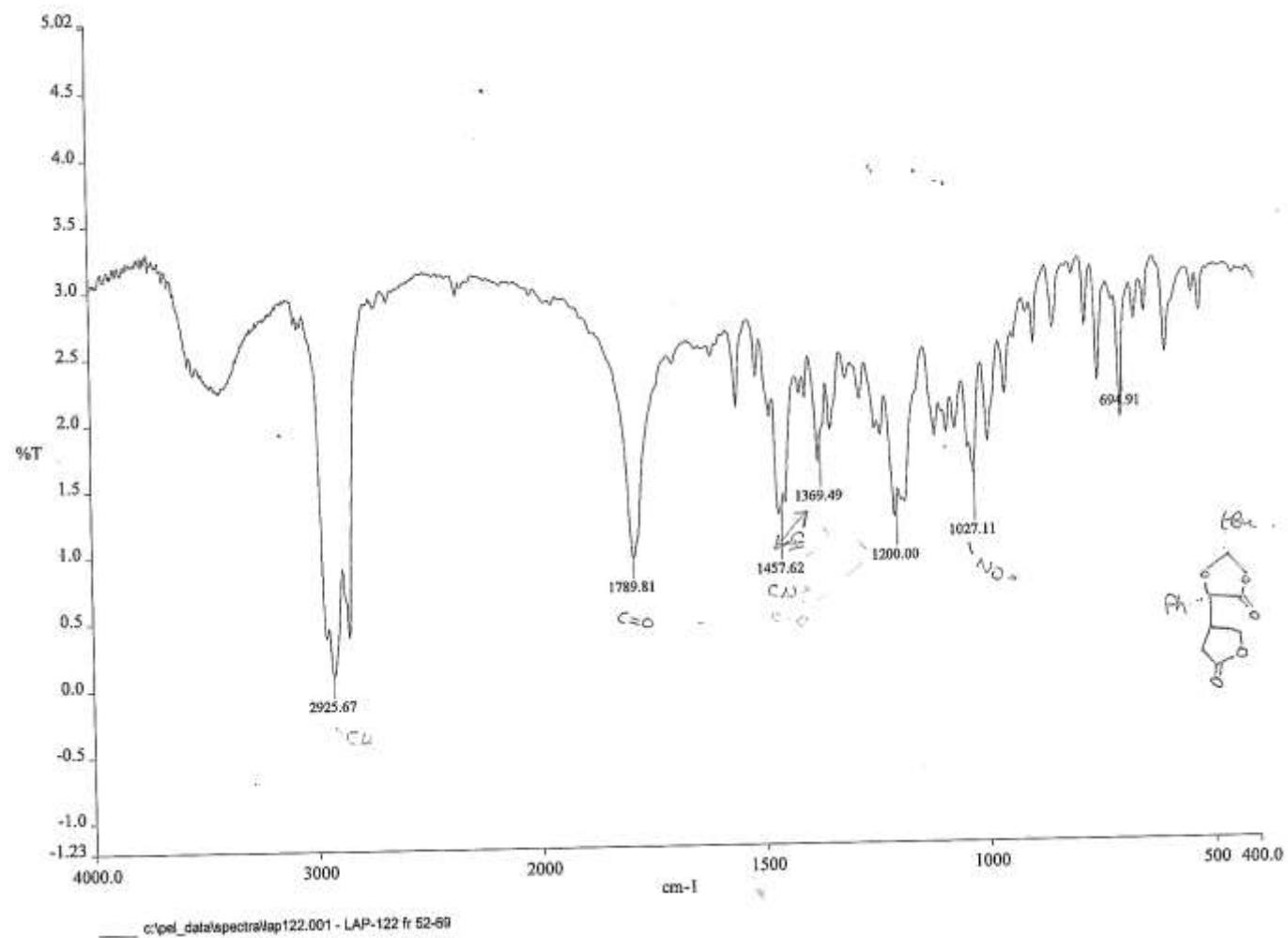


Figure S4. HRMS of **14**

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

26 formula(e) evaluated with 2 results within limits (up to 8 closest results for each mass)

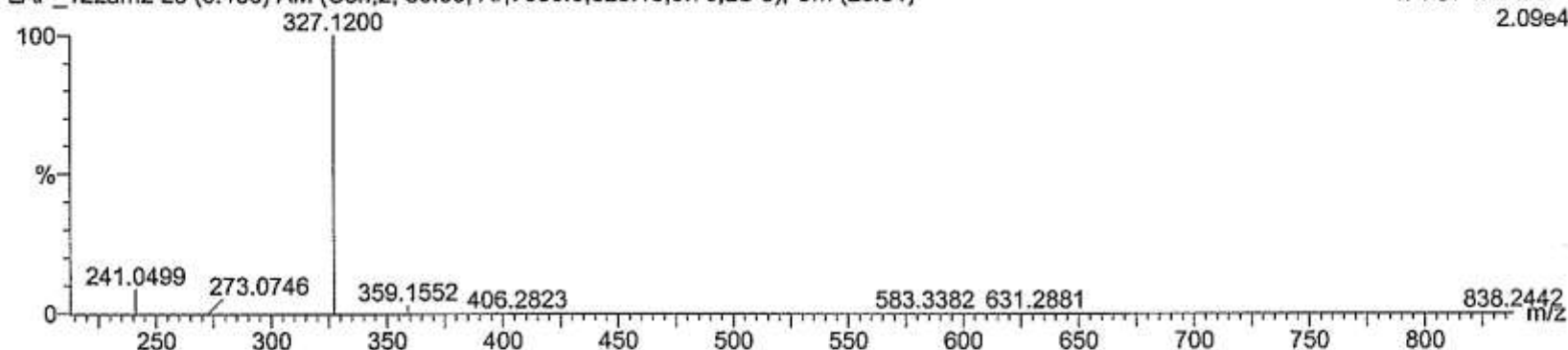
Lynn Power

University of St-Andrews  
School of Chemistry LCTOF

12-Sep-2007 15:03:51

LAP\_122am2 25 (0.486) AM (Cen,2, 80.00, Ar,7000.0,325.19,0.76,LS 5); Cm (25:31)

1: TOF MS ES+  
2.09e4



Minimum: -1.5  
Maximum: 200.0 20.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
327.1200	327.1208	-0.8	-2.5	7.5	1	C17 H20 O5 Na
	327.1232	-3.2	-9.9	10.5	2	C19 H19 O5

Figure S5. 300 MHz  $^1\text{H}$  NMR spectrum of **6a**

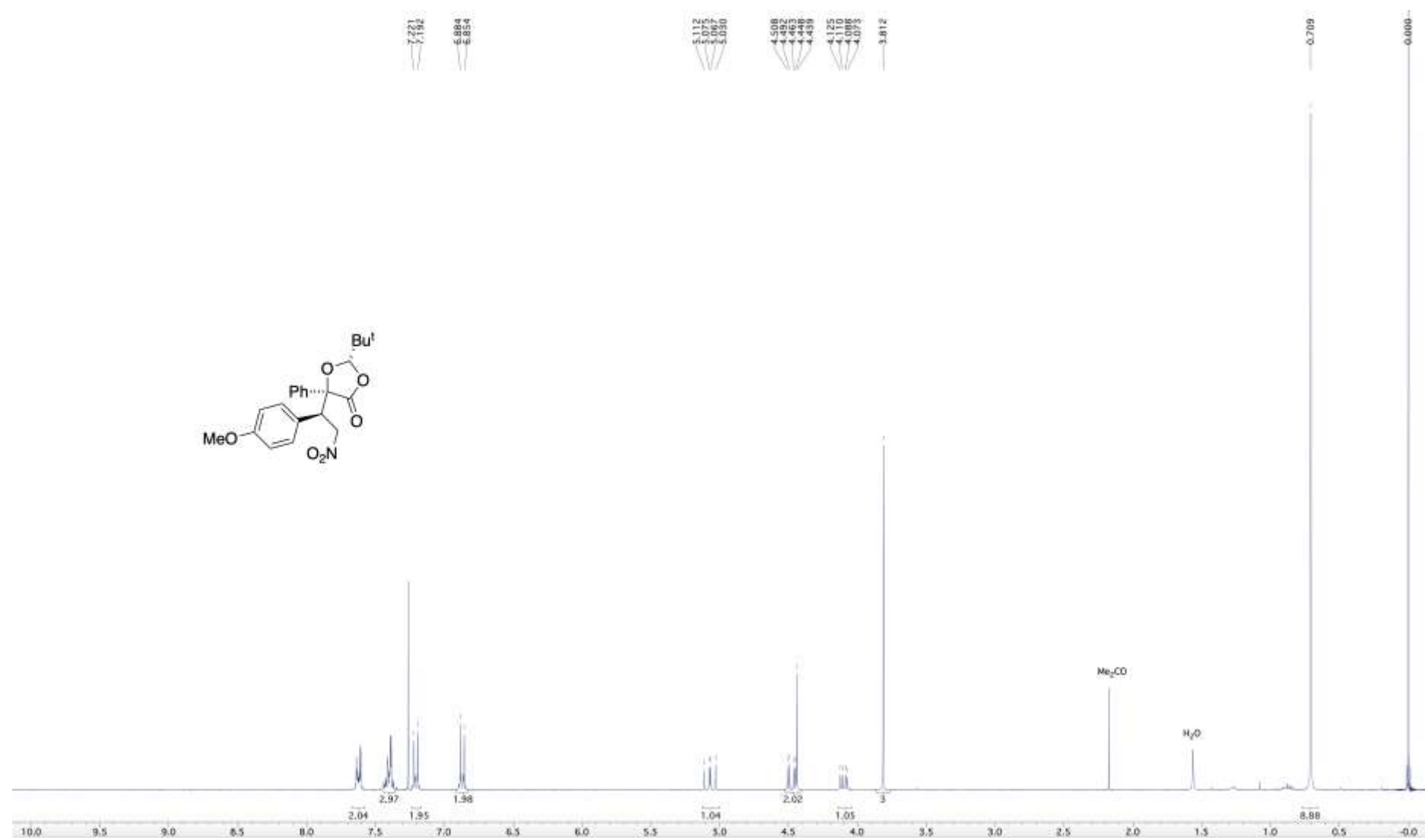


Figure S6. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **6a**

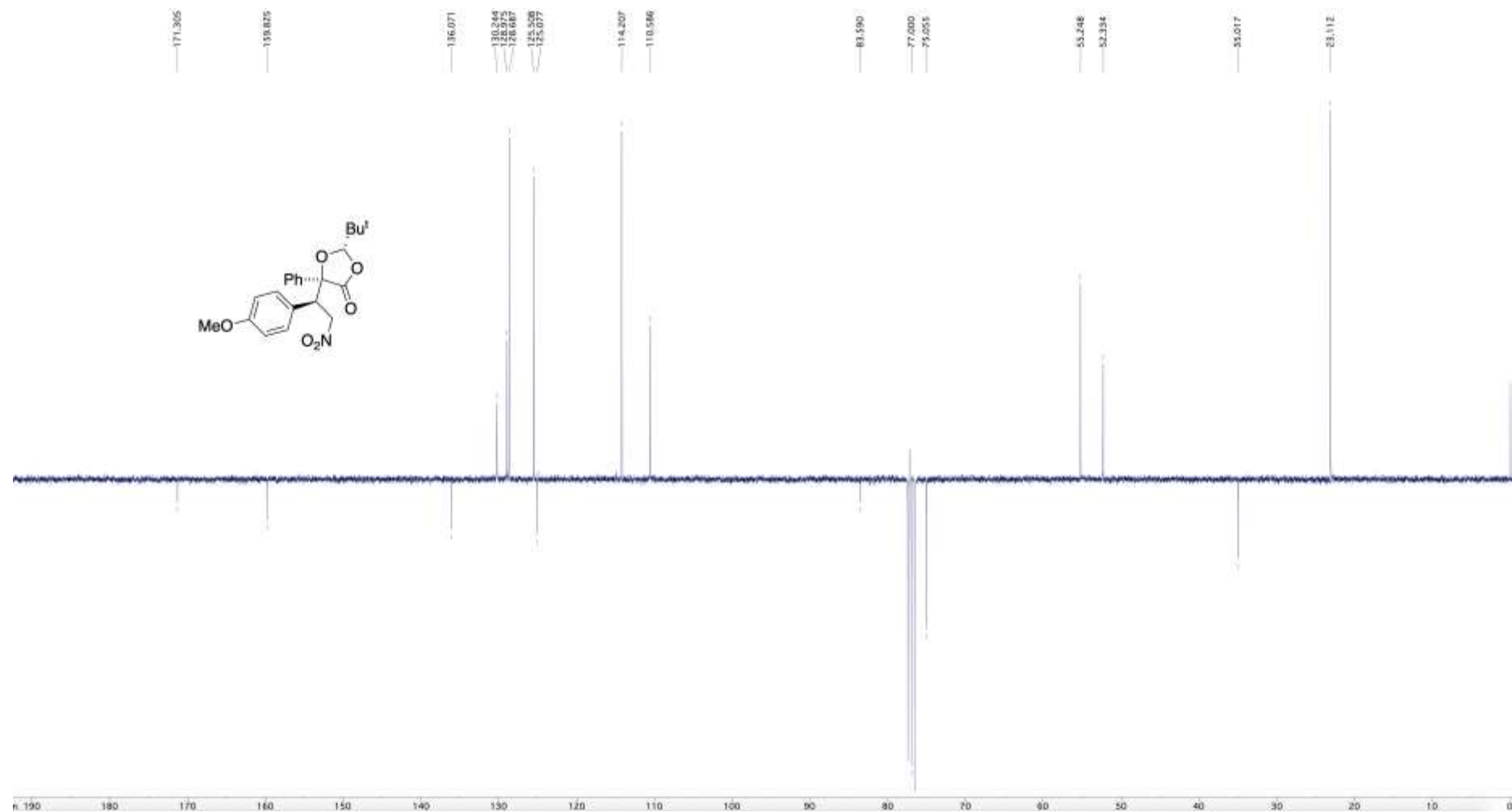


Figure S7. 300 MHz  $^1\text{H}$  NMR spectrum of **6b**

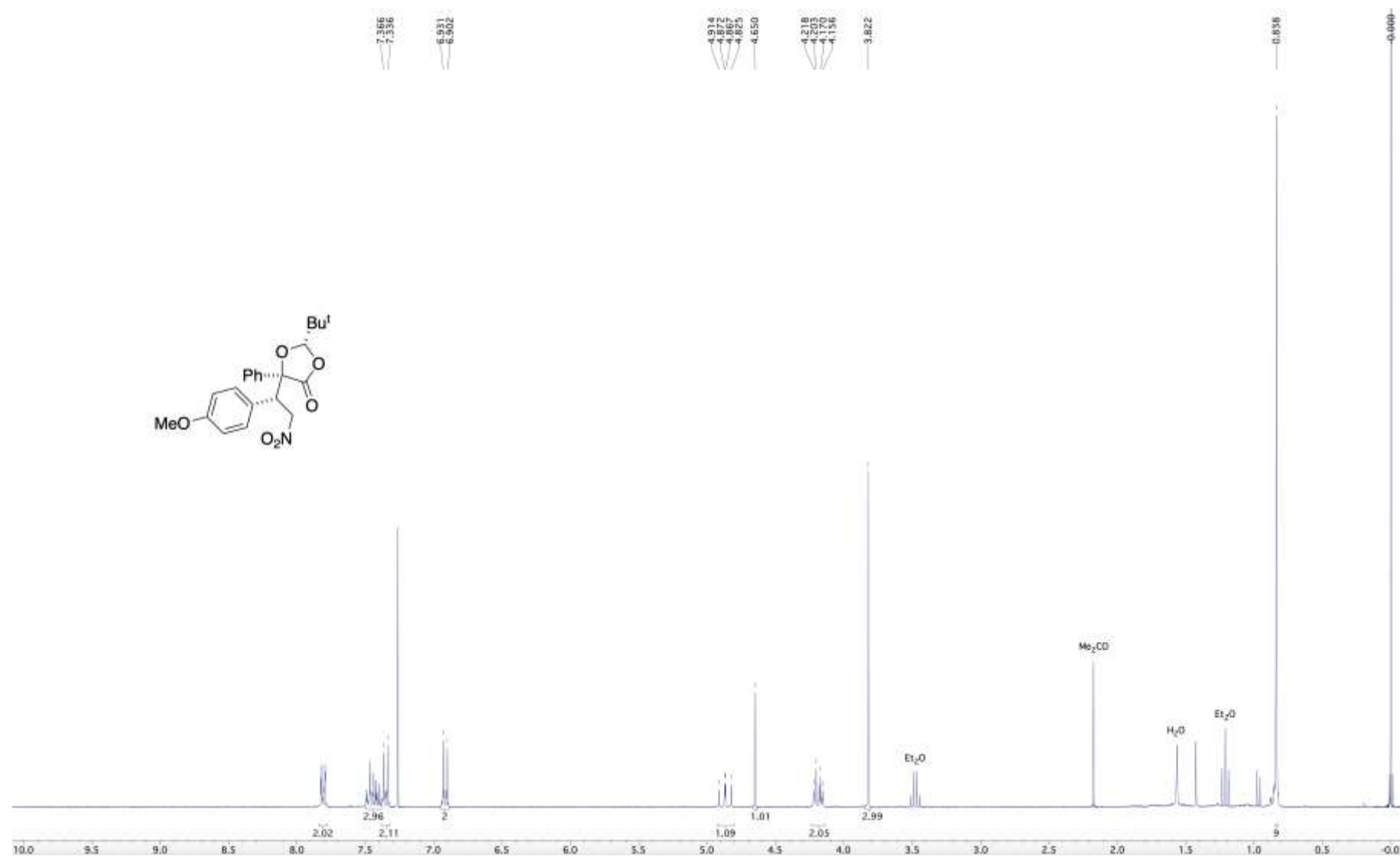




Figure S8. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **6b**

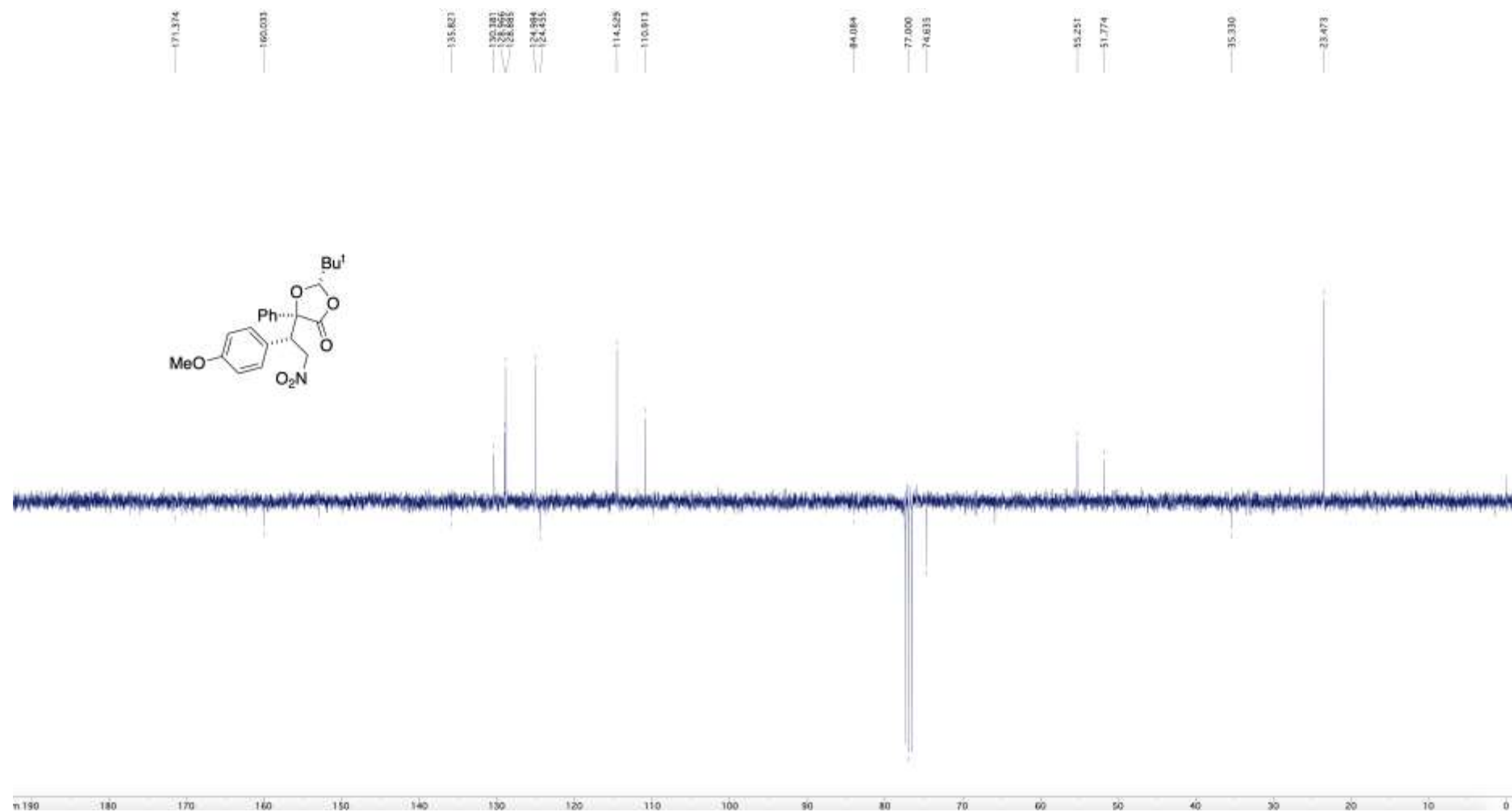


Figure S9. IR spectrum of **6b**

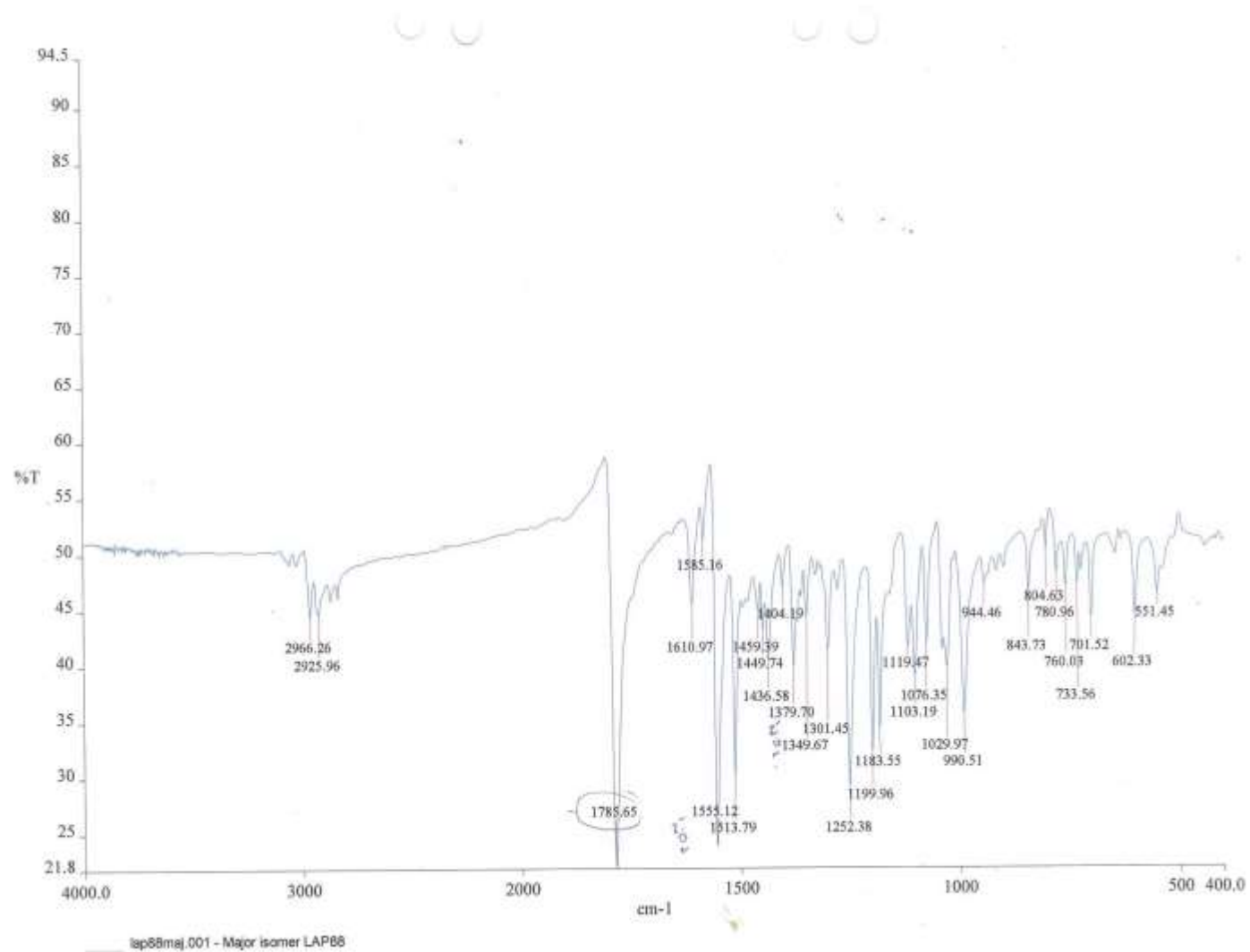


Figure S10. HRMS of 6b

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

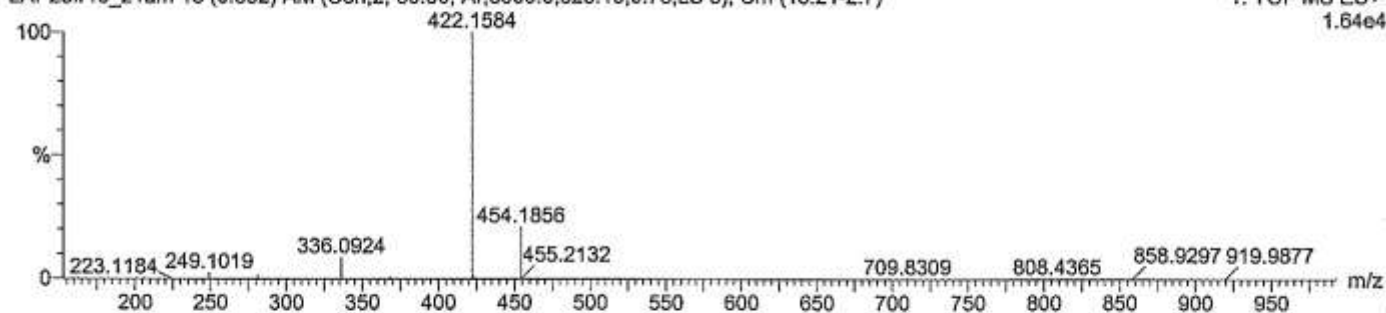
166 formula(e) evaluated with 19 results within limits (up to 8 closest results for each mass)

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10-Nov-2005 11:33:16

LAP25fr19\_21am 18 (0.352) AM (Cen,2, 80.00, Ar,8000.0,325.19,0.76,LS 5); Cm (15:21-2:7)

1: TOF MS ES+  
1.64e4

Minimum: -1.5  
Maximum: 200.0 30.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
422.1584	422.1580	0.5	1.2	10.5	3	C22 H25 N O6 Na
	422.1604	-1.9	-4.5	13.5	4	C24 H24 N O6
	422.1563	2.1	5.0	9.5	2	C19 H24 N3 O8
	422.1606	-2.2	-5.2	15.0	5	C25 H23 N2 O3 Na
	422.1539	4.5	10.7	6.5	1	C17 H25 N3 O8 Na
	422.1630	-4.6	-10.9	18.0	6	C27 H22 N2 O3
	422.1633	-4.9	-11.5	19.5	7	C28 H21 N3 Na
	422.1647	-6.2	-14.7	19.0	8	C30 H23 O Na

Figure S11. 300 MHz  $^1\text{H}$  NMR spectrum of **7a**

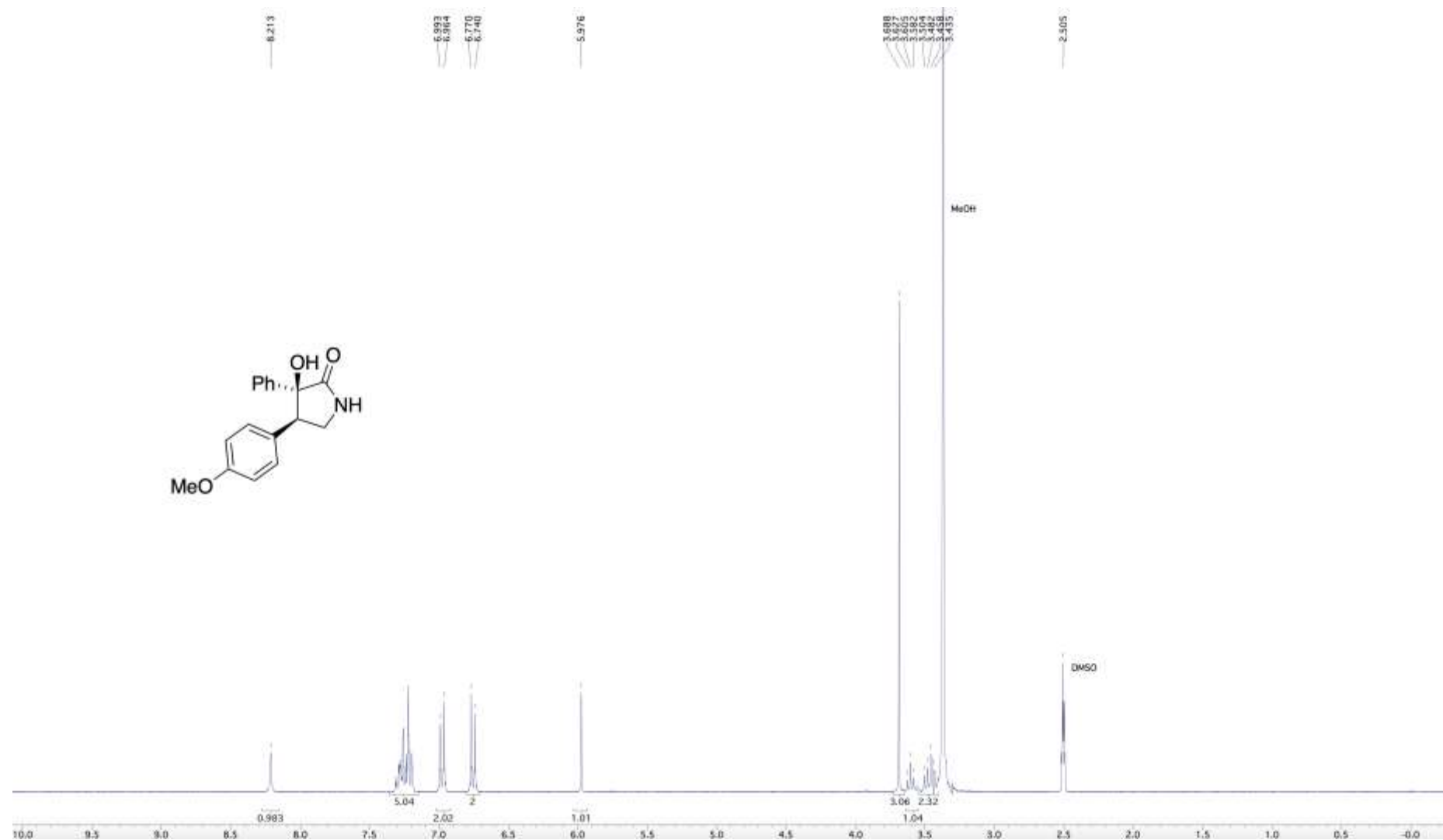


Figure S12. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **7a**

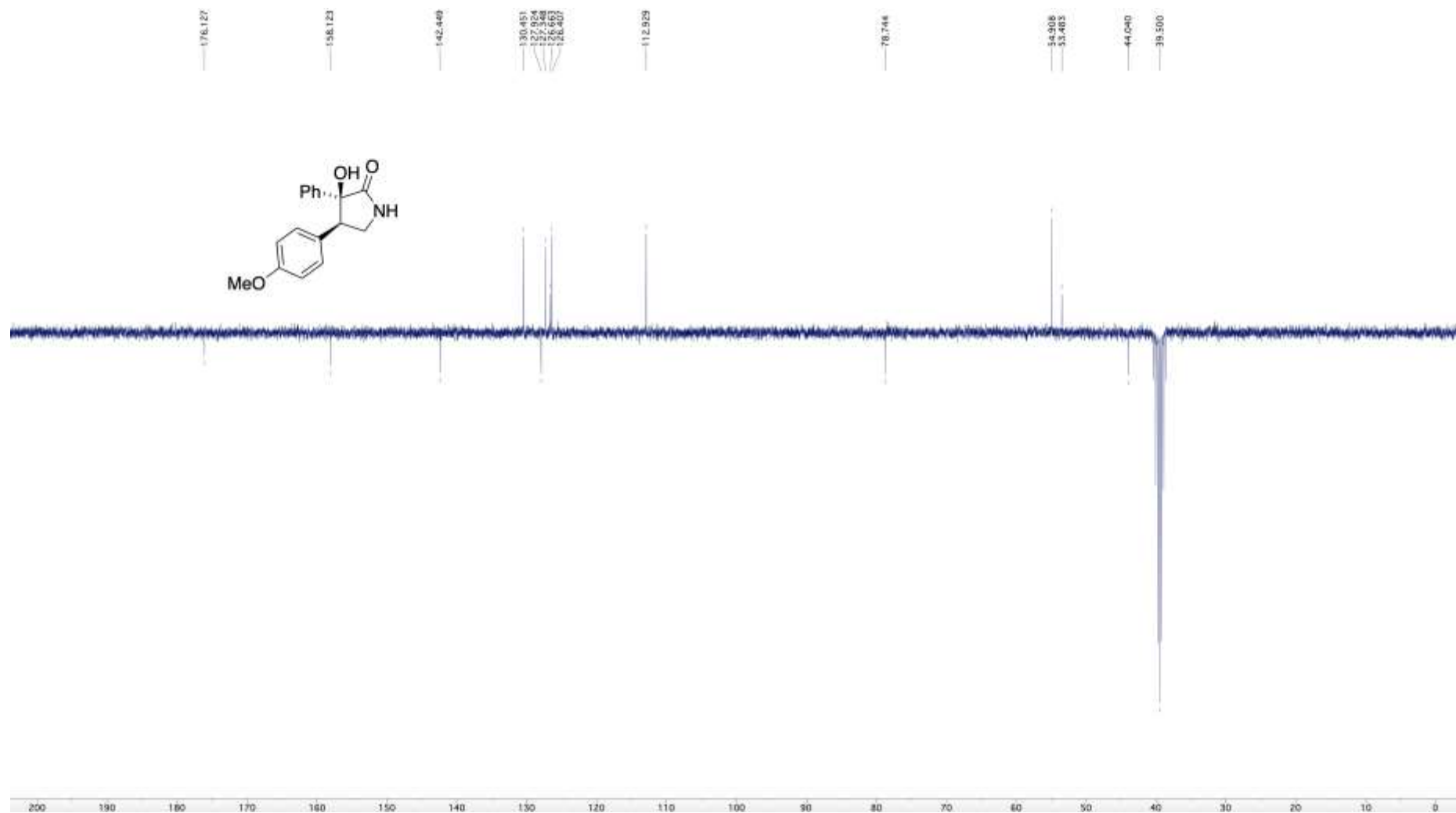


Figure S13. IR spectrum of **7a**

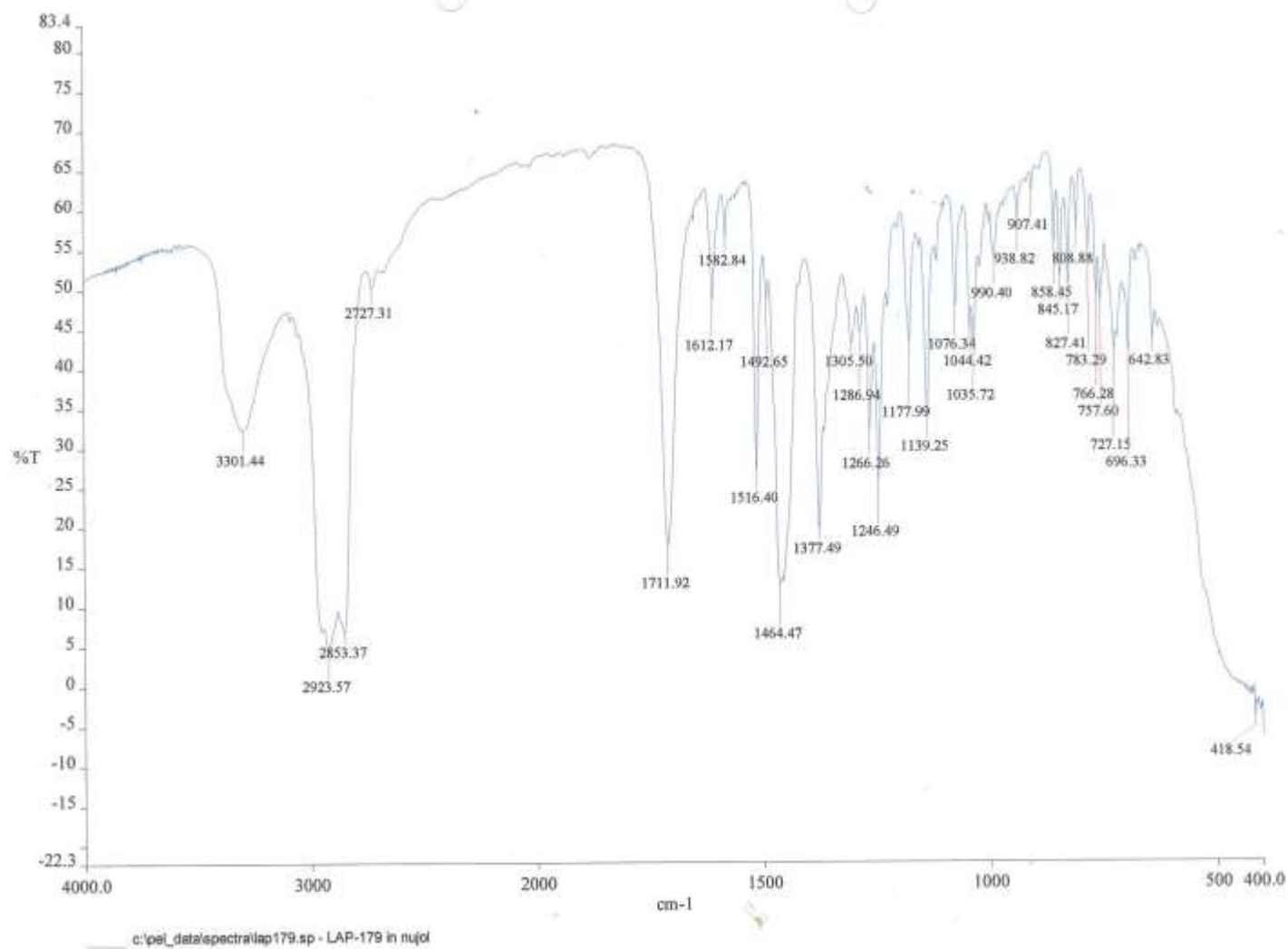


Figure S14. 300 MHz  $^1\text{H}$  NMR spectrum of **7b**

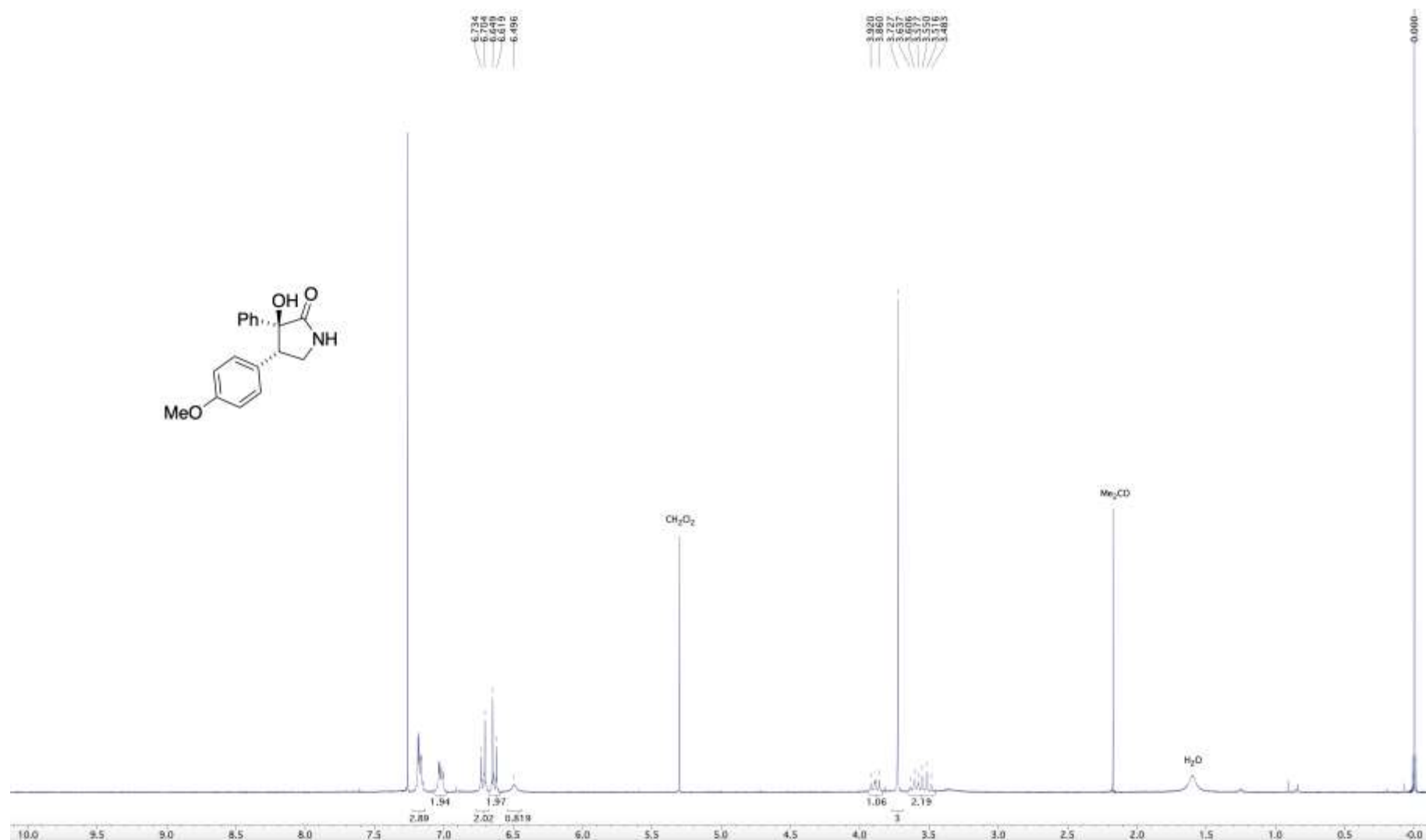


Figure S15. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **7b**

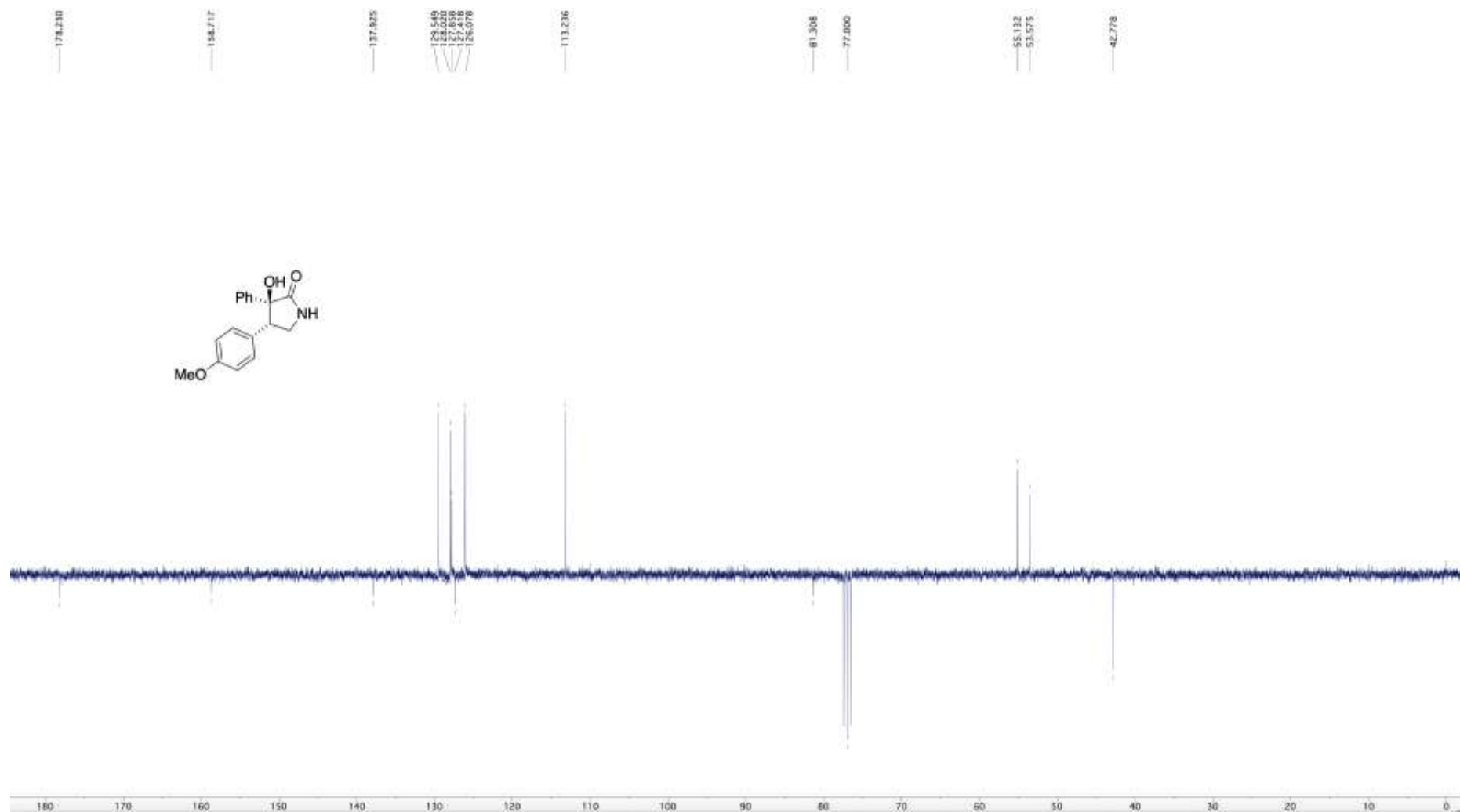




Figure S16. IR spectrum of **7b**

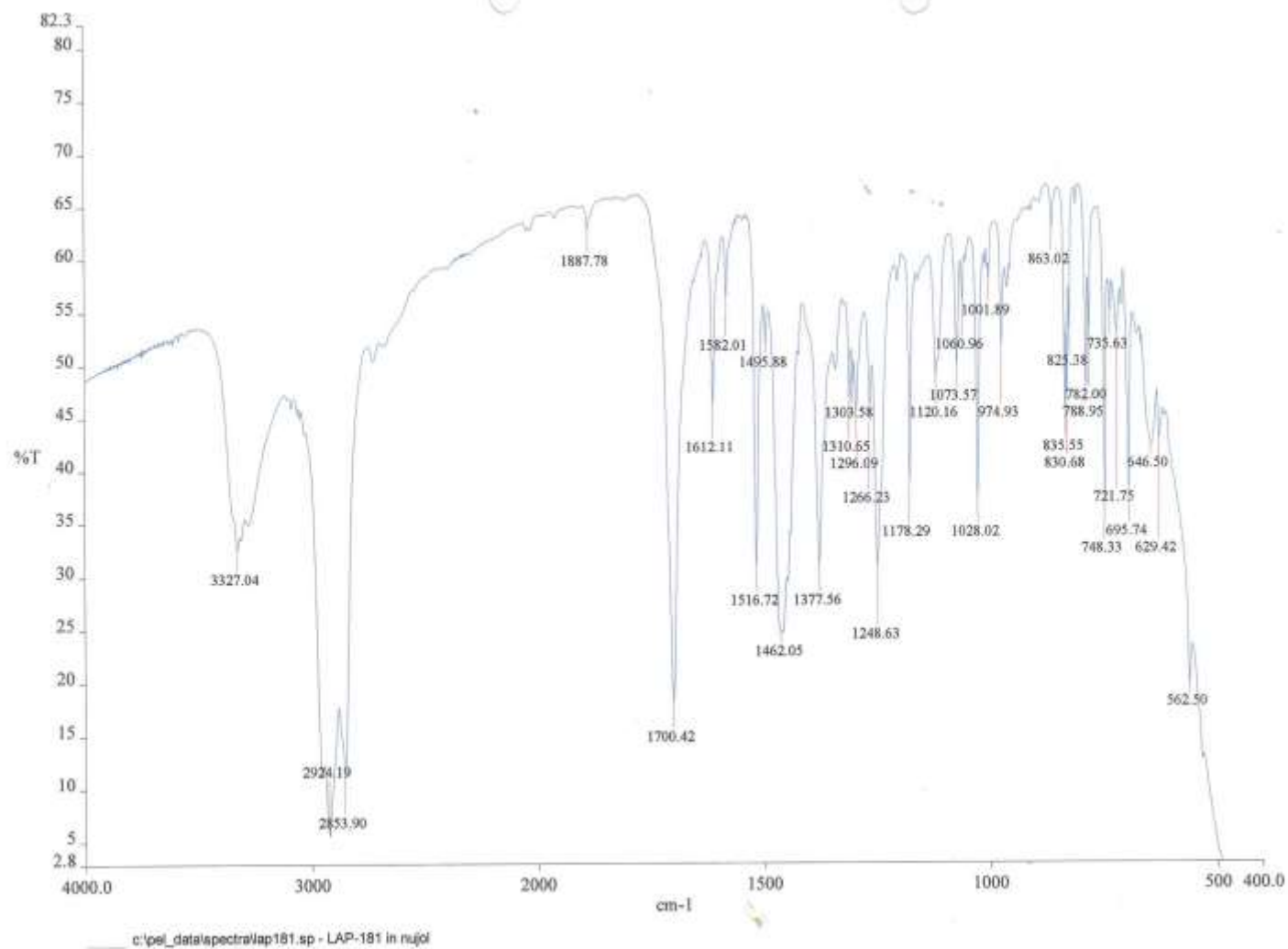


Figure S17. 300 MHz  $^1\text{H}$  NMR spectrum of **16**

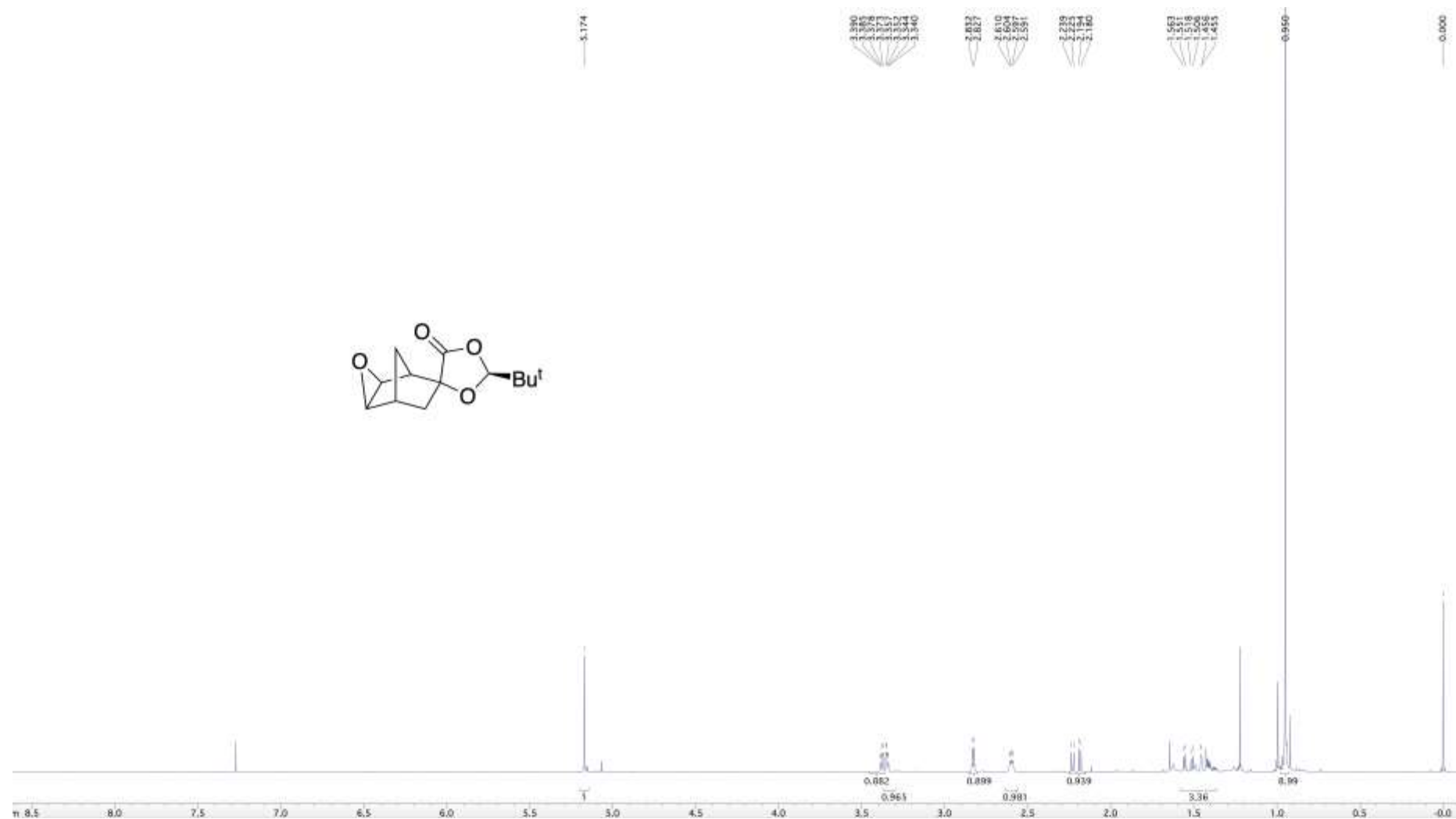


Figure S18. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **16**

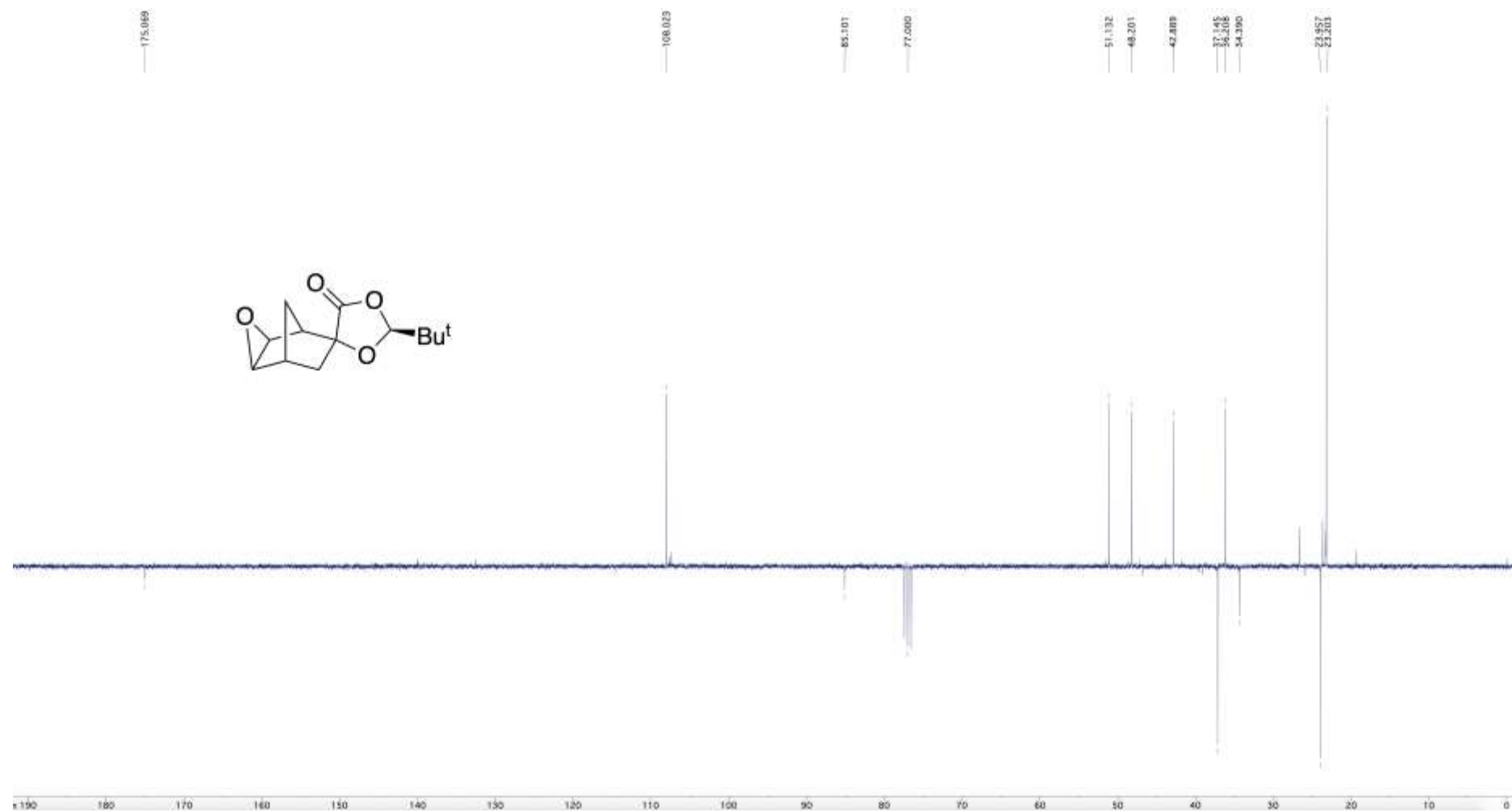


Figure S19. 300 MHz  $^1\text{H}$  NMR spectrum of **17**

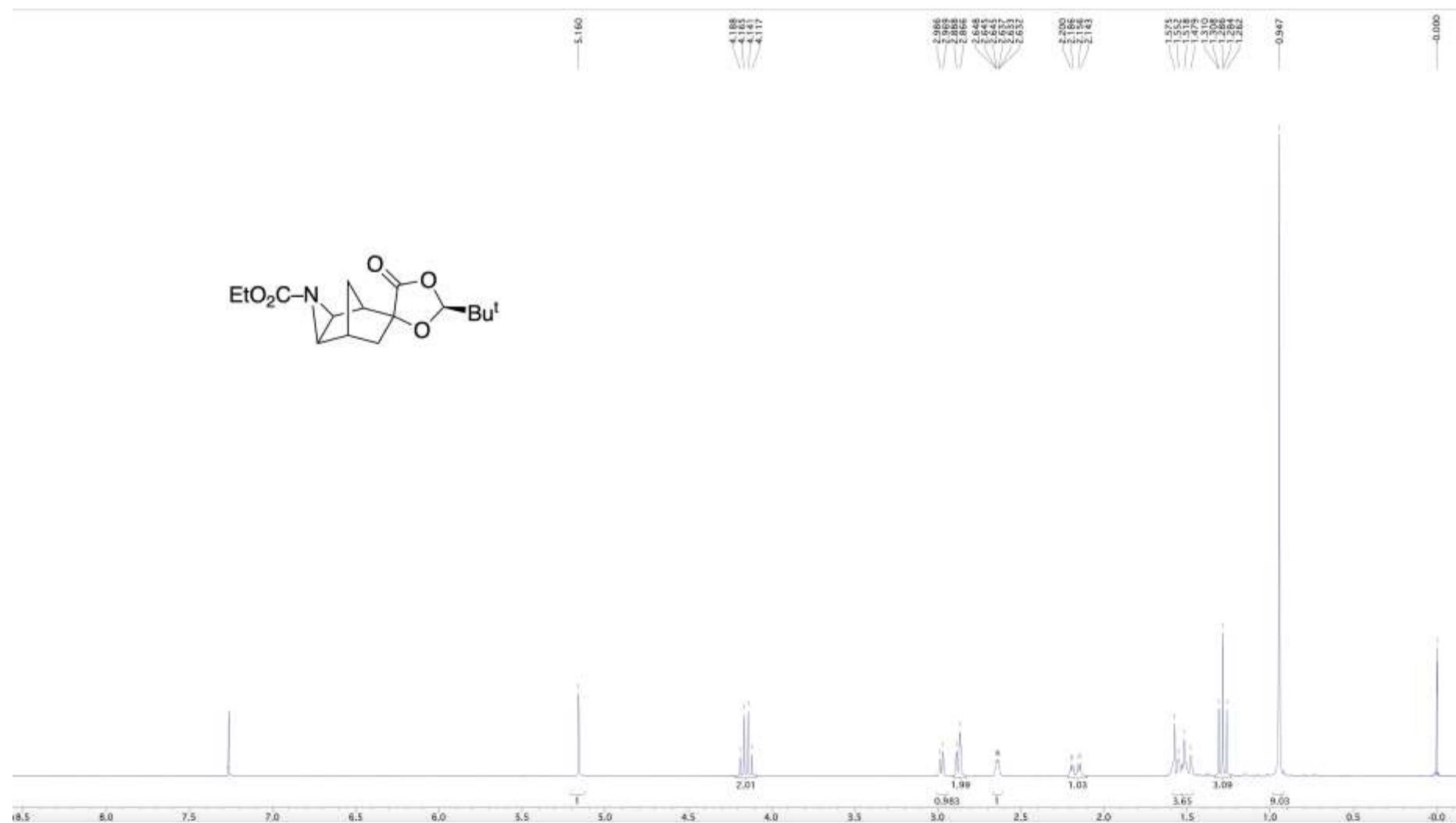


Figure S20. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **17**

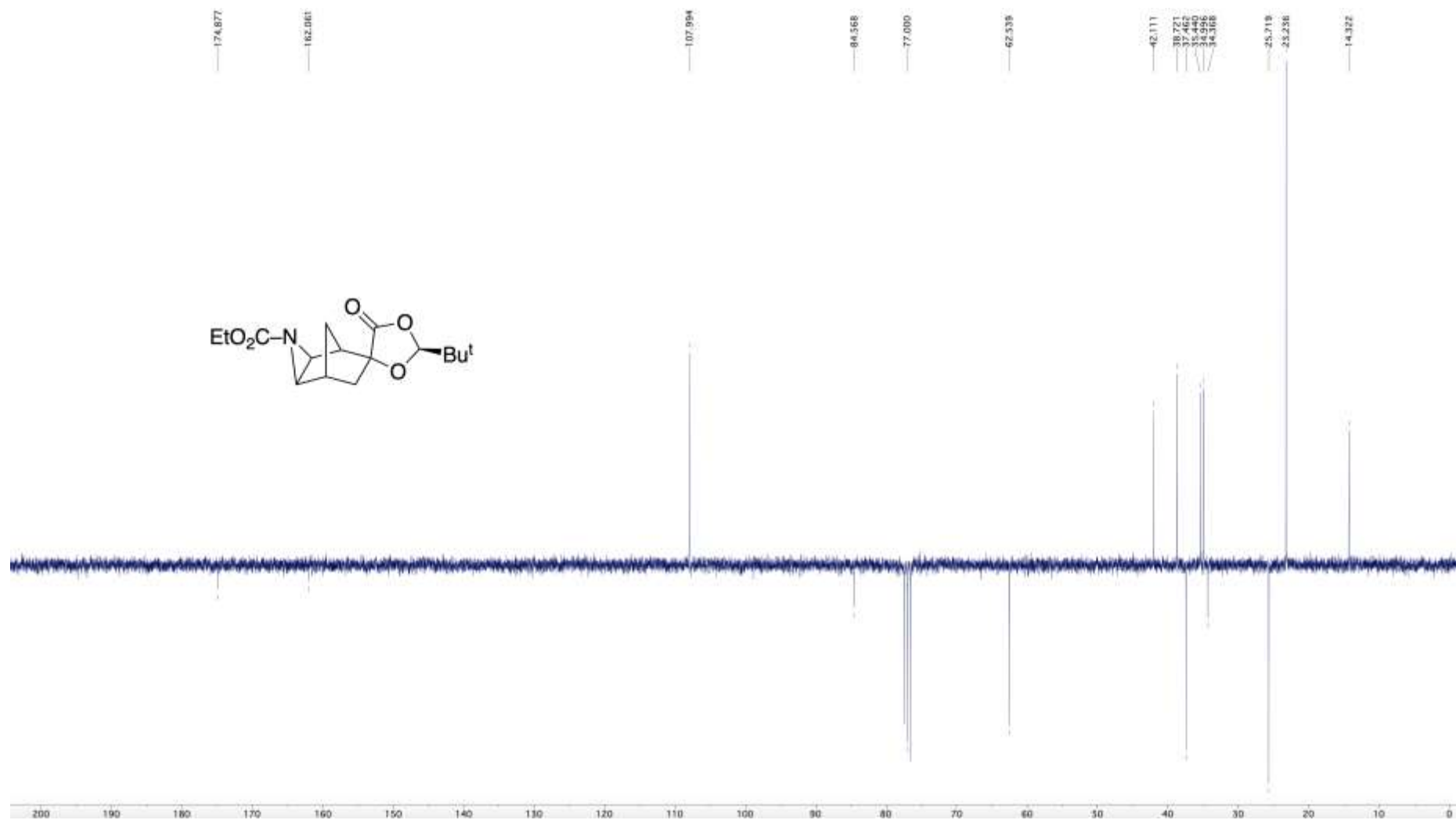


Figure S21. IR spectrum of **17**

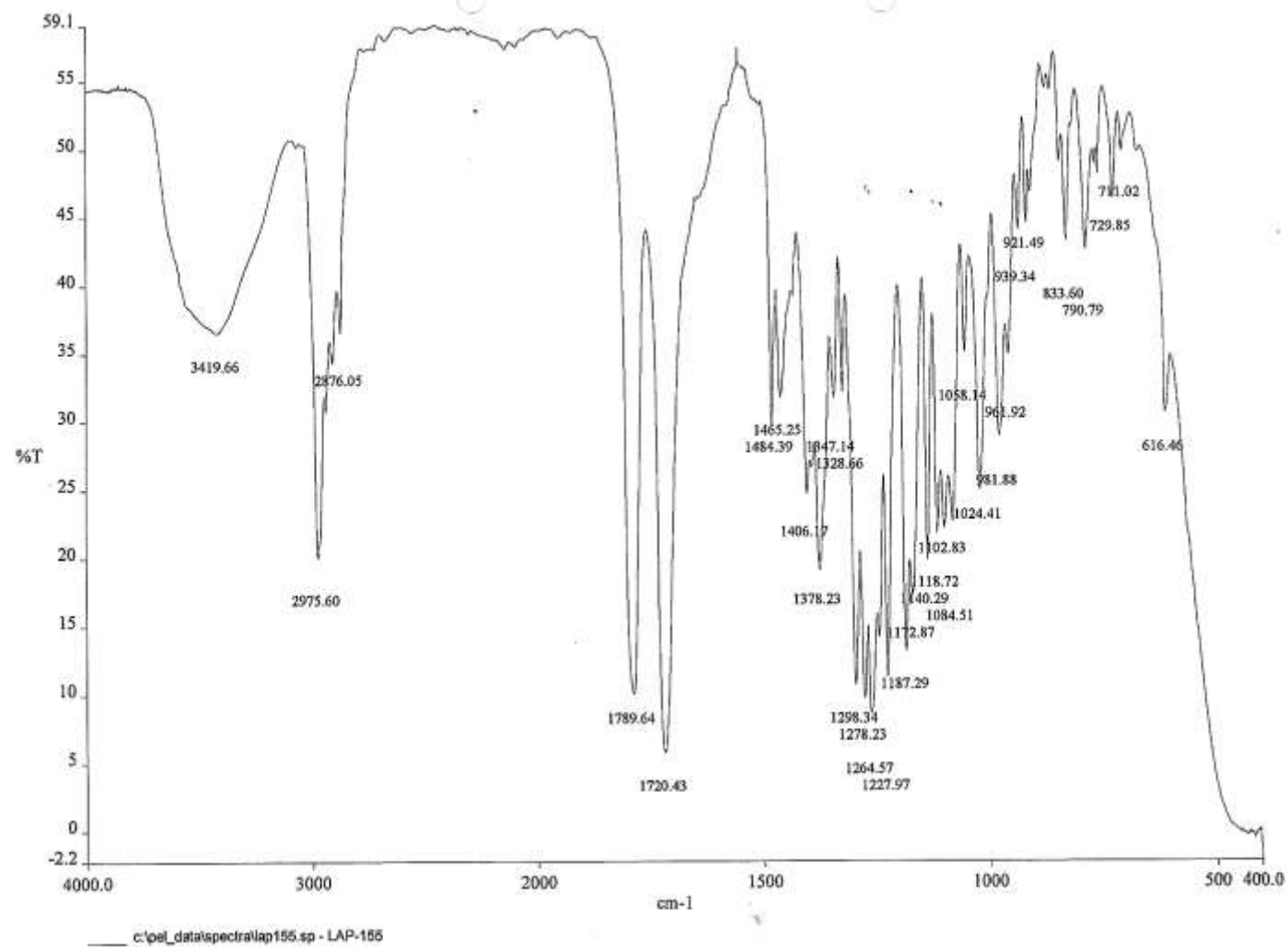
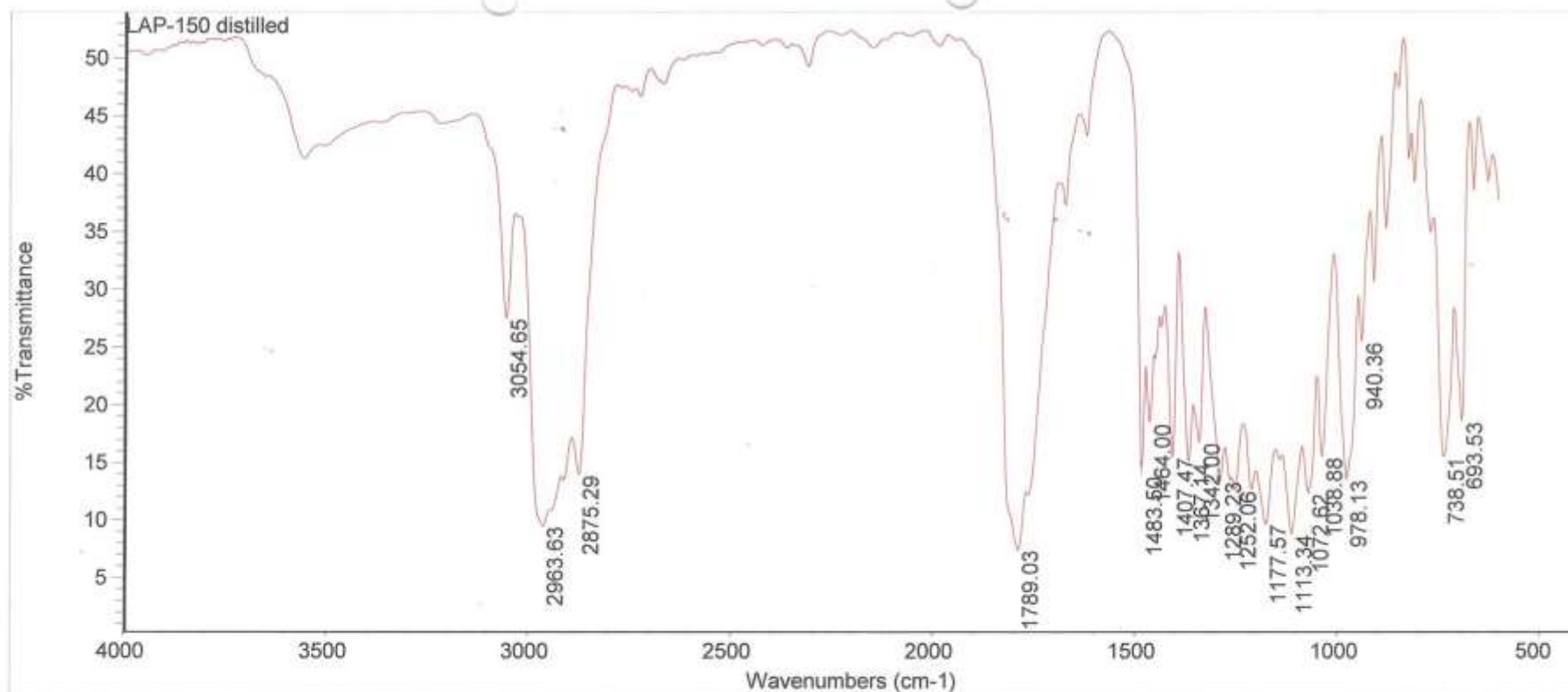


Figure S22. IR spectrum of **18**



Fri Jul 06 13:59:47 2007 (GMT+01:00)

FIND PEAKS:

Spectrum: LAP-150 distilled  
Region: 4000.00 400.00  
Absolute threshold: 29.882

Figure S23. HRMS of **18**

# Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 8 closest results for each mass)

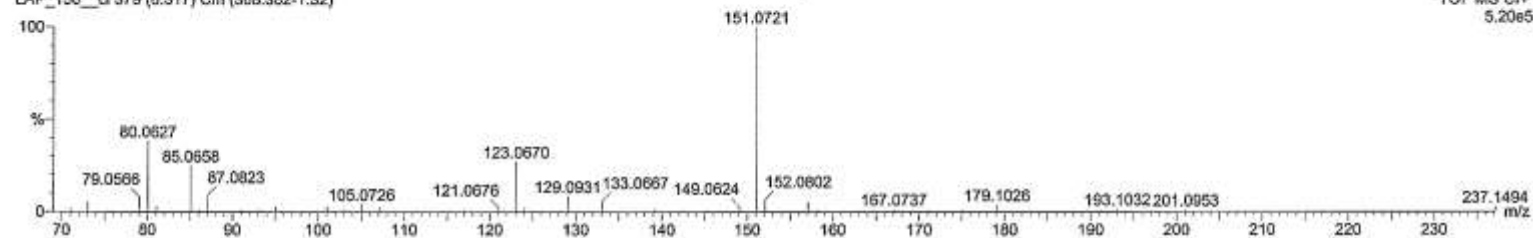
Lynn Power

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09-Jul-2007 11:44:41

LAP\_150\_ci 379 (8.317) Cm (388:382-1:32)

TOF MS Cl+  
5.20e5



Minimum: -1.5  
Maximum: 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
237.1494	237.1491	0.3	1.4	4.5	1	C14 H21 O3 + H



Figure S24. 300 MHz  $^1\text{H}$  NMR spectrum of **19**

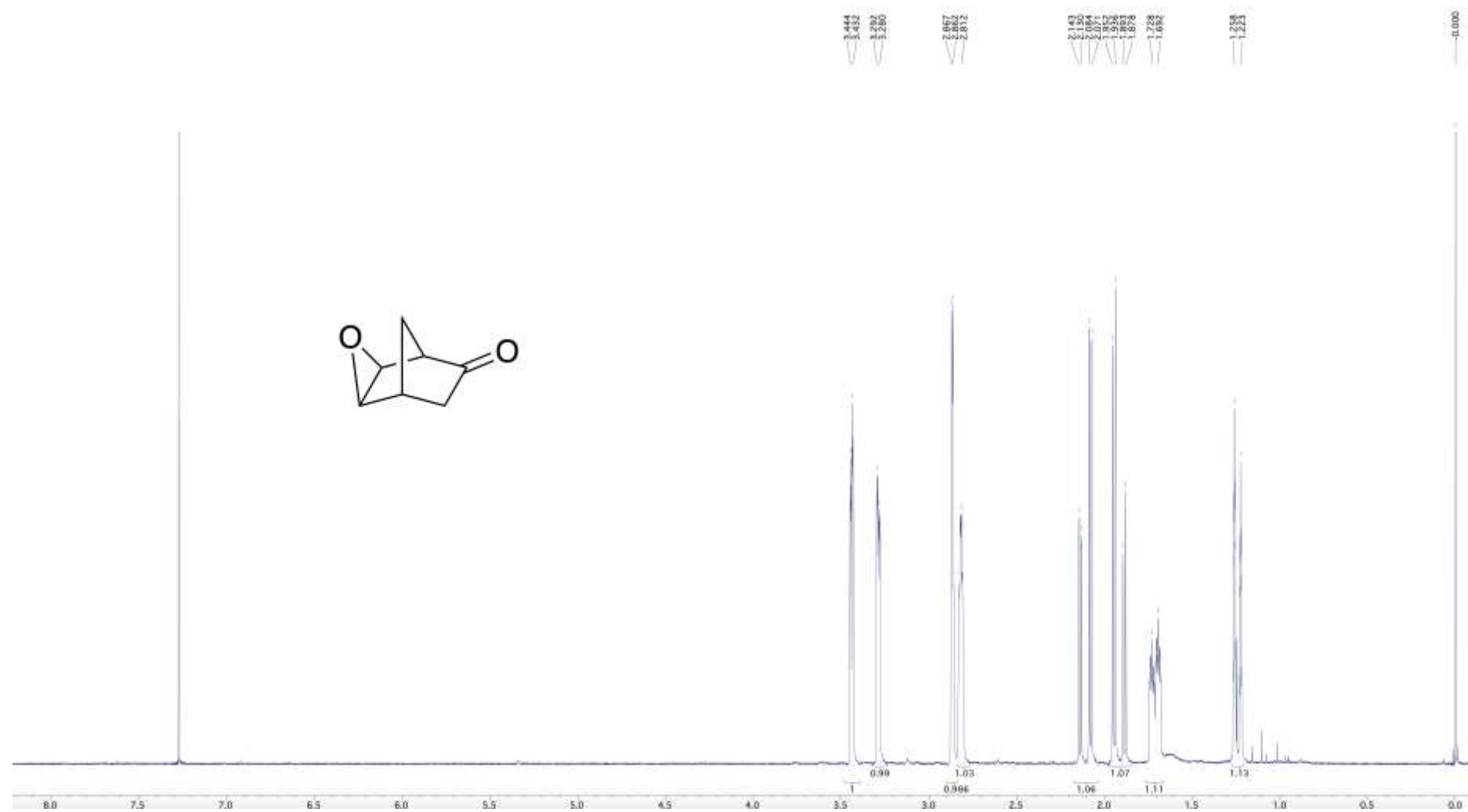


Figure S25. 300 MHz  $^1\text{H}$  NMR spectrum of **20**

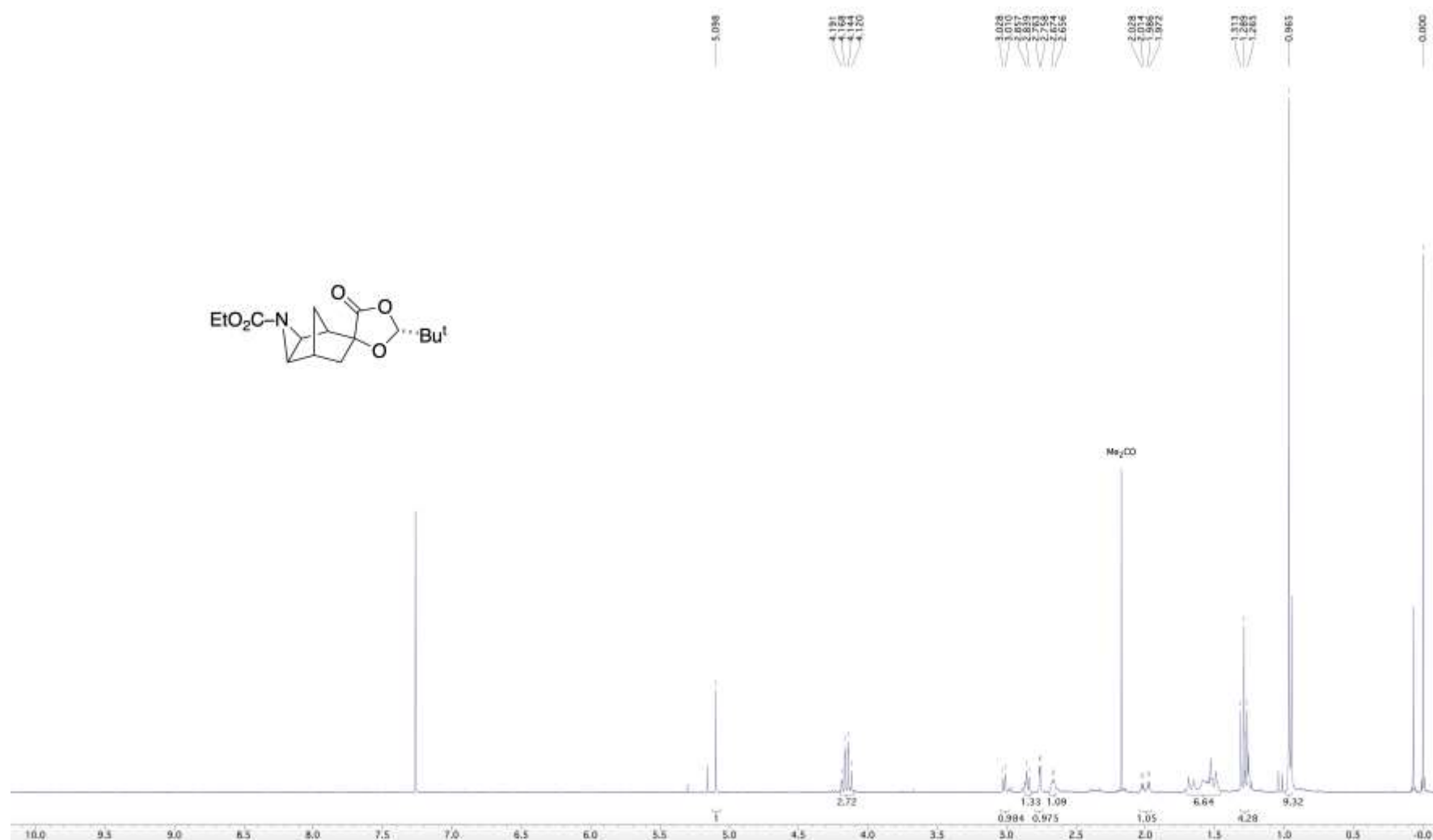


Figure S26. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **20**

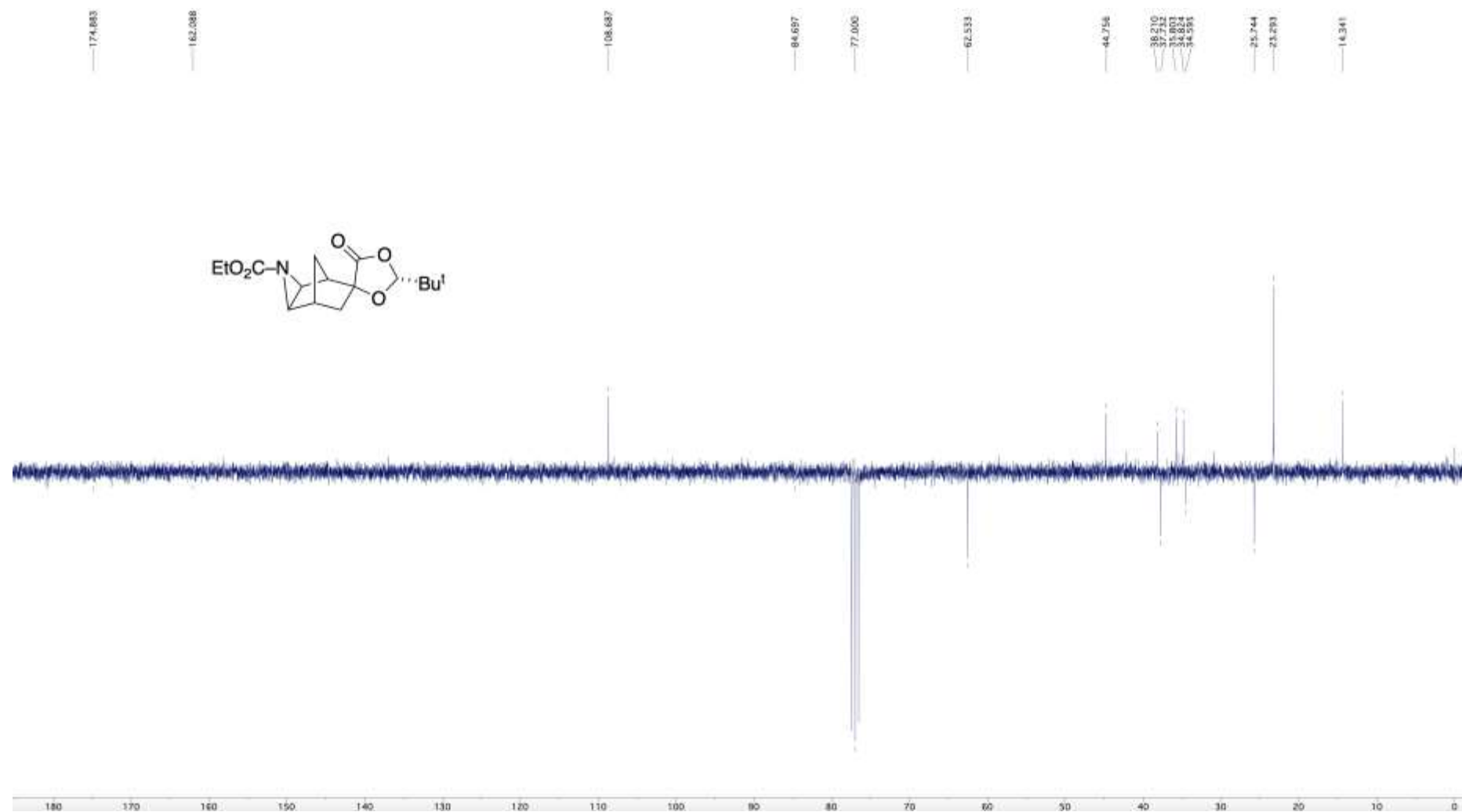


Figure S27. HRMS of **20**

# Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

65 formula(e) evaluated with 10 results within limits (up to 8 closest results for each mass)

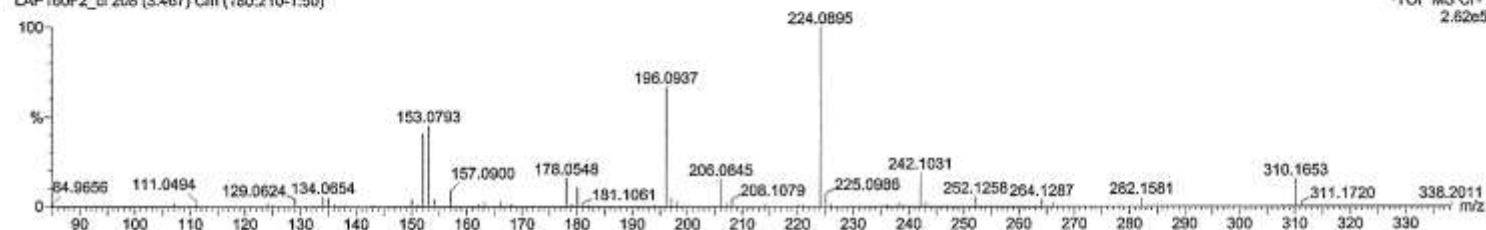
Lynn Power

University of St-Andrews  
School of Chemistry GCTOF

12-Sep-2007 11:12:58

LAP160F2\_ci 208 (3.467) Cm (180:210-1:50)

TOF MS CI+  
2.62e5



Minimum: -1.5  
Maximum: 200.0 50.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
310.1653	310.1654	-0.1	-0.5	5.5	5	C16 H24 N O5
	310.1681	-2.8	-9.1	10.0	7	C19 H22 N2 O2
	310.1614	3.9	12.5	1.5	1	C11 H24 N3 O7
	310.1569	8.4	27.1	10.0	8	C20 H22 O3
	310.1740	-8.7	-28.1	1.0	2	C12 H26 N2 O7
	310.1556	9.7	31.4	10.5	6	C18 H20 N3 O2
	310.1767	-11.4	-36.7	5.5	4	C15 H24 N3 O4
	310.1529	12.4	40.1	6.0	3	C15 H22 N2 O5

Figure S28. 300 MHz  $^1\text{H}$  NMR spectrum of **21**

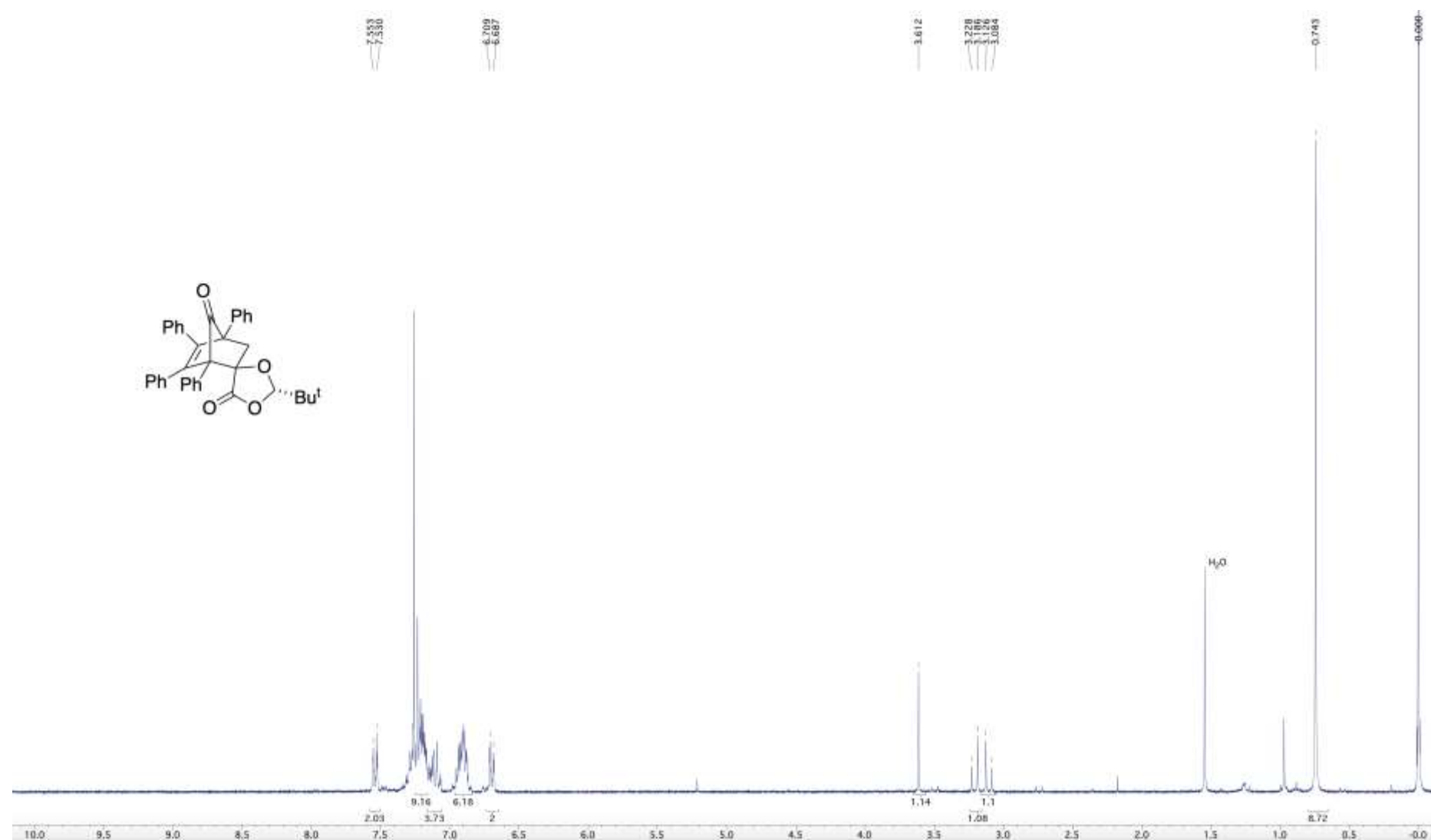


Figure S29. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **21**

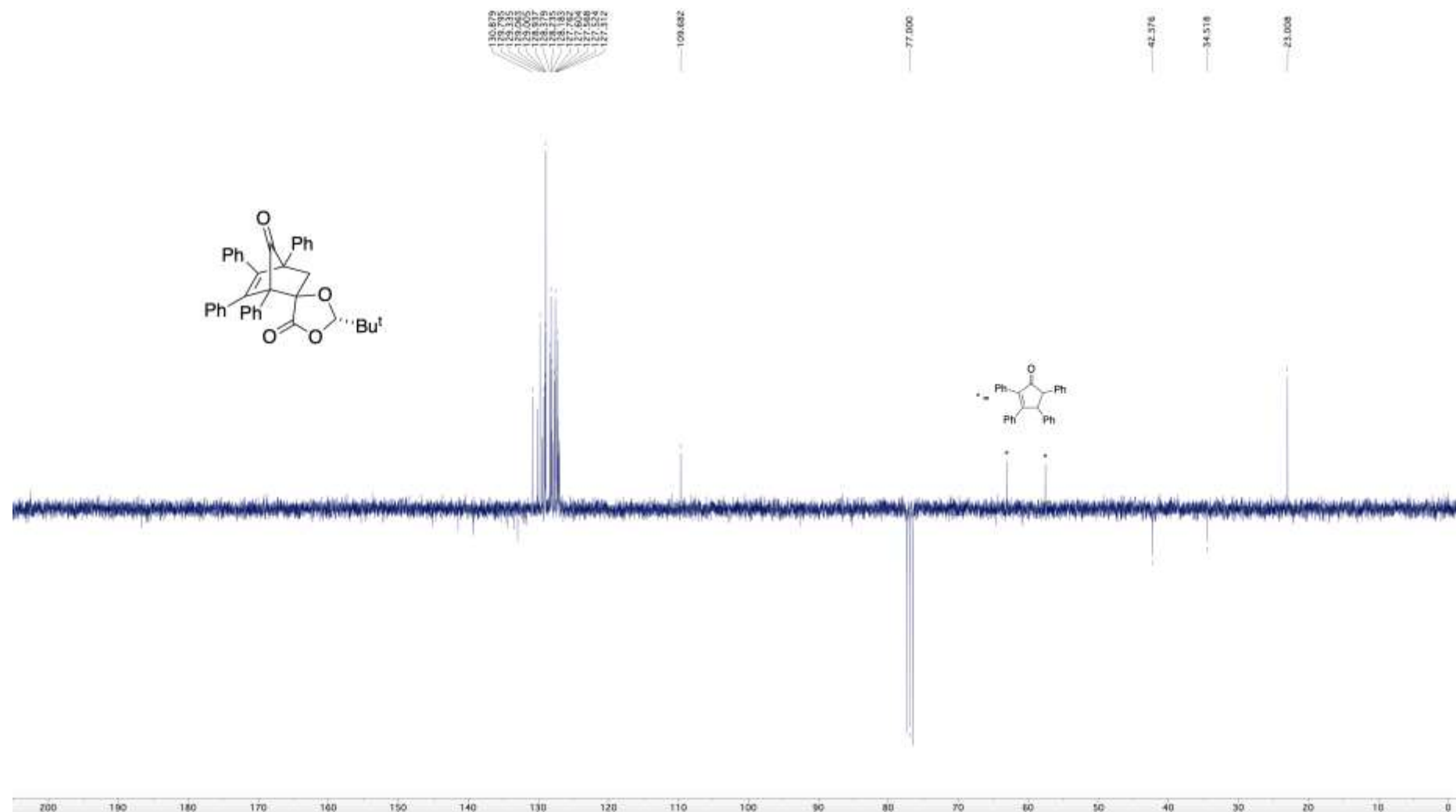


Figure S30. IR spectrum of **21**

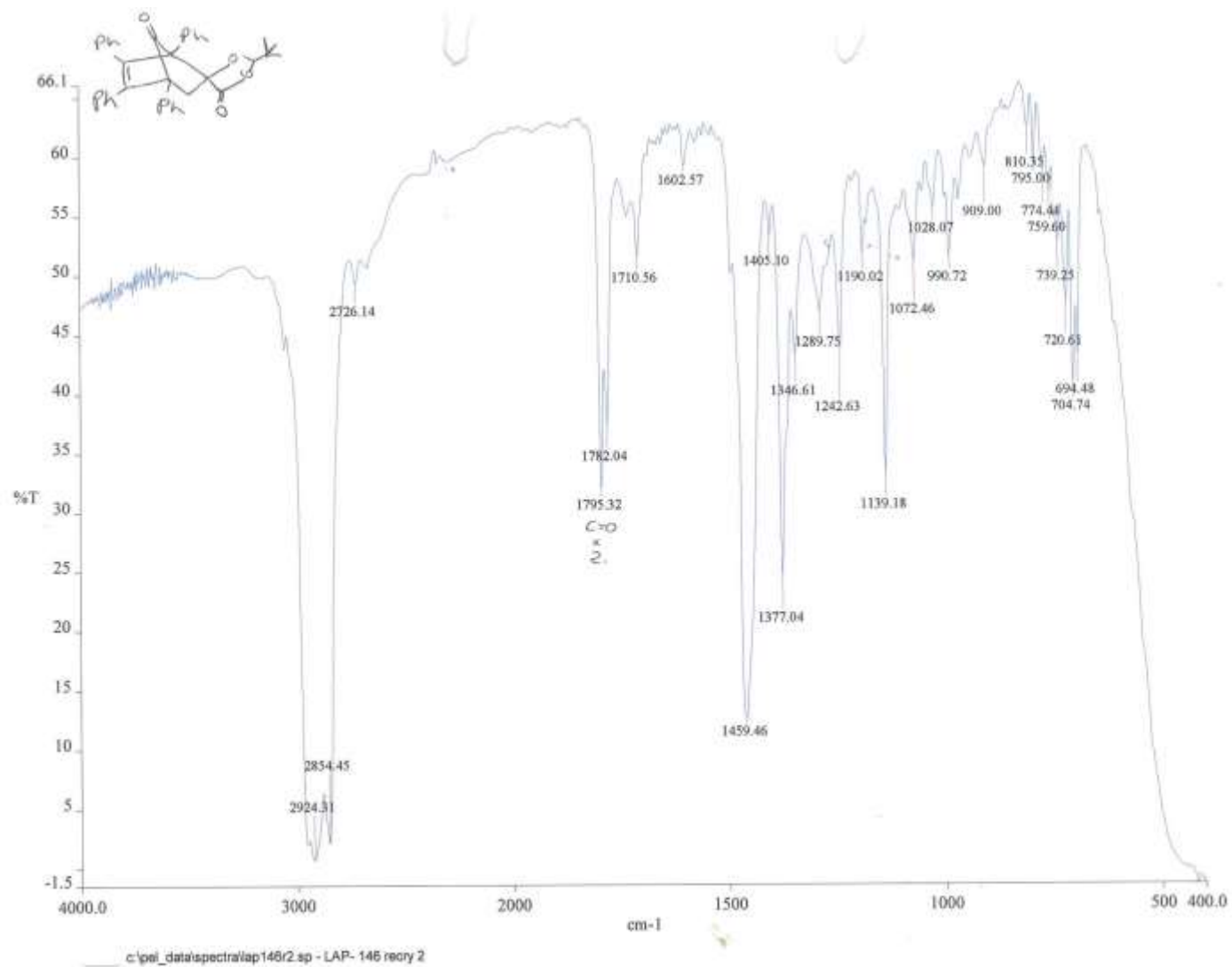


Figure S31. HRMS of 21

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

27 formula(e) evaluated with 5 results within limits (up to 8 closest results for each mass)

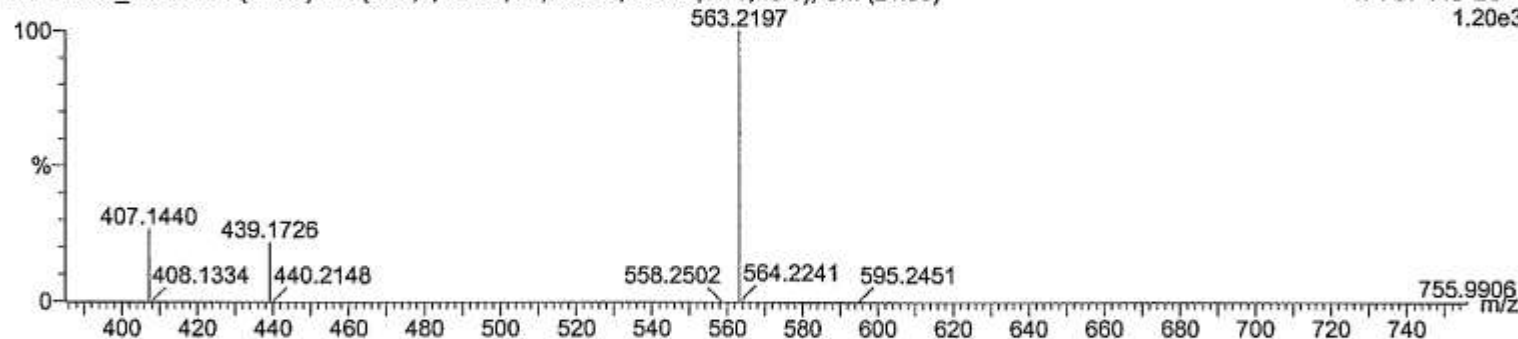
Lynn Power

University of St-Andrews  
School of Chemistry LCTOF

10-Mar-2006 10:24:05

LAP146fr6\_14am3 21 (0.402) AM (Cen,2, 80.00, Ar,7000.0,556.28,0.76,LS 5); Cm (21:30)

1: TOF MS ES+  
1.20e3



Minimum: -1.5

Maximum: 200.0 50.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
563.2197	563.2198	-0.2	-0.3	21.5	3	C37 H32 O4 Na
	563.2222	-2.6	-4.6	24.5	4	C39 H31 O4
	563.1987	21.0	37.2	26.5	5	C40 H28 O2 Na
	563.2410	-21.3	-37.8	16.5	1	C34 H36 O6 Na
	563.2434	-23.7	-42.1	19.5	2	C36 H35 O6



Figure S32. 300 MHz  $^1\text{H}$  NMR spectrum of **22a**

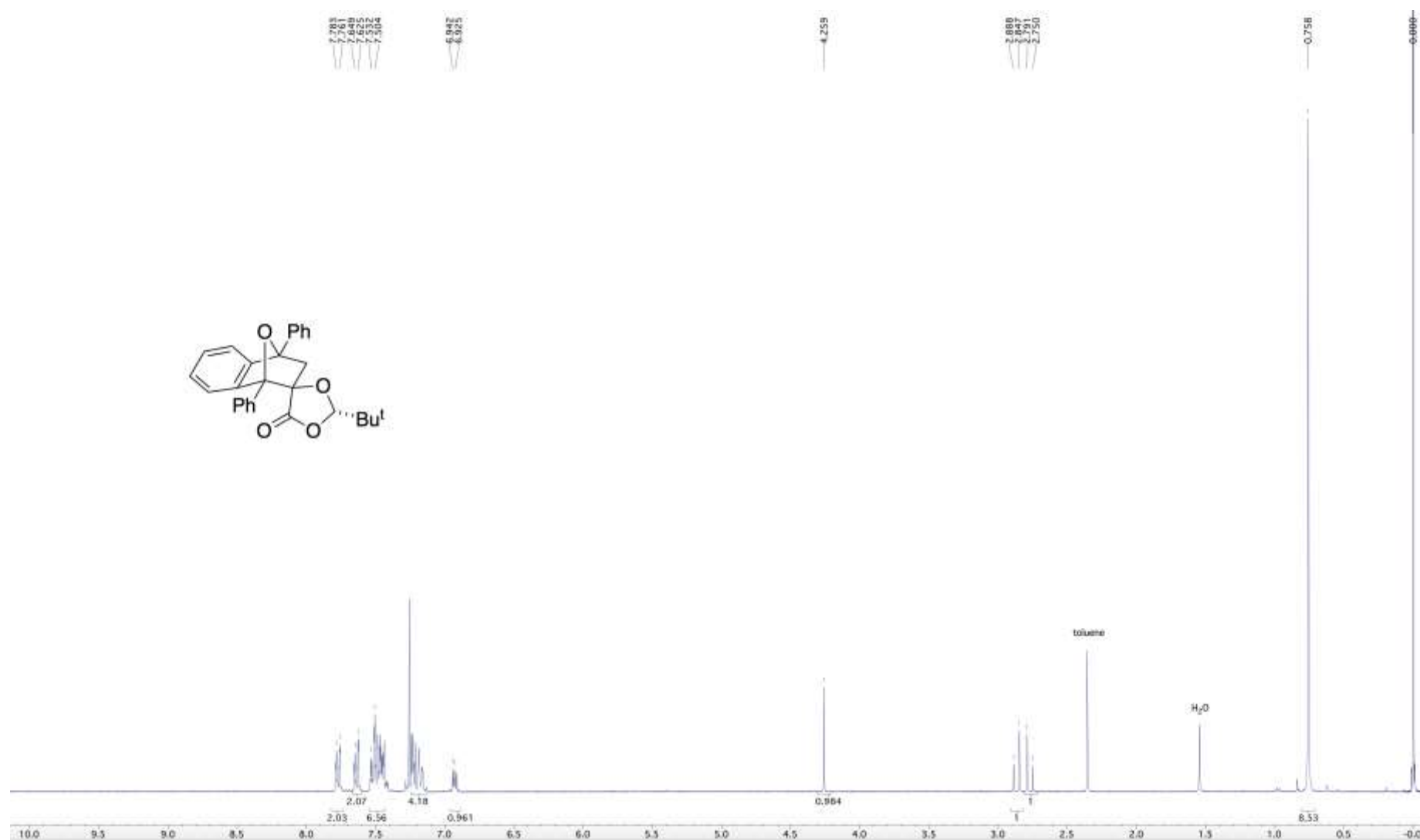


Figure S33. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **22a**

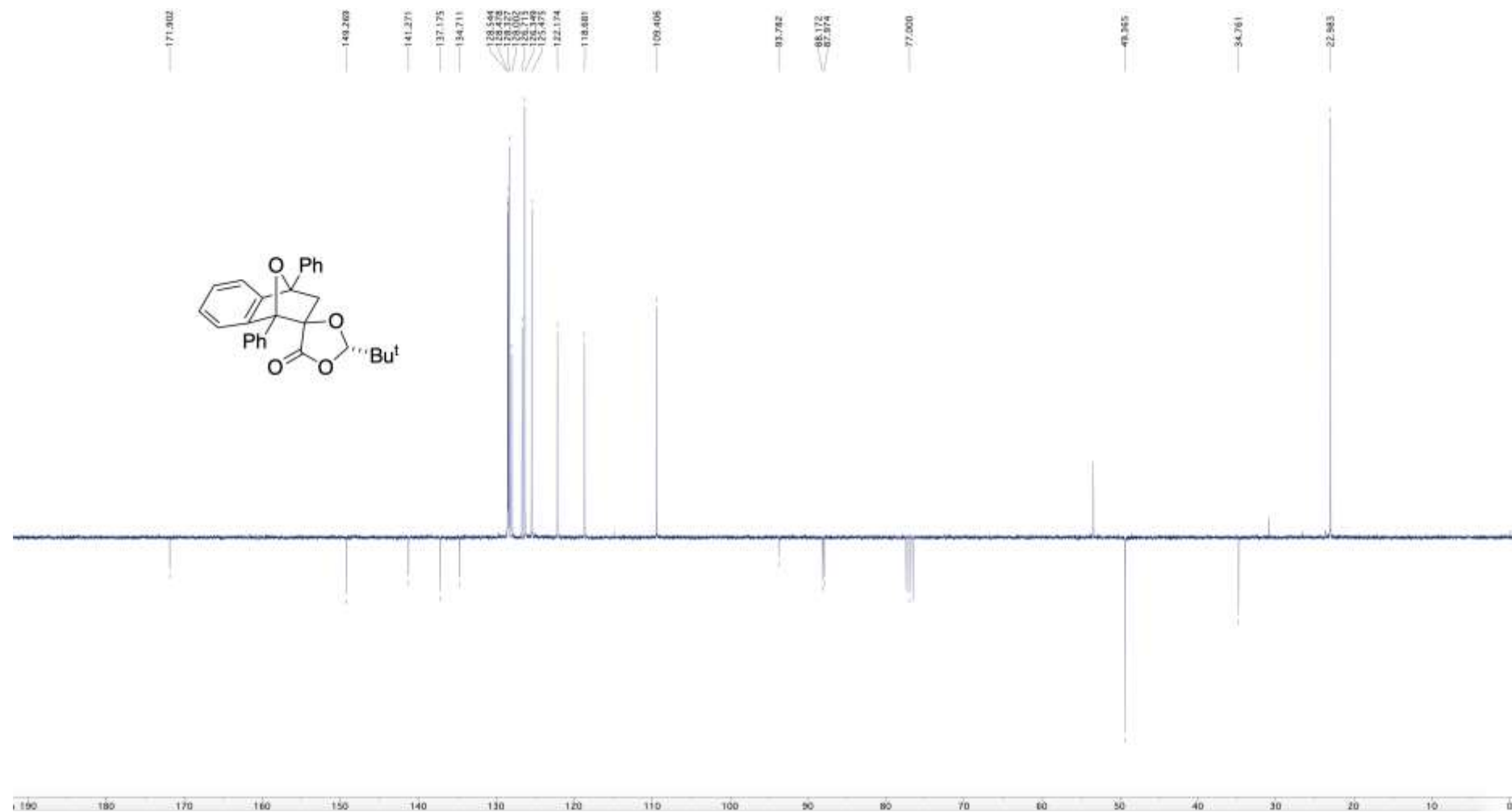


Figure S34. IR spectrum of **22a**

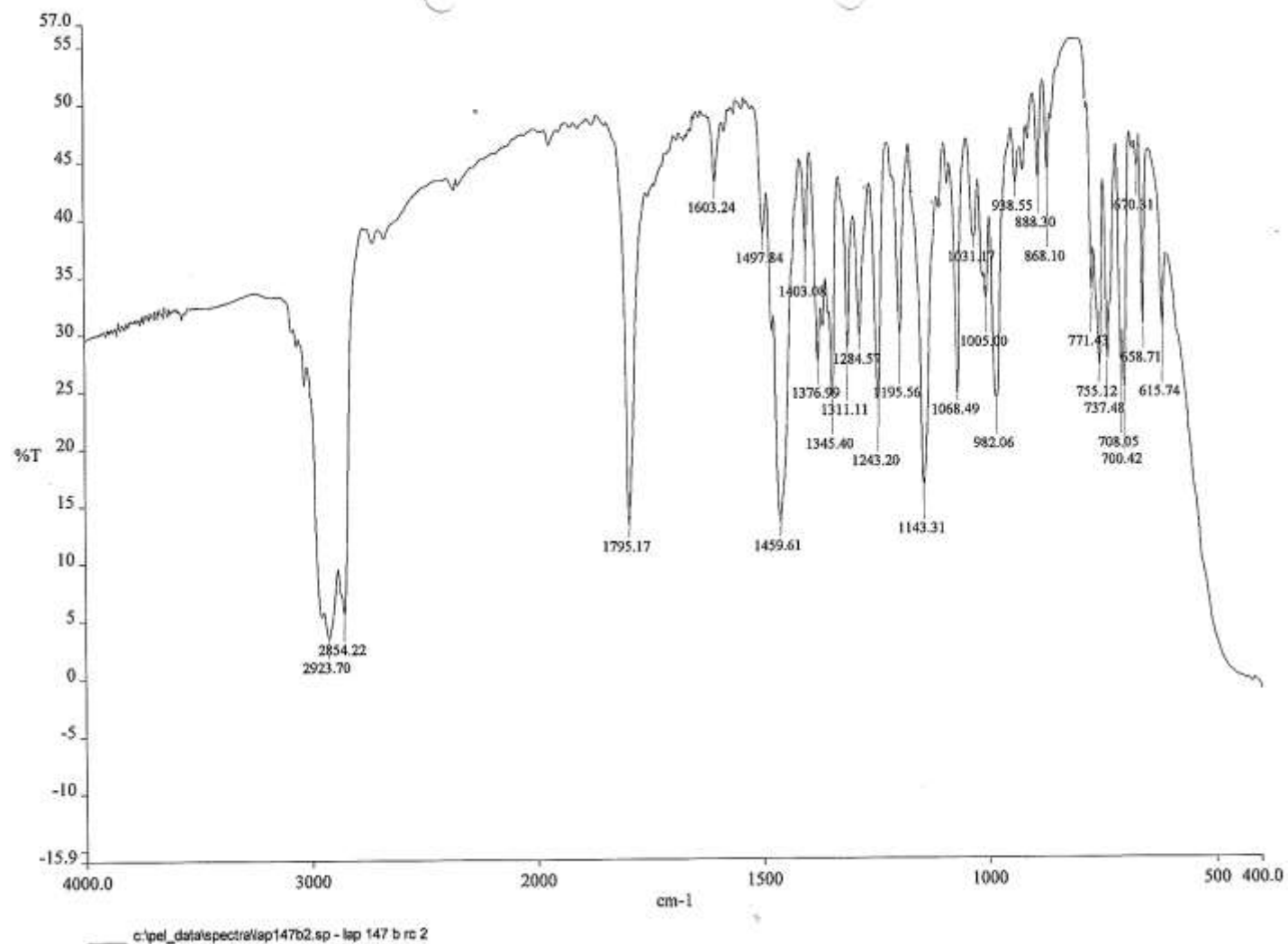


Figure S35. 300 MHz  $^1\text{H}$  NMR spectrum of **24**

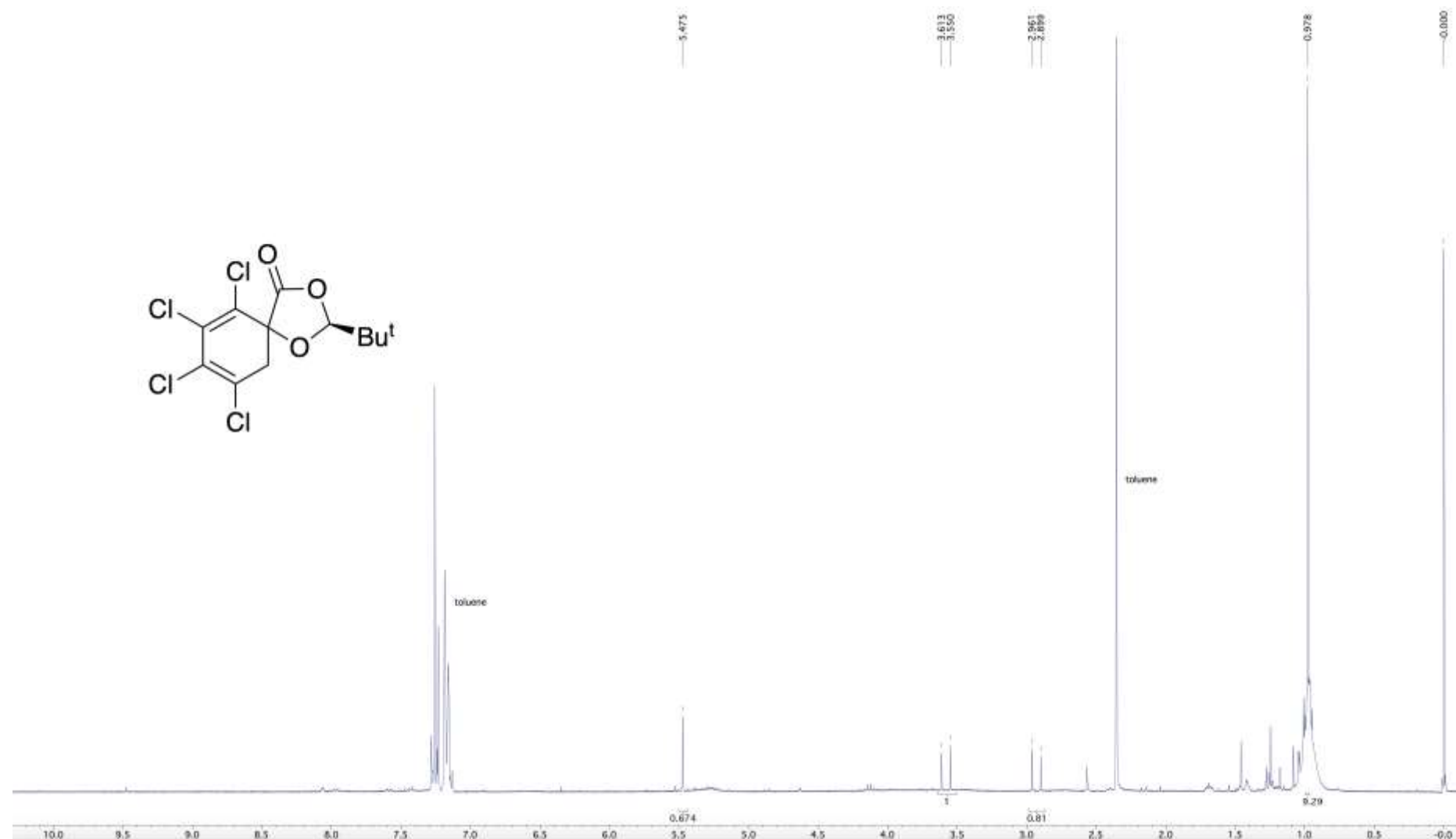


Figure S36. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **24**

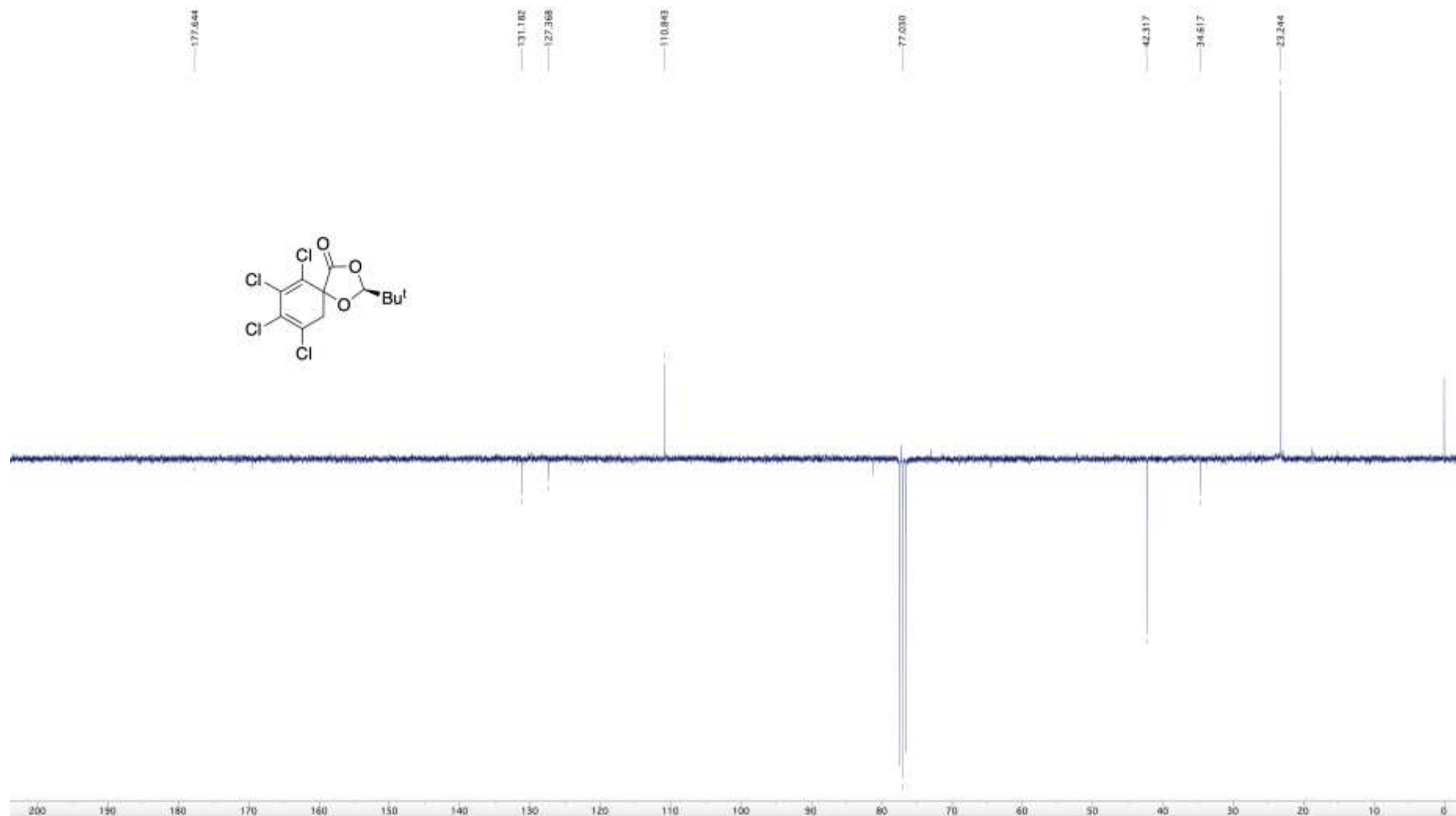


Figure 37. IR spectrum of **24**

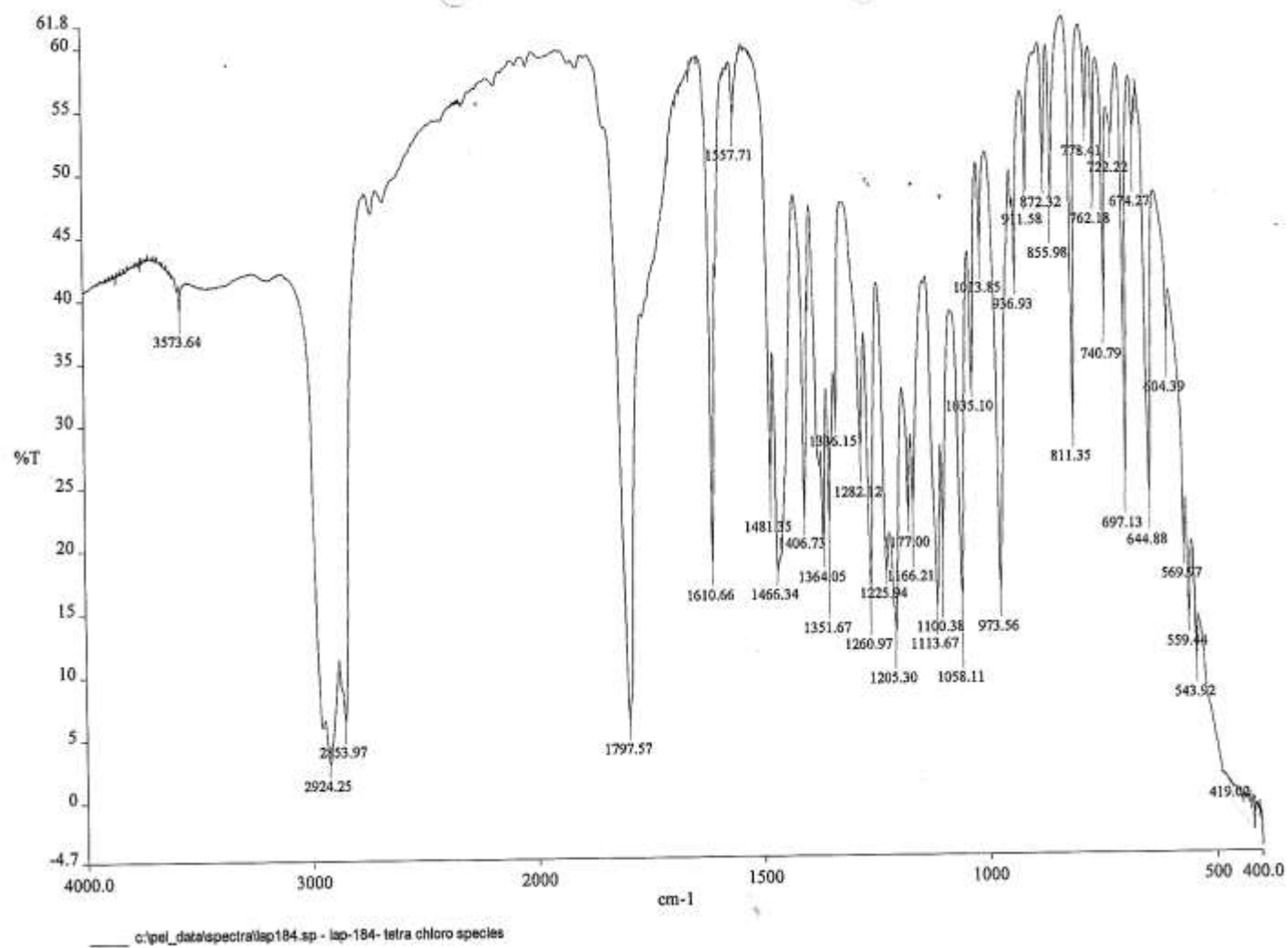


Figure S38. 300 MHz  $^1\text{H}$  NMR spectrum of **25**

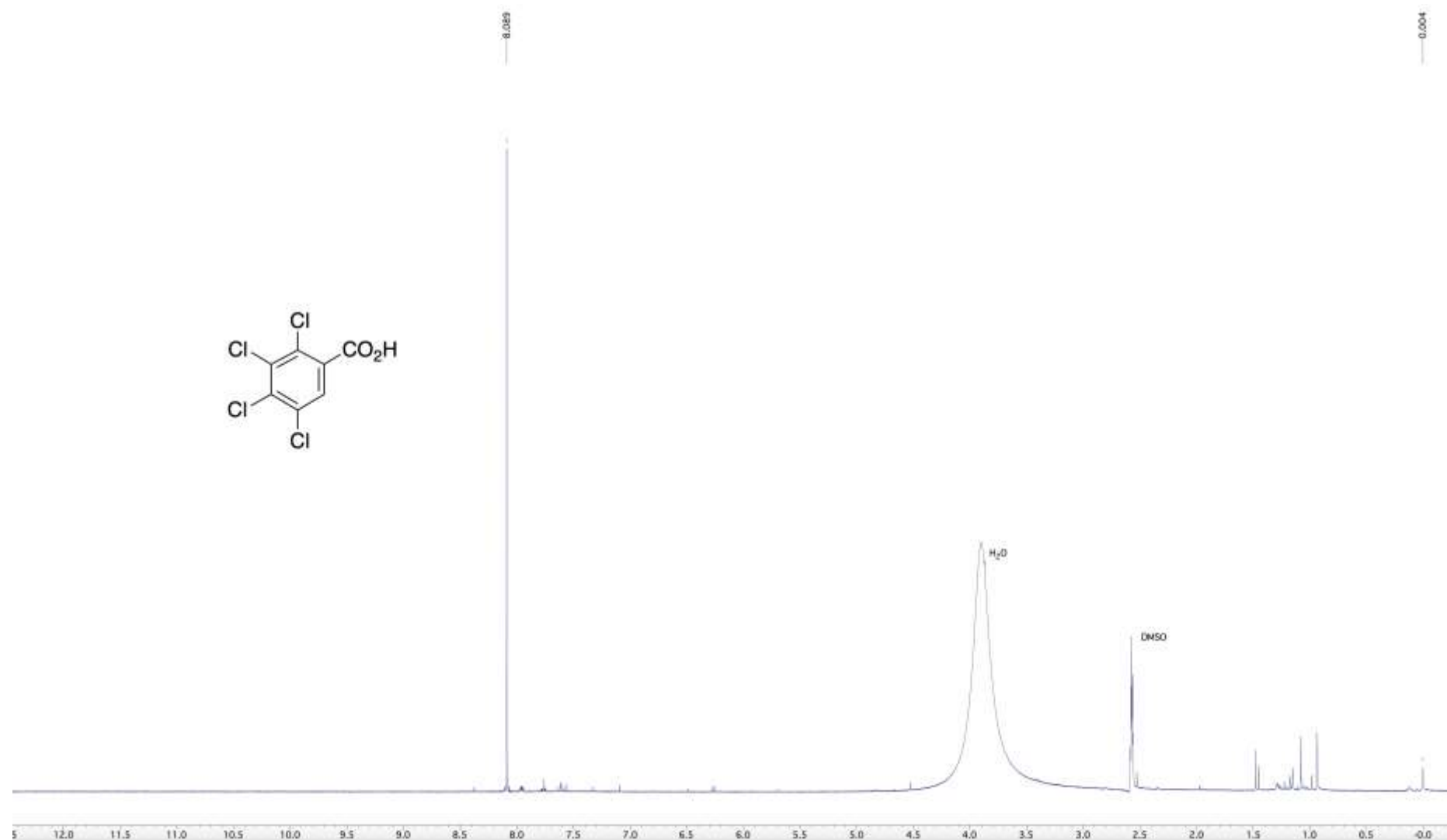


Figure S39. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **25**

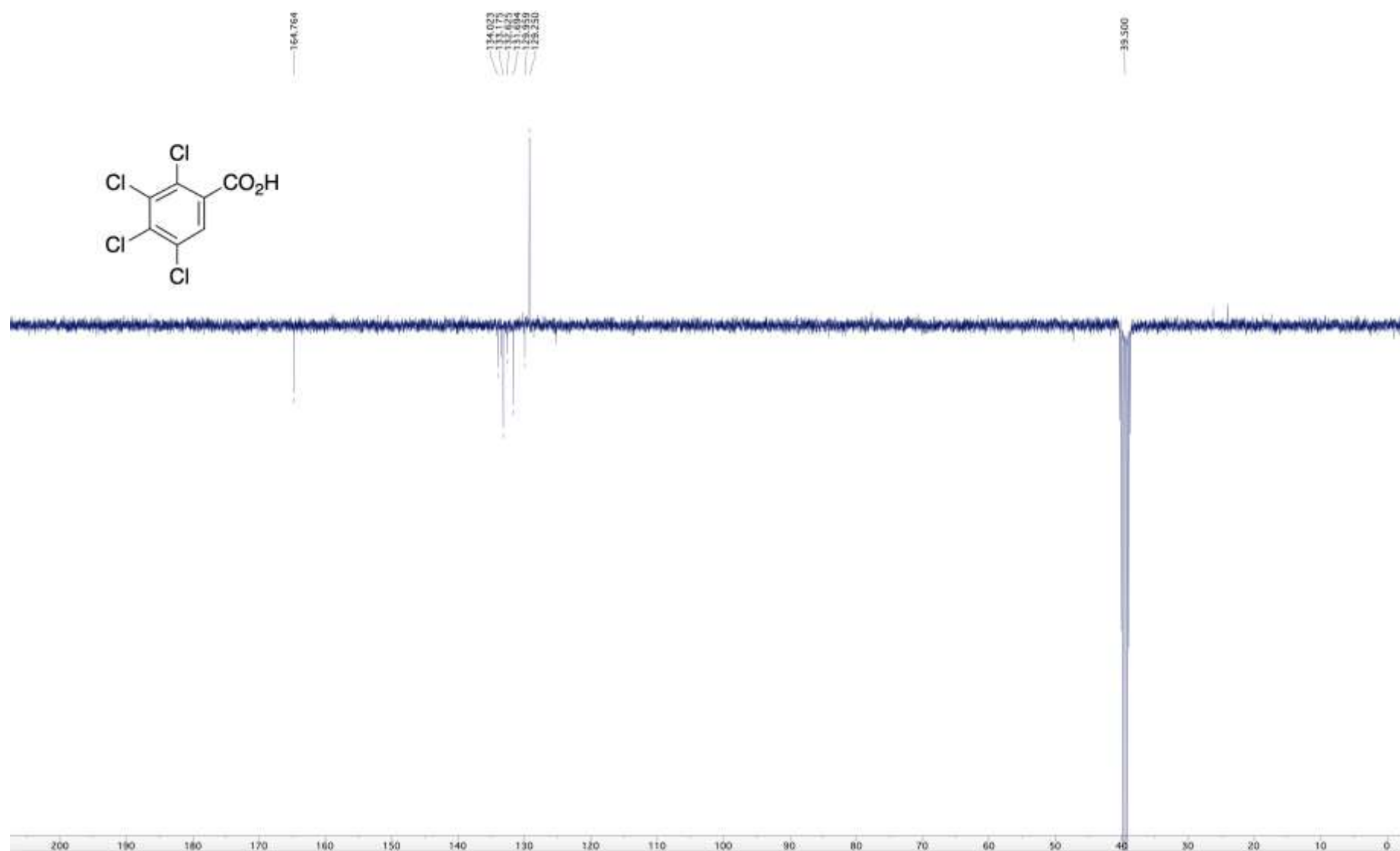




Figure S40. 300 MHz  $^1\text{H}$  NMR spectrum of **27**

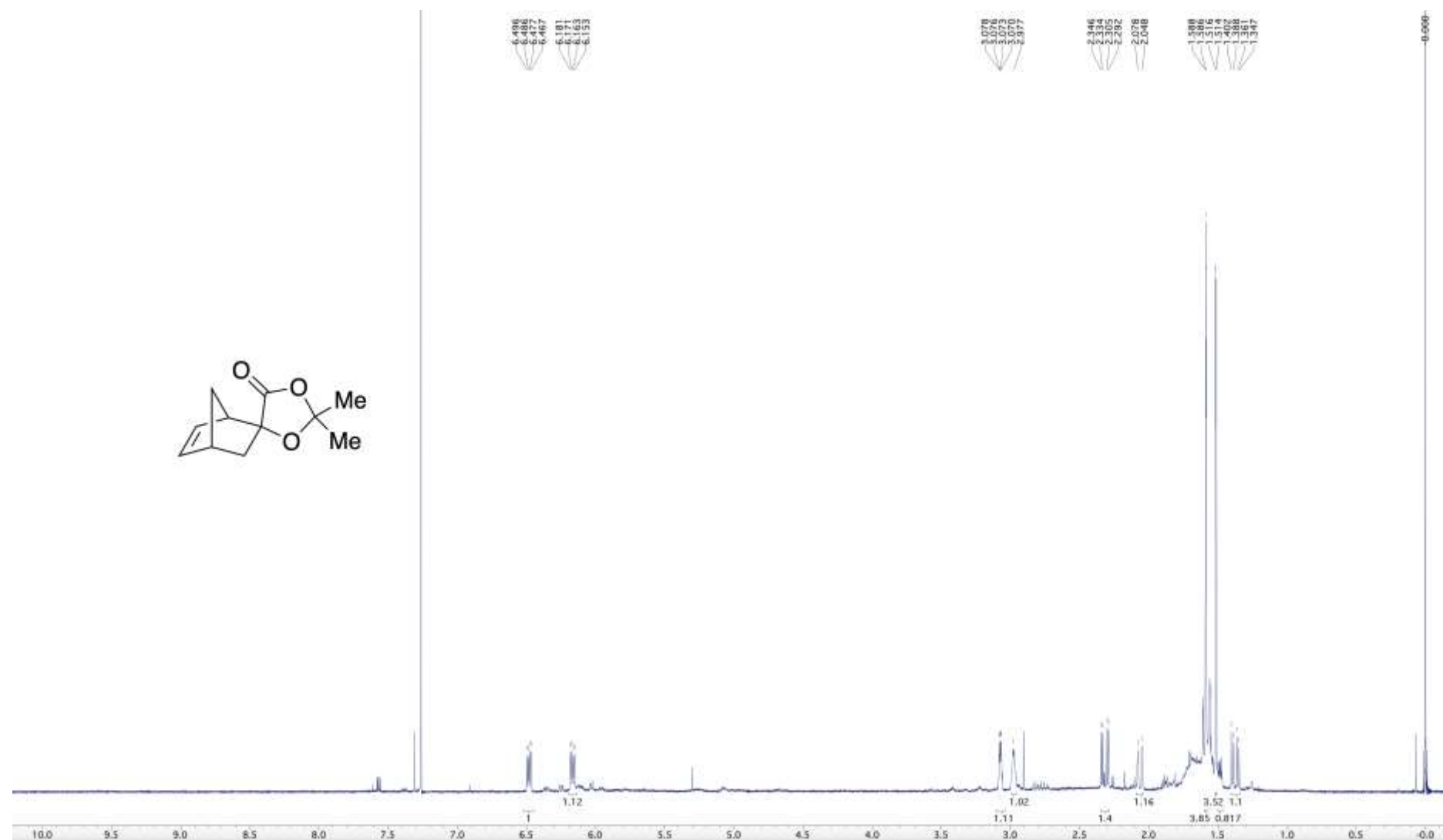


Figure S41. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **27**

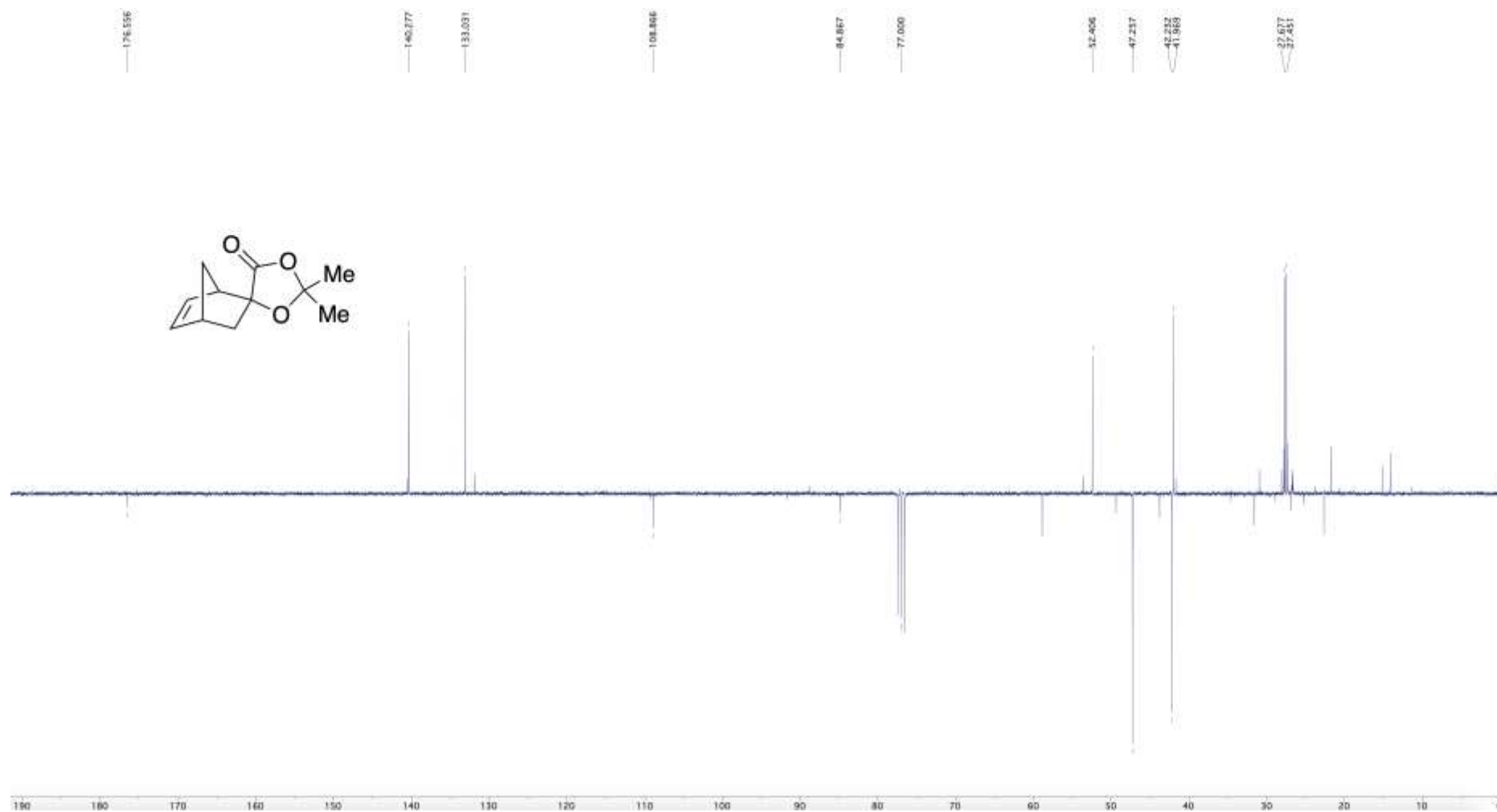


Figure S42. 300 MHz  $^1\text{H}$  NMR spectrum of **28**

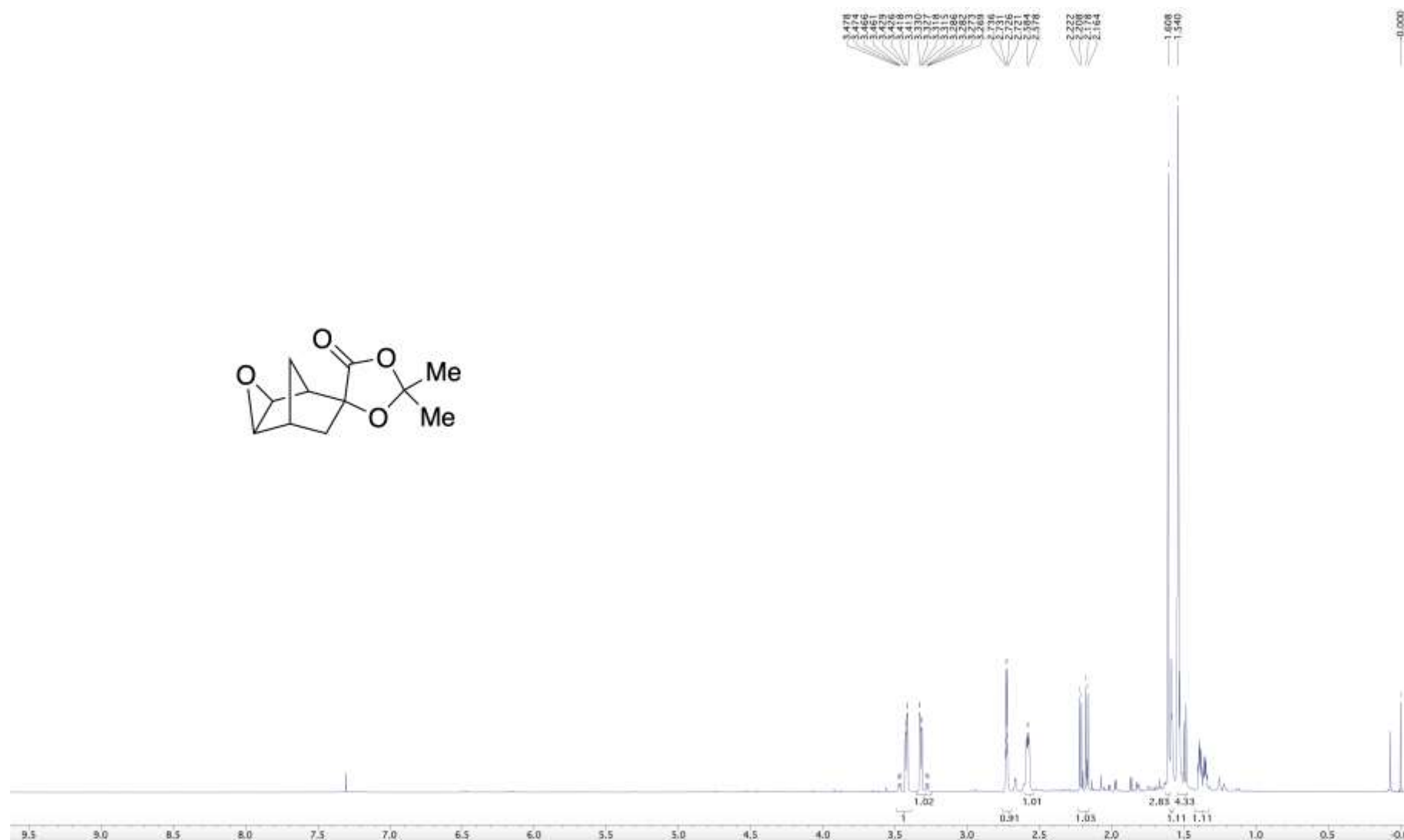


Figure S43. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **28**

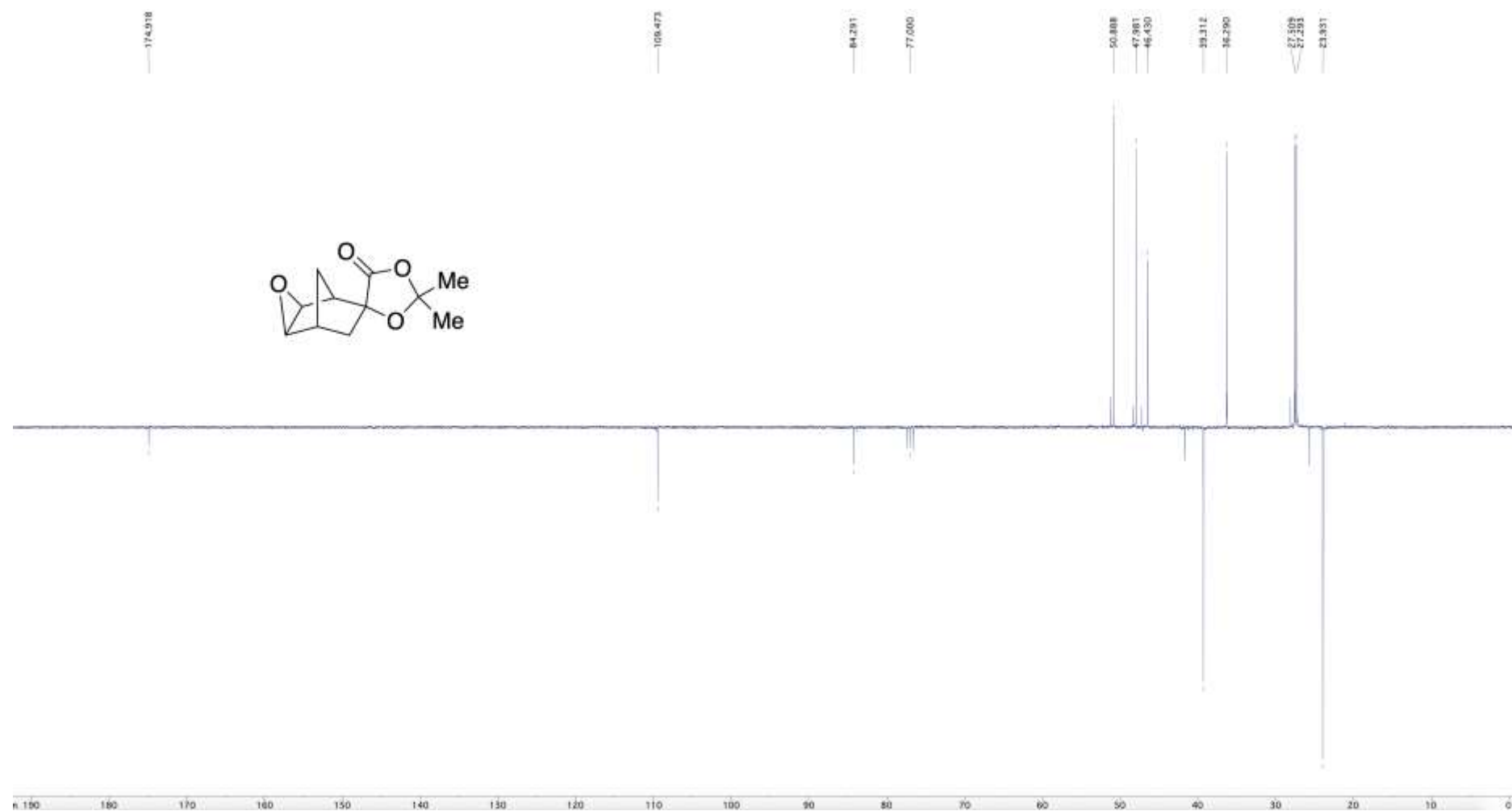


Figure S44. HRMS of 28

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 40.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

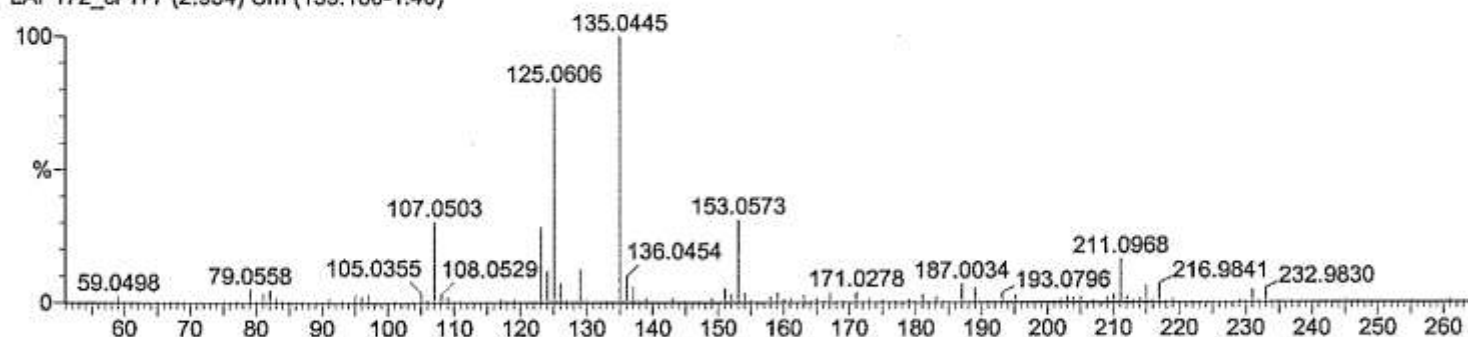
Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 8 closest results for each mass)

Lynn Power

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School of Chemistry GCTOF

LAP172\_ci 177 (2.934) Cm (159:180-1:40)



Minimum: -1.5  
Maximum: 200.0 20.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
211.0968	211.0970	-0.2	-1.1	4.5	1	C11 H15 O4

Figure S45. 300 MHz  $^1\text{H}$  NMR spectrum of **29a**

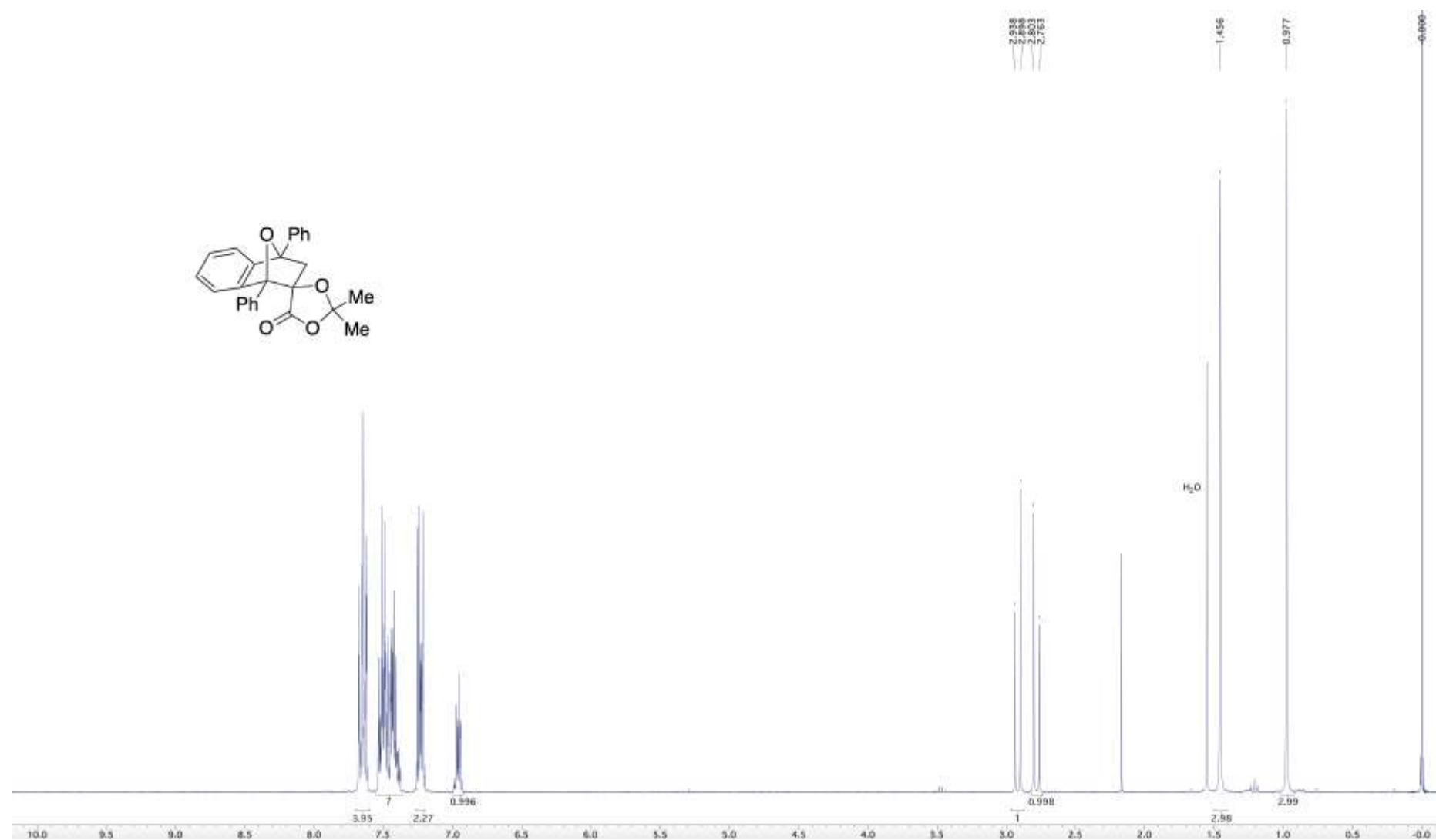


Figure S46. 75 MHz DEPTQ  $^{13}\text{C}$  NMR spectrum of **29a**

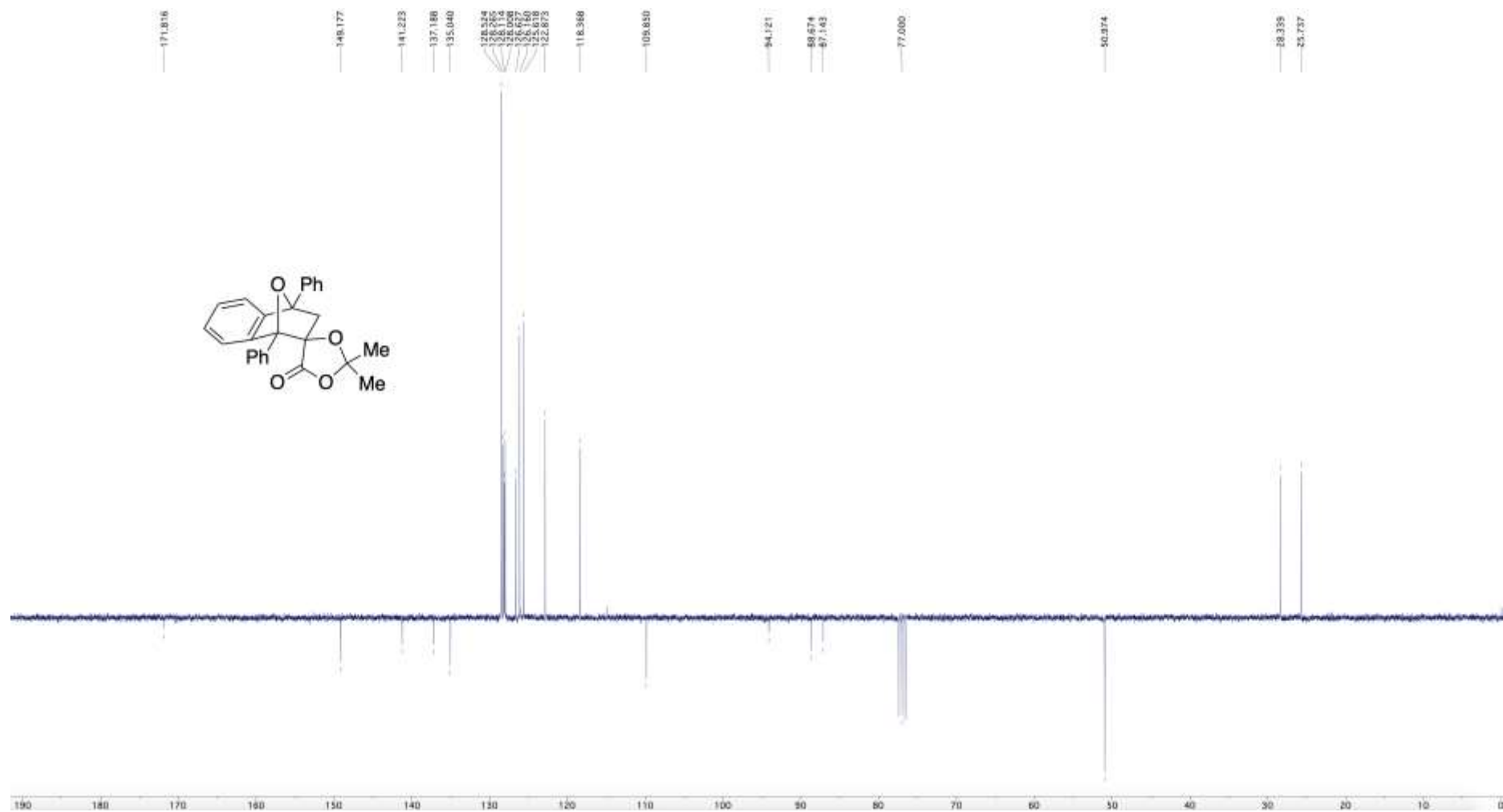


Figure S47. IR spectrum of **29a**

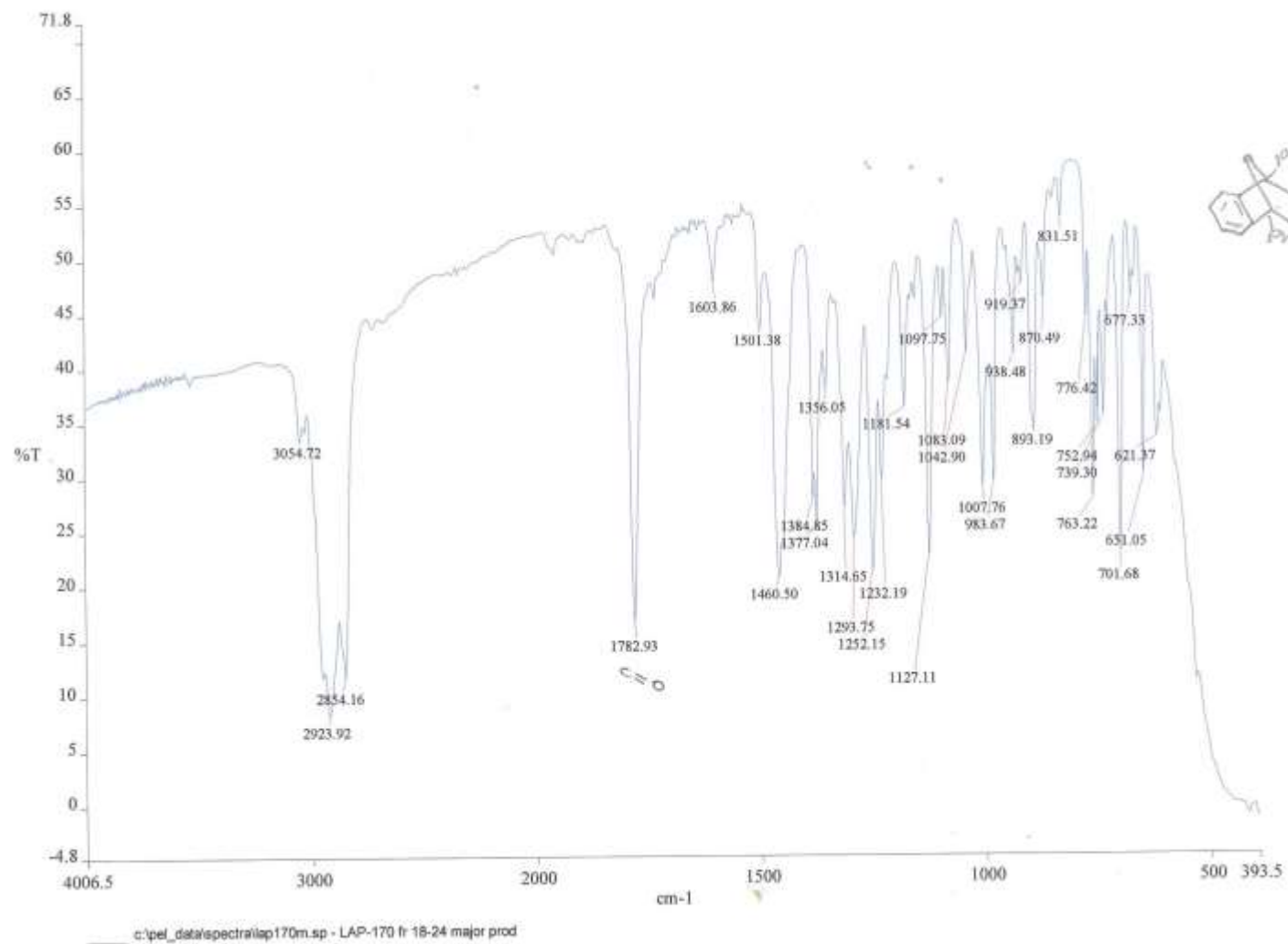




Figure S48. 300 MHz  $^1\text{H}$  NMR spectrum of **29b**

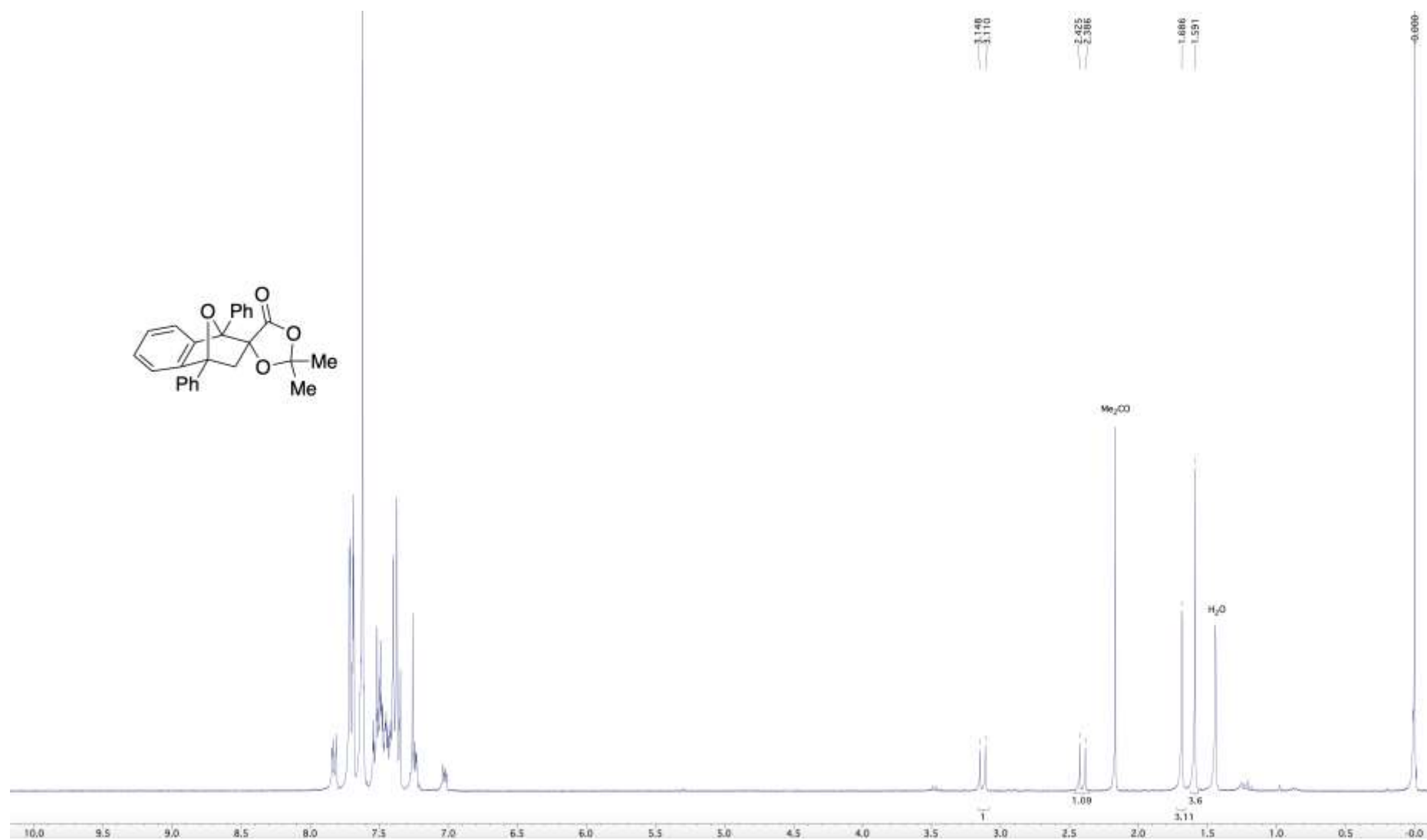


Figure S49. IR spectrum of **29b**

