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S U P P L E M E N T A R Y M A T E R I A L

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B E L O N G I N G T O T H E P A P E R

## **AMVN Mediated Expedient Synthesis of Biaryls from Unactivated Arenes and heteroarenes with Aryl Iodides**

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MP, India 462 023

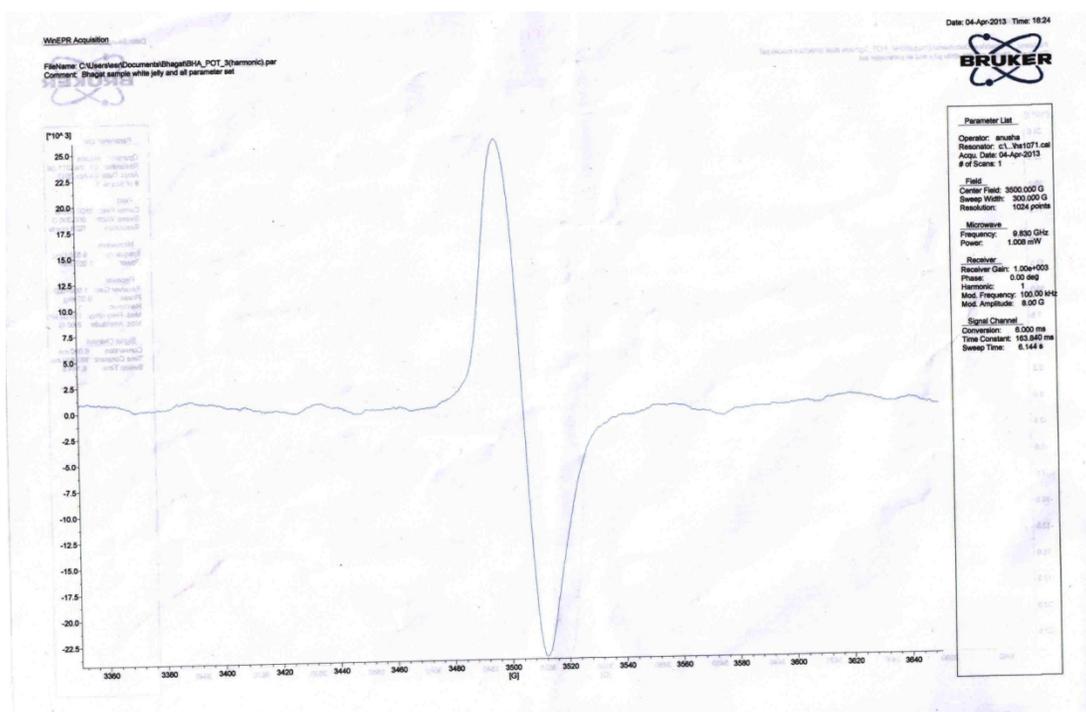
[sangitkumar@iiserb.ac.in](mailto:sangitkumar@iiserb.ac.in)

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$^1\text{H}$ , $^{13}\text{C}$ , and $^{13}\text{C}$ DEPT-135 NMR spectra for biaryls	S4-S116

## EPR Experiments on potassium *tert*-butoxide mediate intermolecular biaryl coupling.

**Sample preparation for EPR experiment:** KO<sup>t</sup>Bu (561 mg, 5.0 mmol) was heated in benzene (5 mL) in a sealed tube for 1.5 h at 110 °C. After this reaction mixture was cooled to room temperature. White color precipitate which was settled in sealed tube, was transferred to EPR tube under nitrogen. one signal was observed in EPR which suggests that the radical present in the mixture of KO<sup>t</sup>Bu and benzene. Reaction mixture of KO<sup>t</sup>Bu and benzene without any heating does not show any peak in EPR spectrum.



**Figure S1.** EPR spectrum of KO<sup>t</sup>Bu after reflux in benzene for 1.5 h.

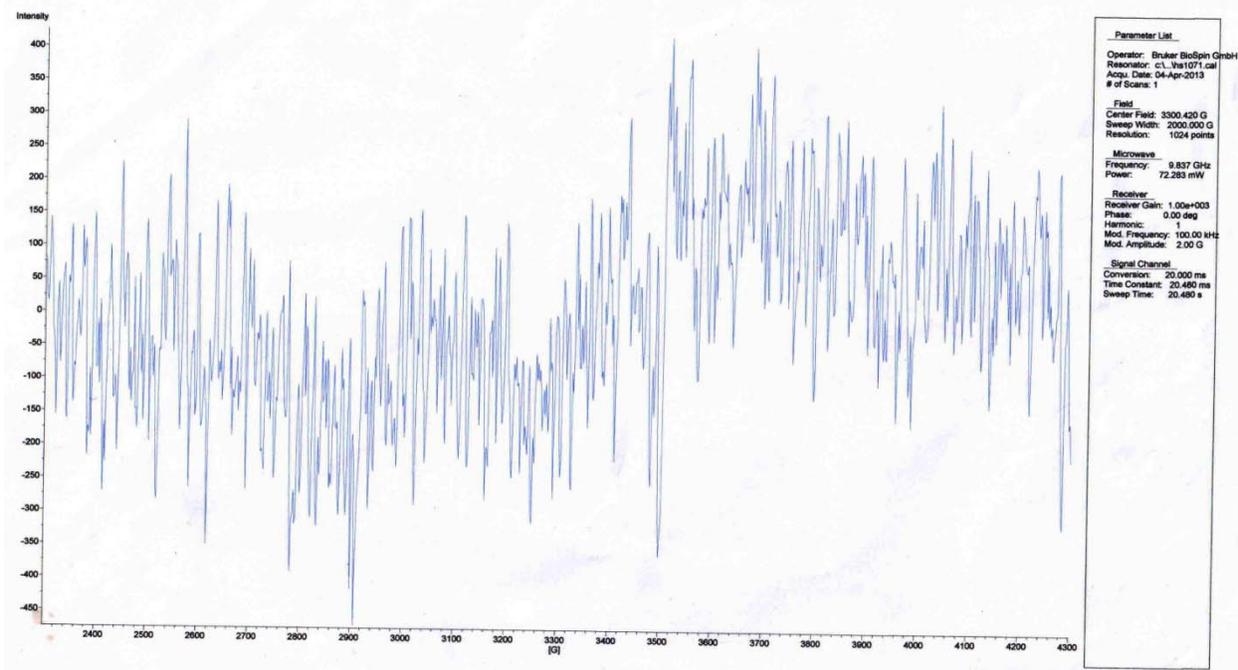


Figure S2. EPR spectrum of precipitate from reaction mixture after 1 h.



Figure S3. EPR spectrum of solution from reaction mixture after 3h

Figure S4  $^1\text{H}$  NMR of **1**

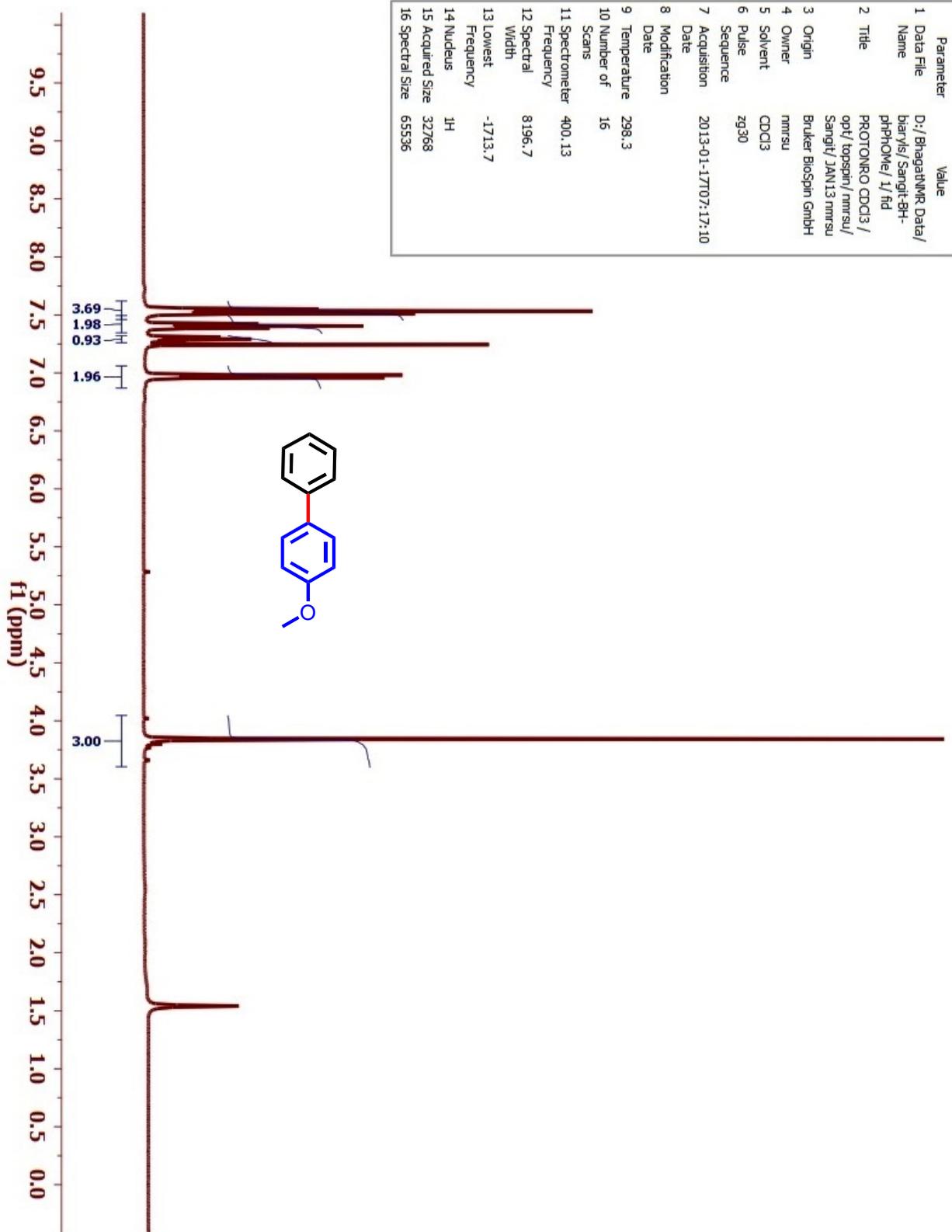


Figure S5  $^{13}\text{C}$  NMR spectrum of **1**

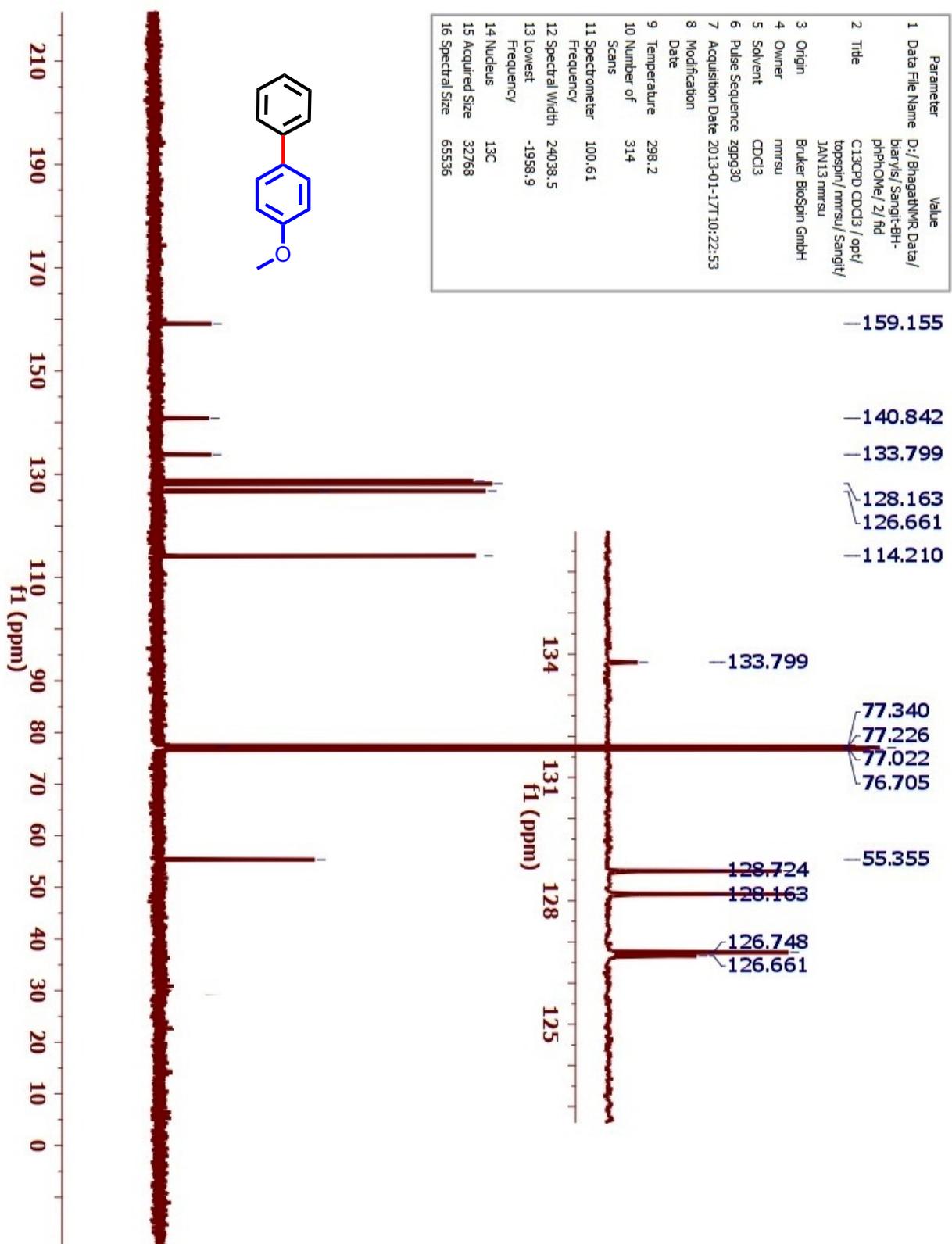


Figure S6  $^{13}\text{C}$  NMR DEPT-135 of **1**

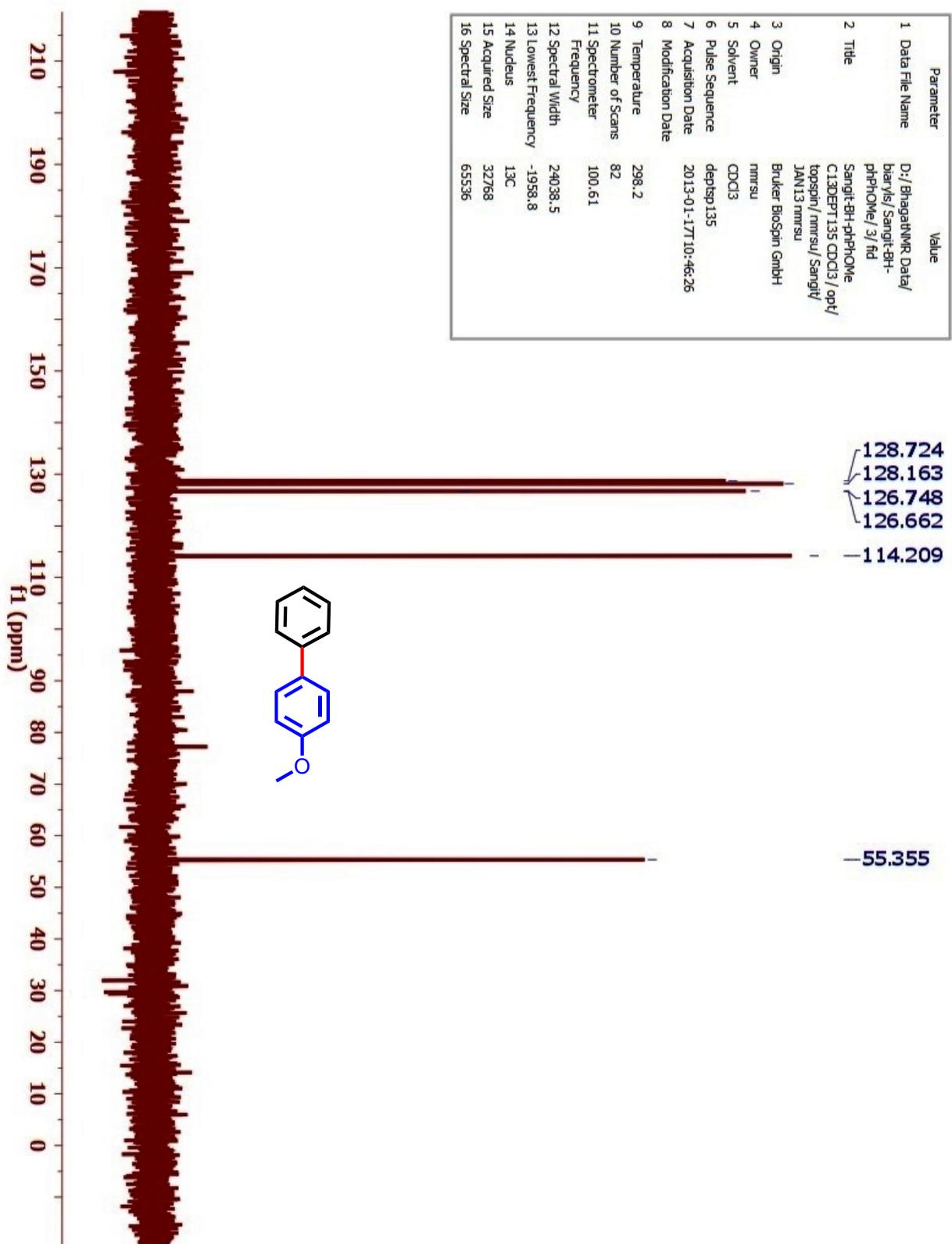


Figure S7  $^1\text{H}$  NMR of **2**

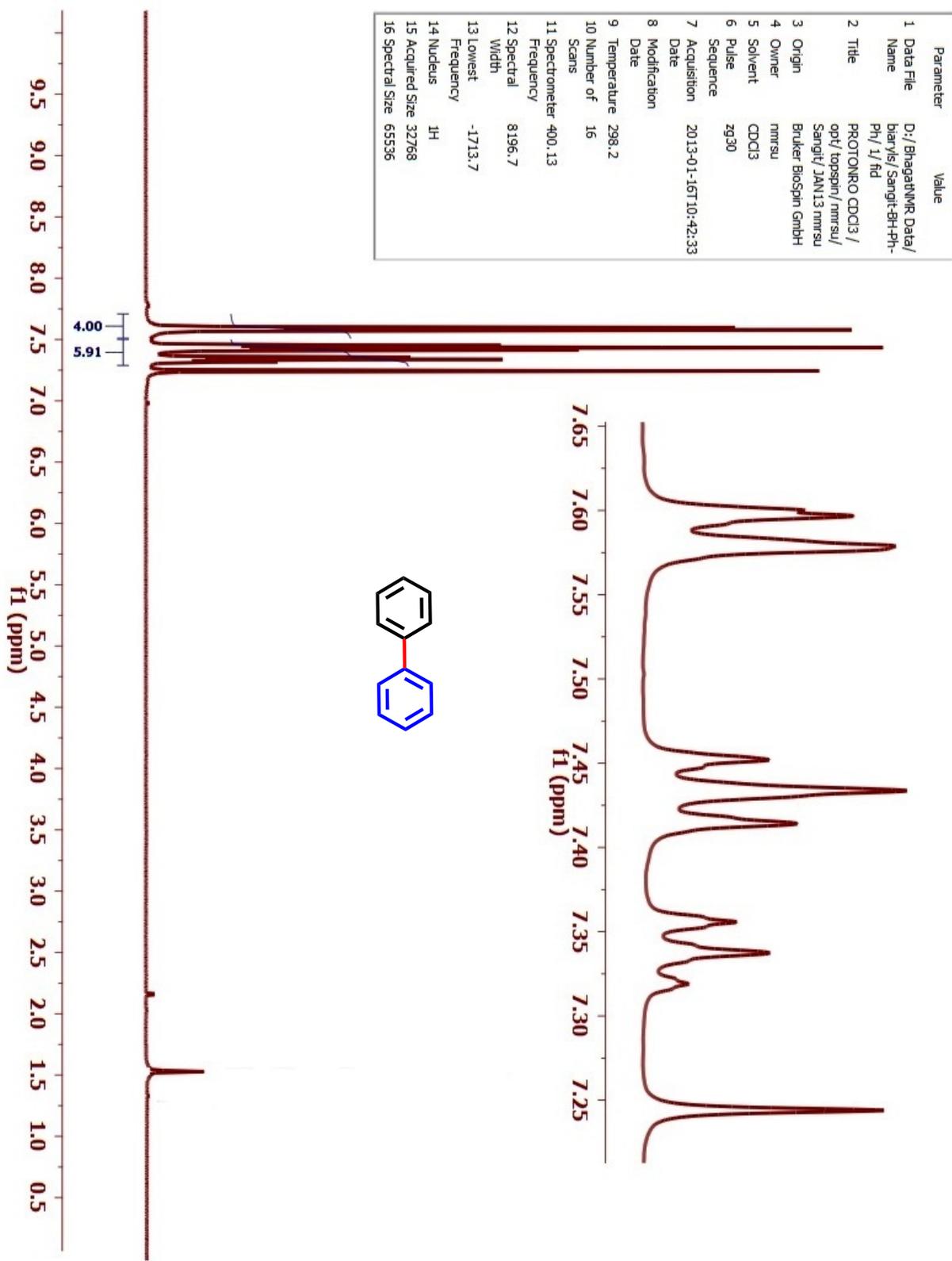


Figure S8  $^{13}\text{C}$  NMR spectrum of **2**

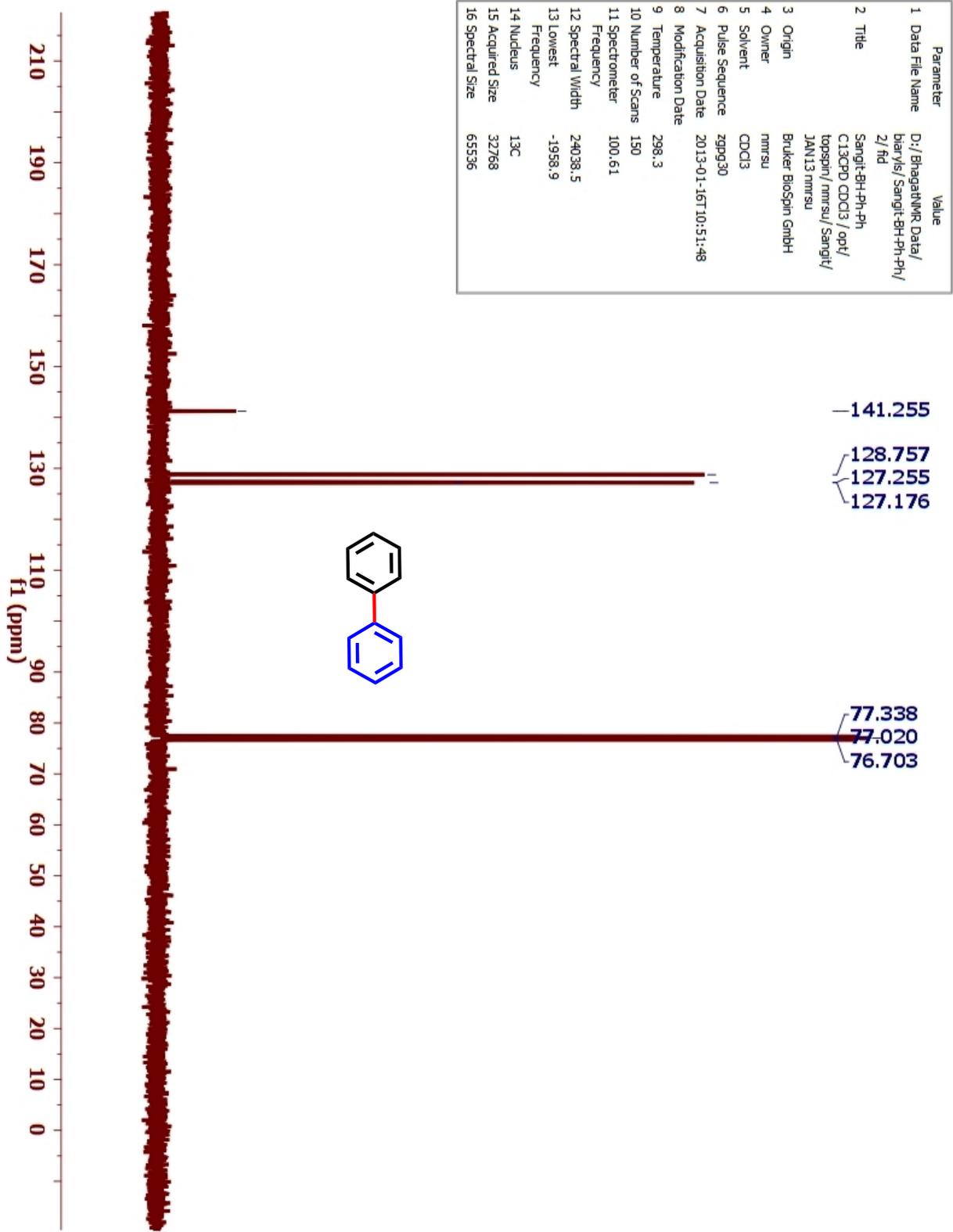


Figure S9  $^{13}\text{C}$  NMR DEPT-135 of **2**

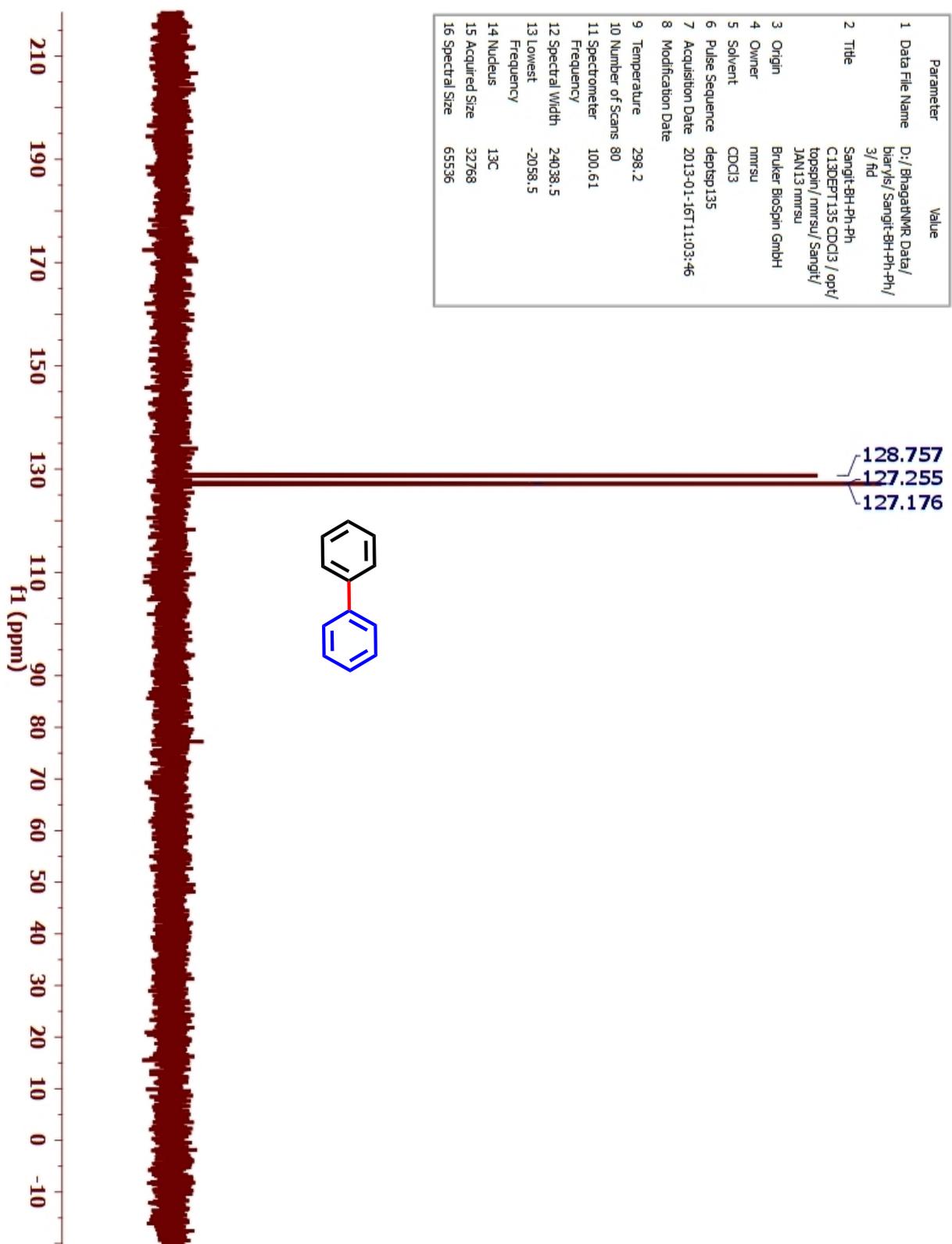


Figure S10 <sup>1</sup>H NMR of 3

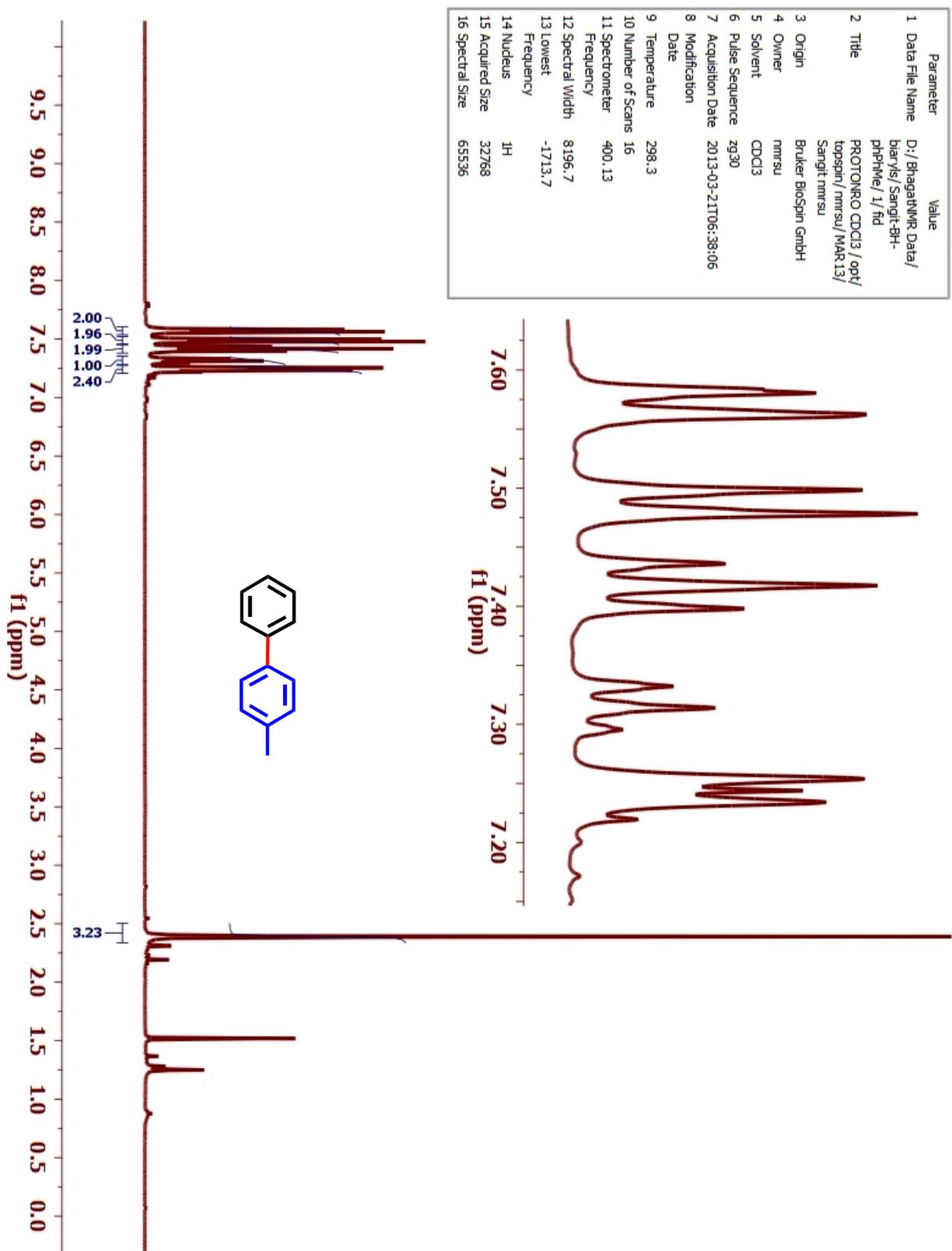


Figure S11  $^{13}\text{C}$  NMR spectrum of **3**

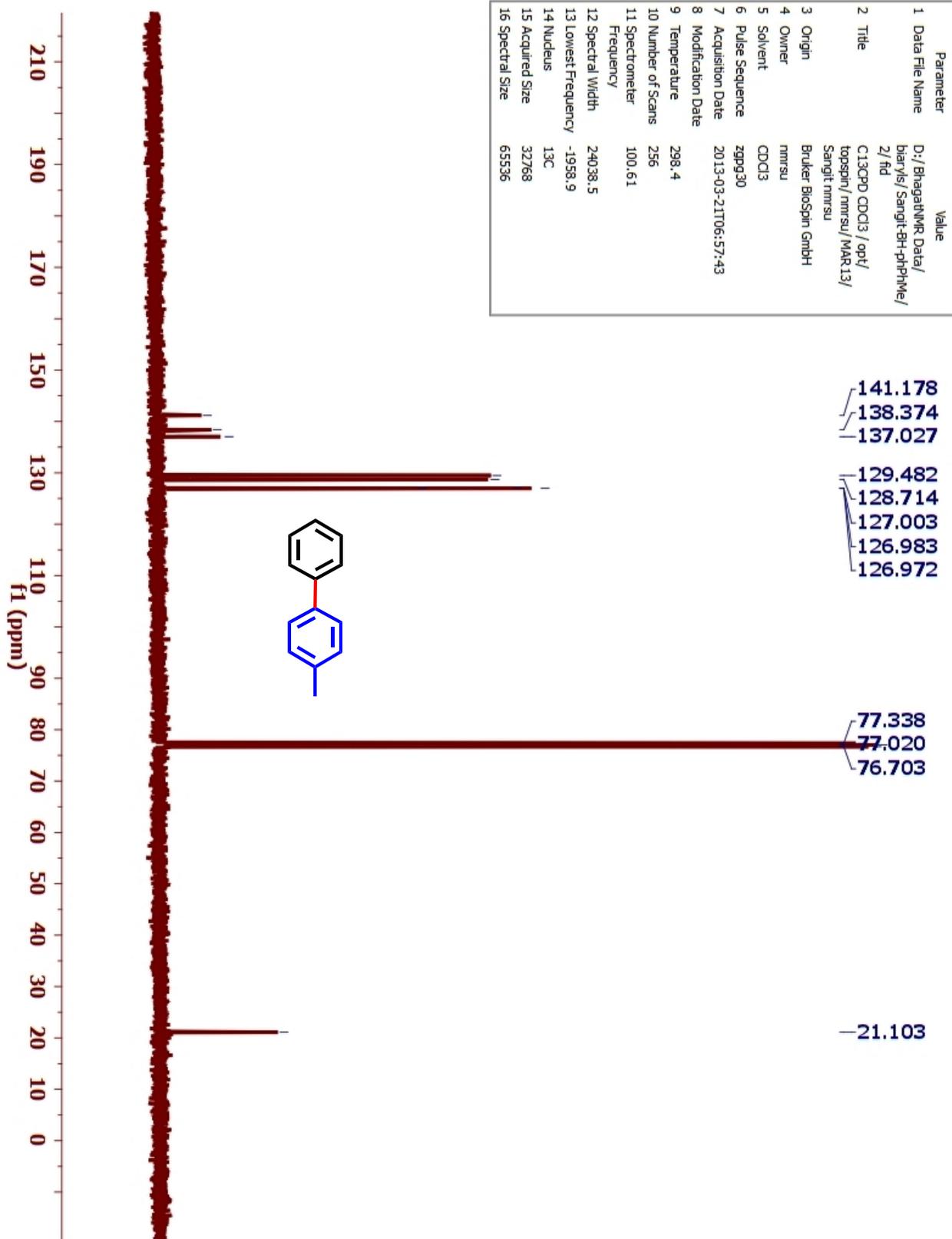


Figure S12  $^{13}\text{C}$  NMR DEPT-135 of **3**

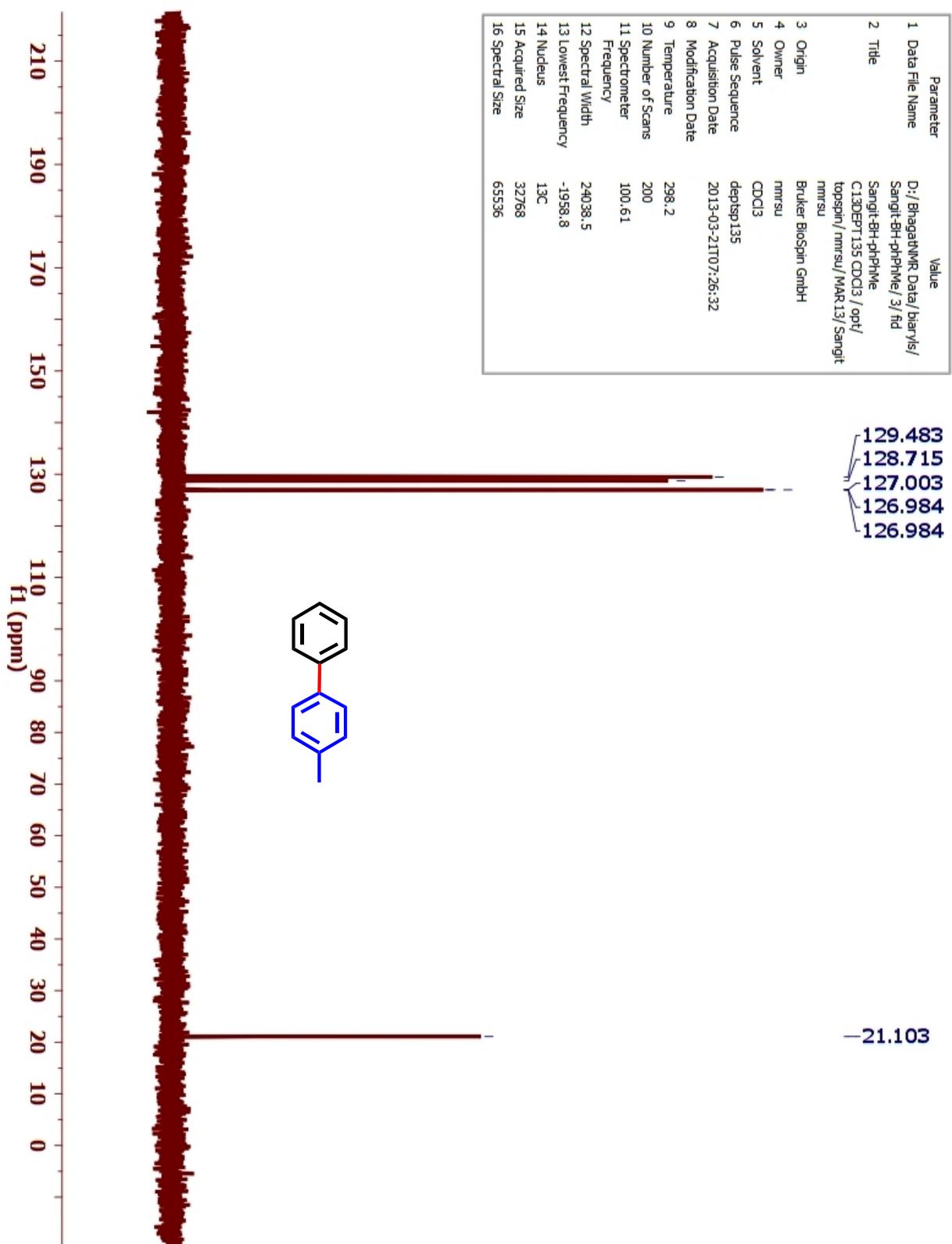


Figure S13 <sup>1</sup>H NMR of **4**

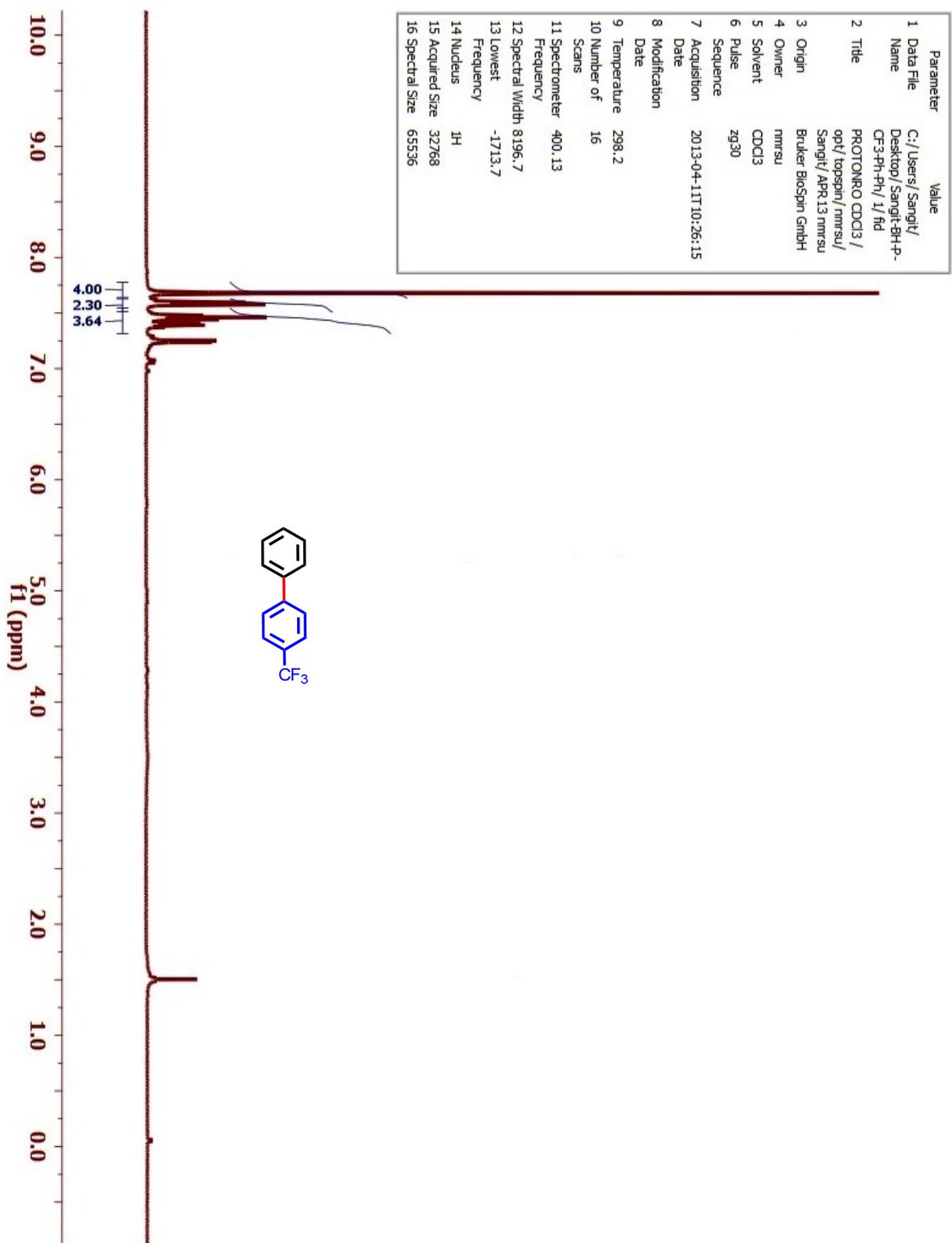


Figure S14  $^{13}\text{C}$  NMR spectrum of **4**

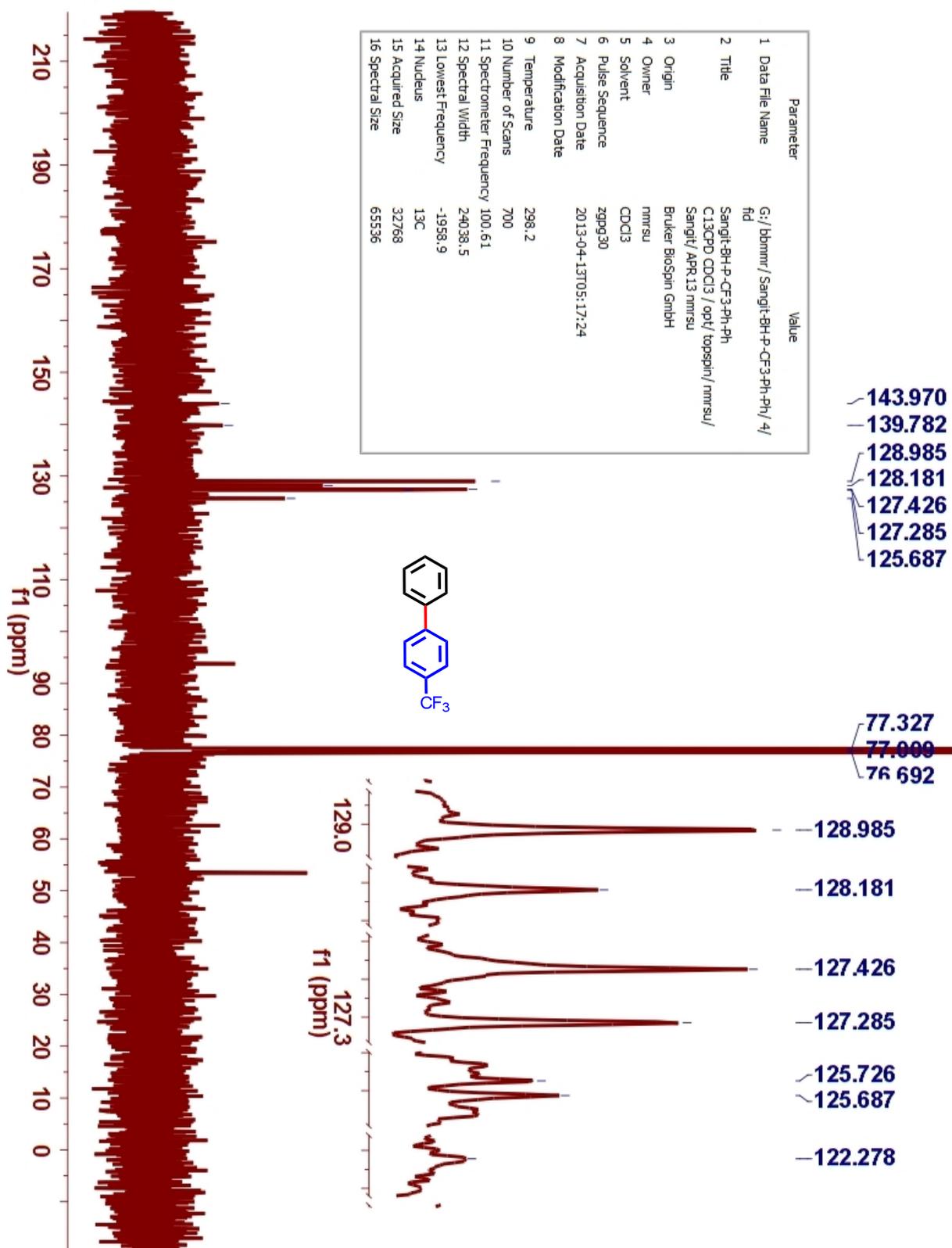


Figure S15  $^{13}\text{C}$  NMR DEPT-135 of **4**

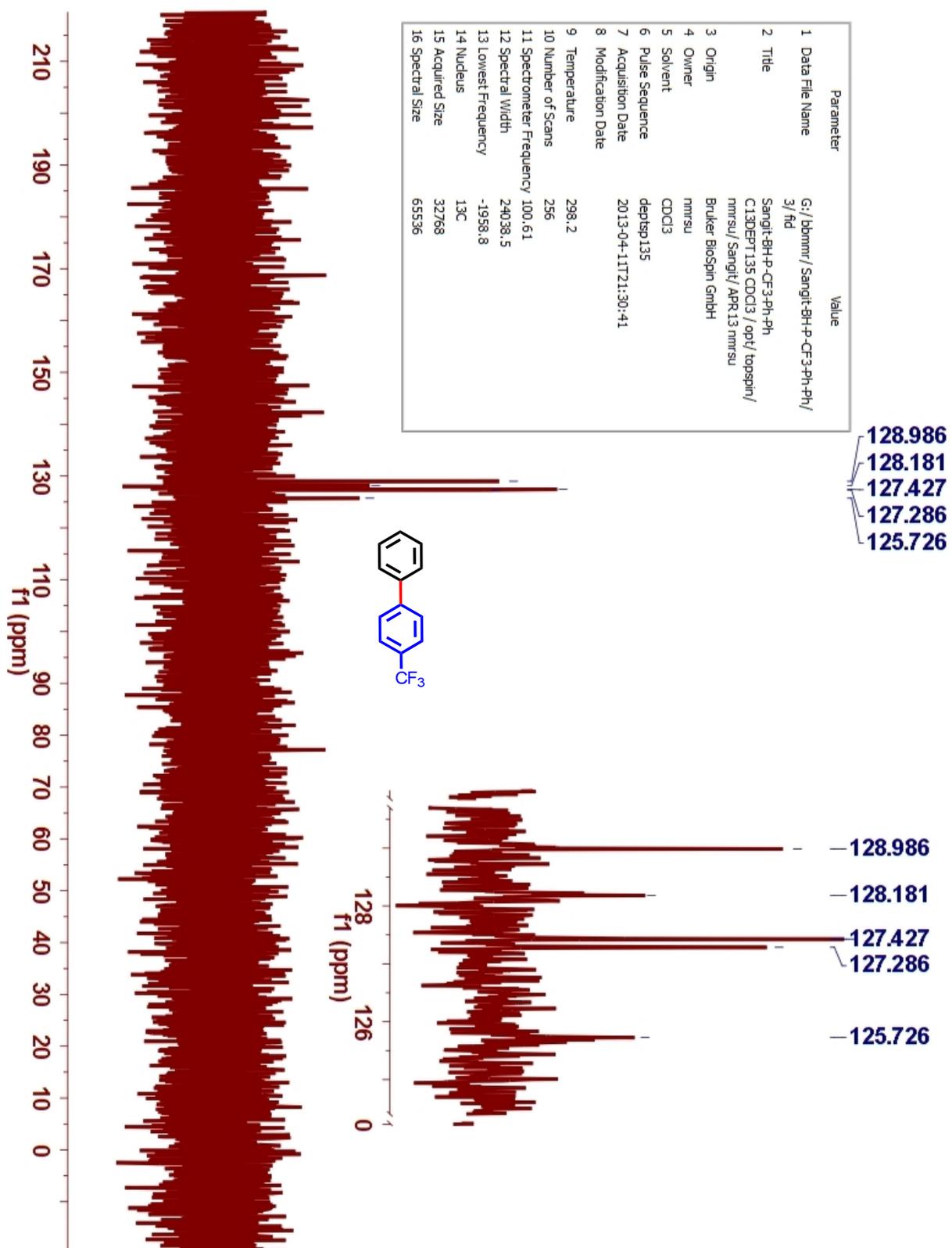


Figure S16  $^1\text{H}$  NMR of **5**

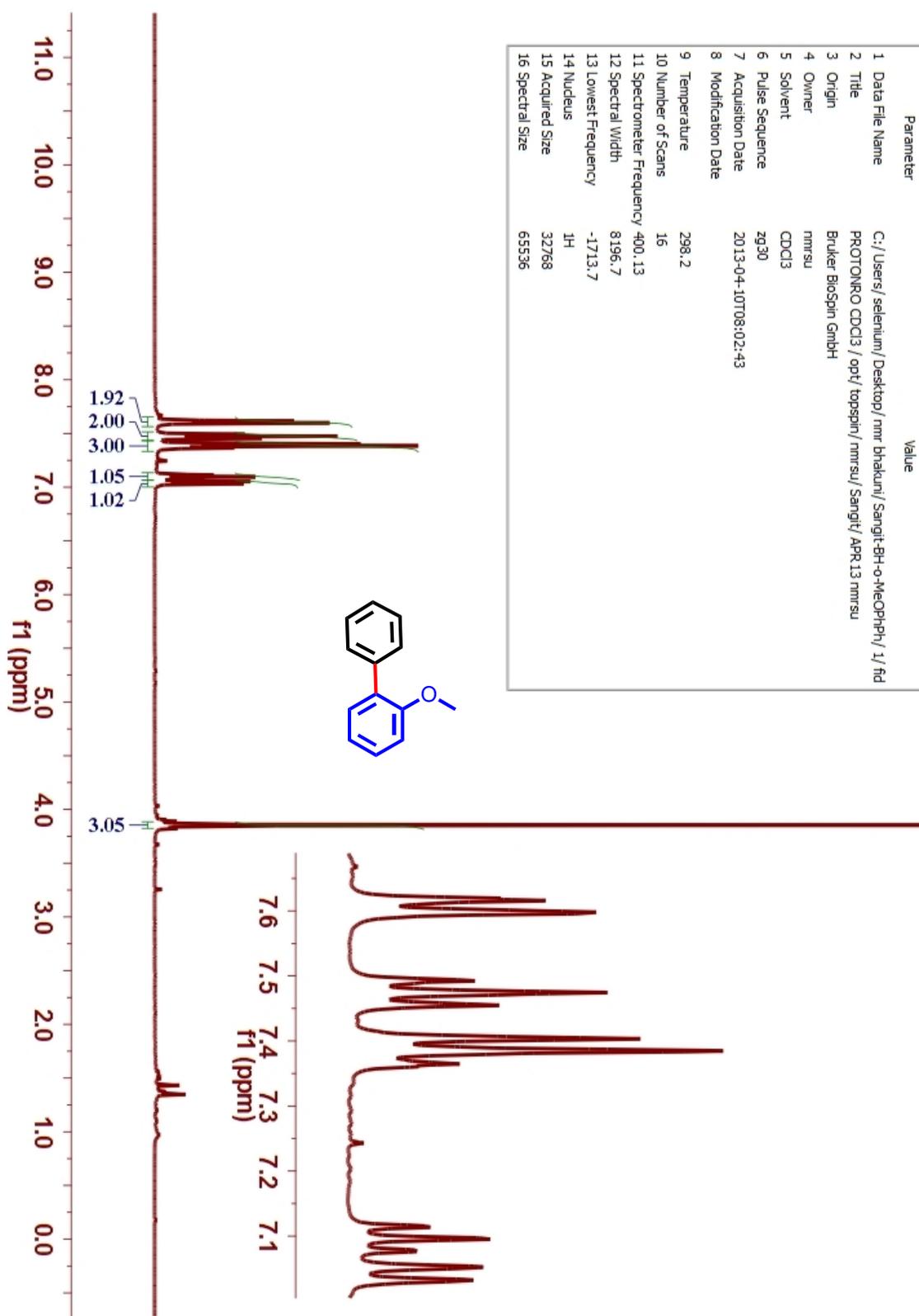


Figure S17  $^{13}\text{C}$  NMR spectrum of **5**

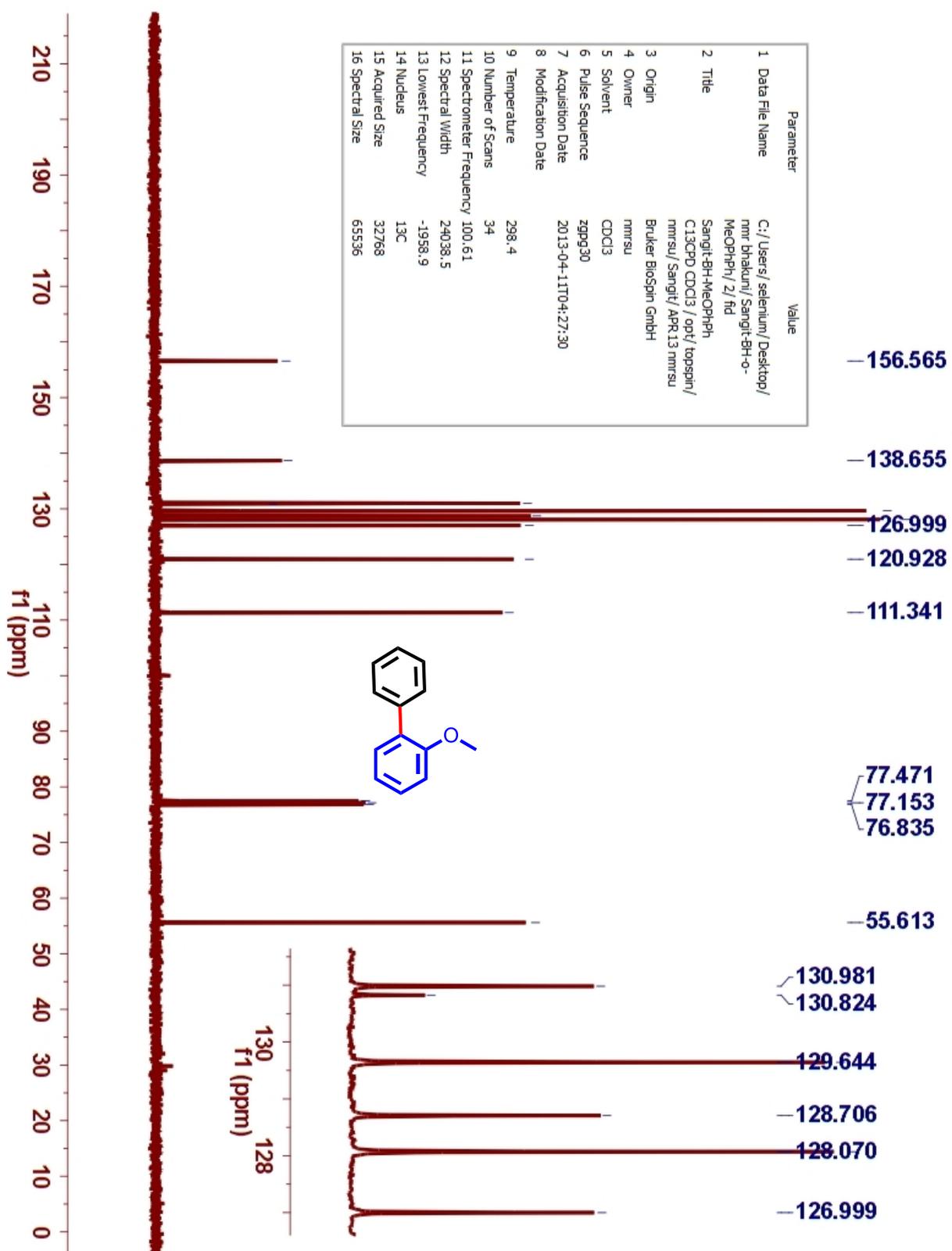


Figure S18  $^{13}\text{C}$  NMR DEPT-135 of **5**

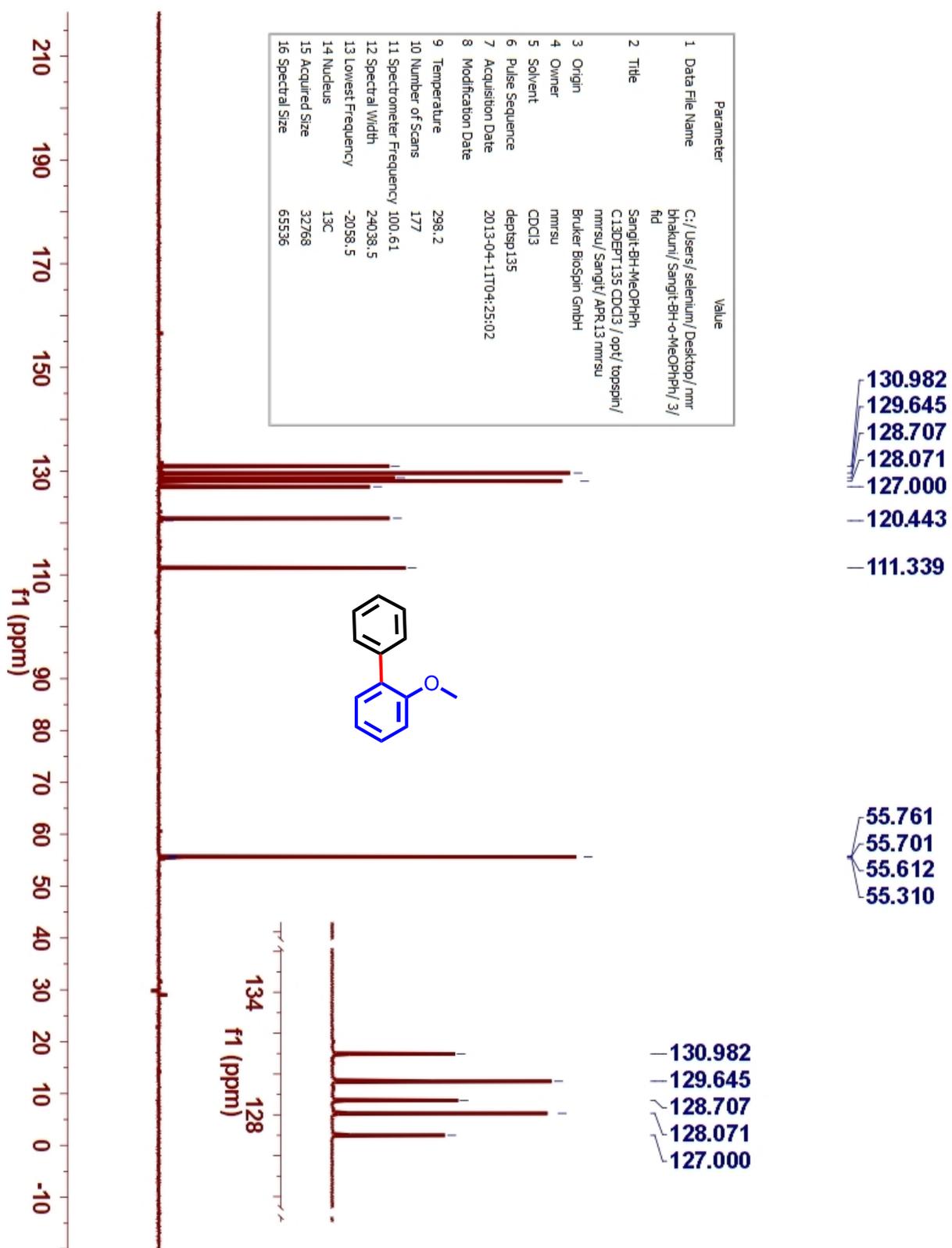


Figure S19 <sup>1</sup>H NMR of 6

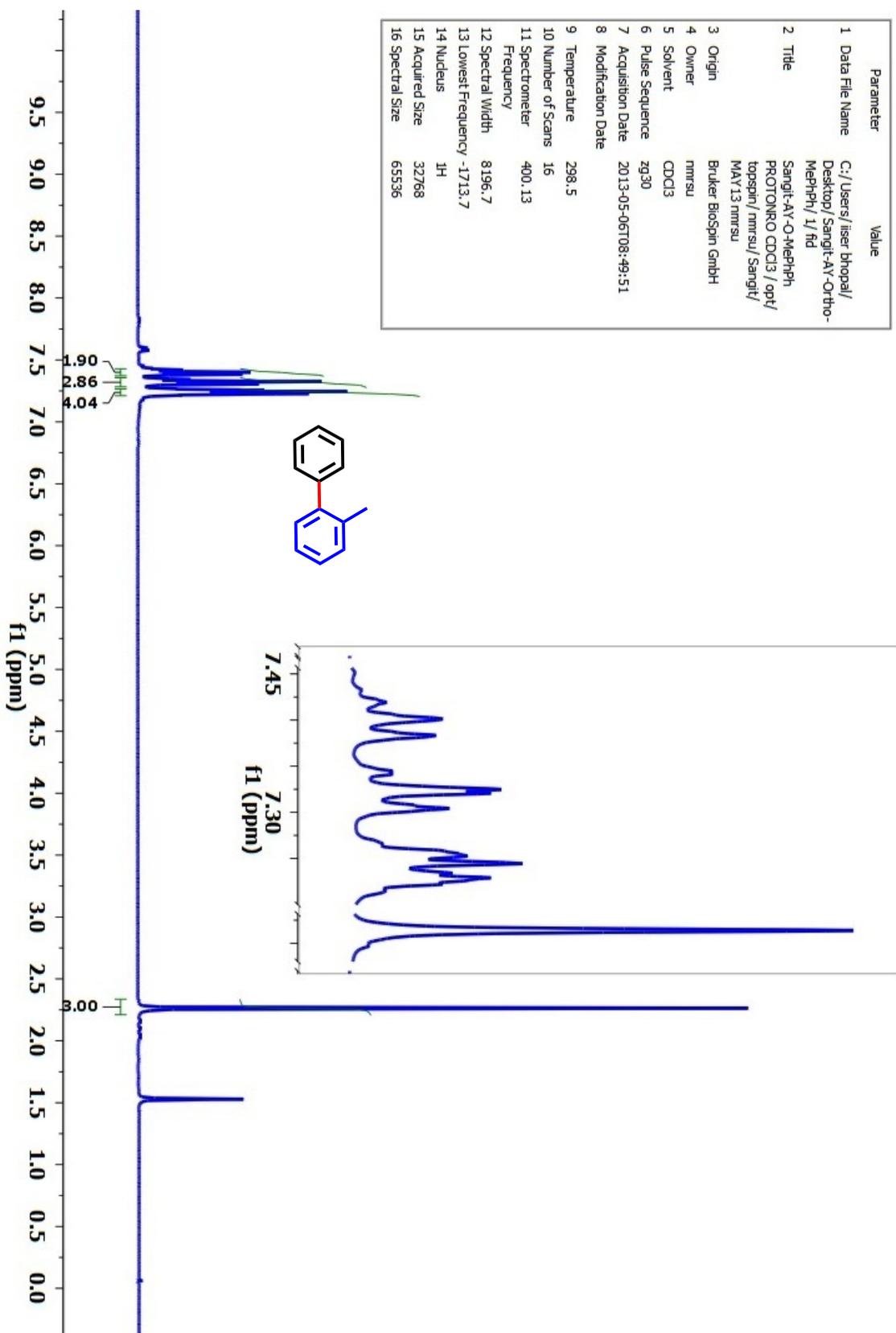


Figure S20  $^{13}\text{C}$  NMR spectrum of **6**

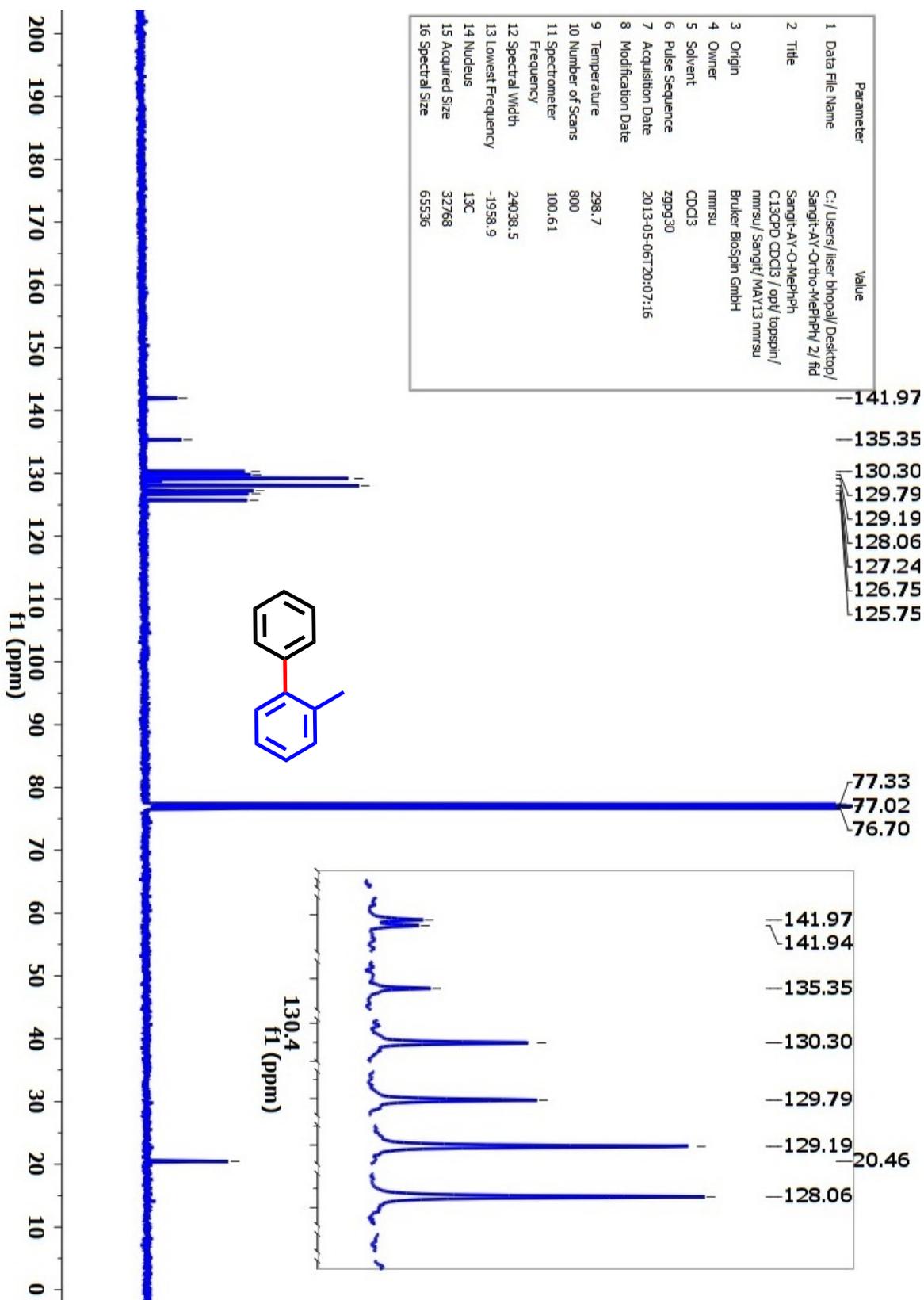


Figure S21  $^{13}\text{C}$  NMR DEPT-135 spectrum of **6**

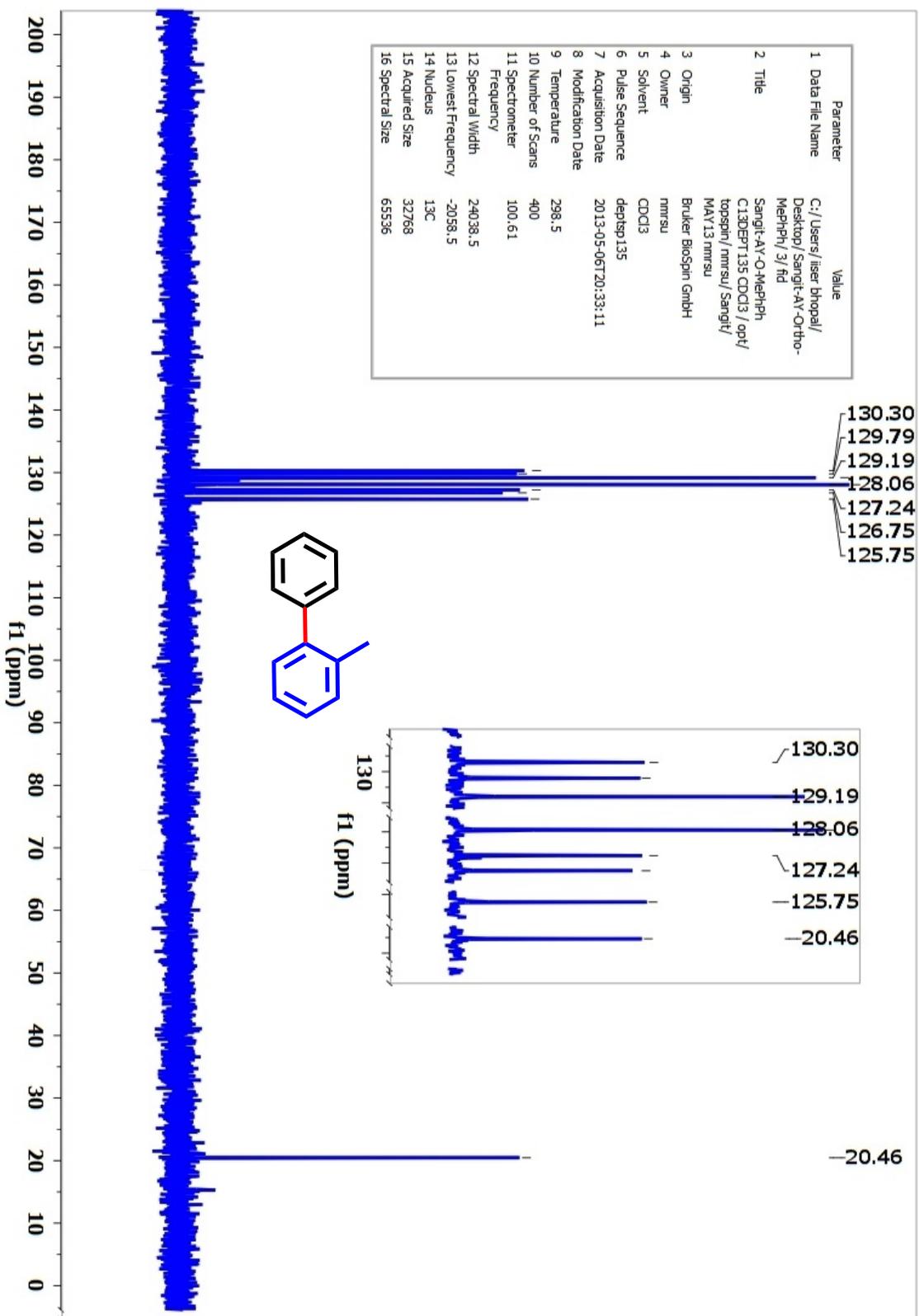


Figure S22 <sup>1</sup>H NMR of 7

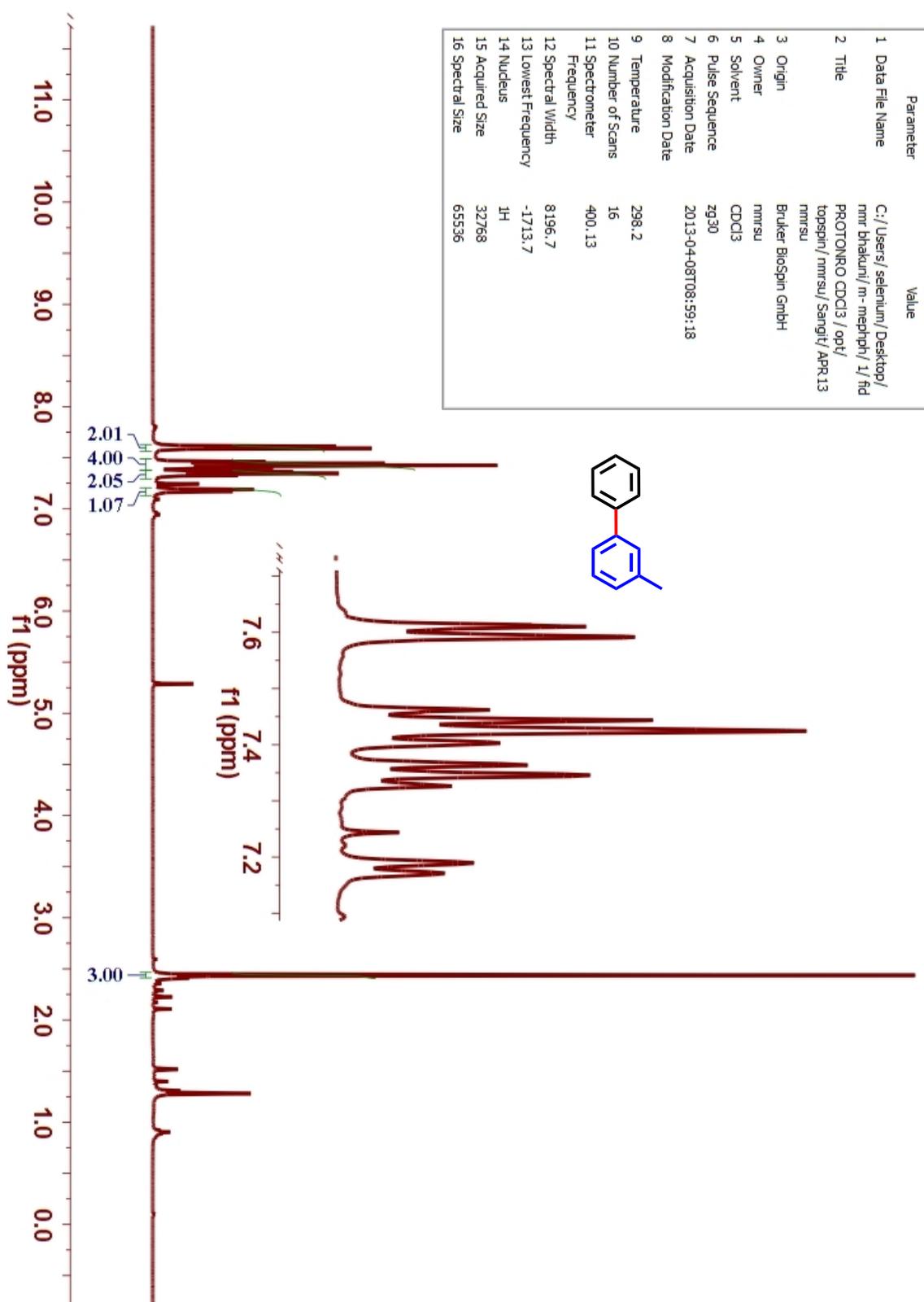


Figure S23 <sup>13</sup>C NMR spectrum of 7

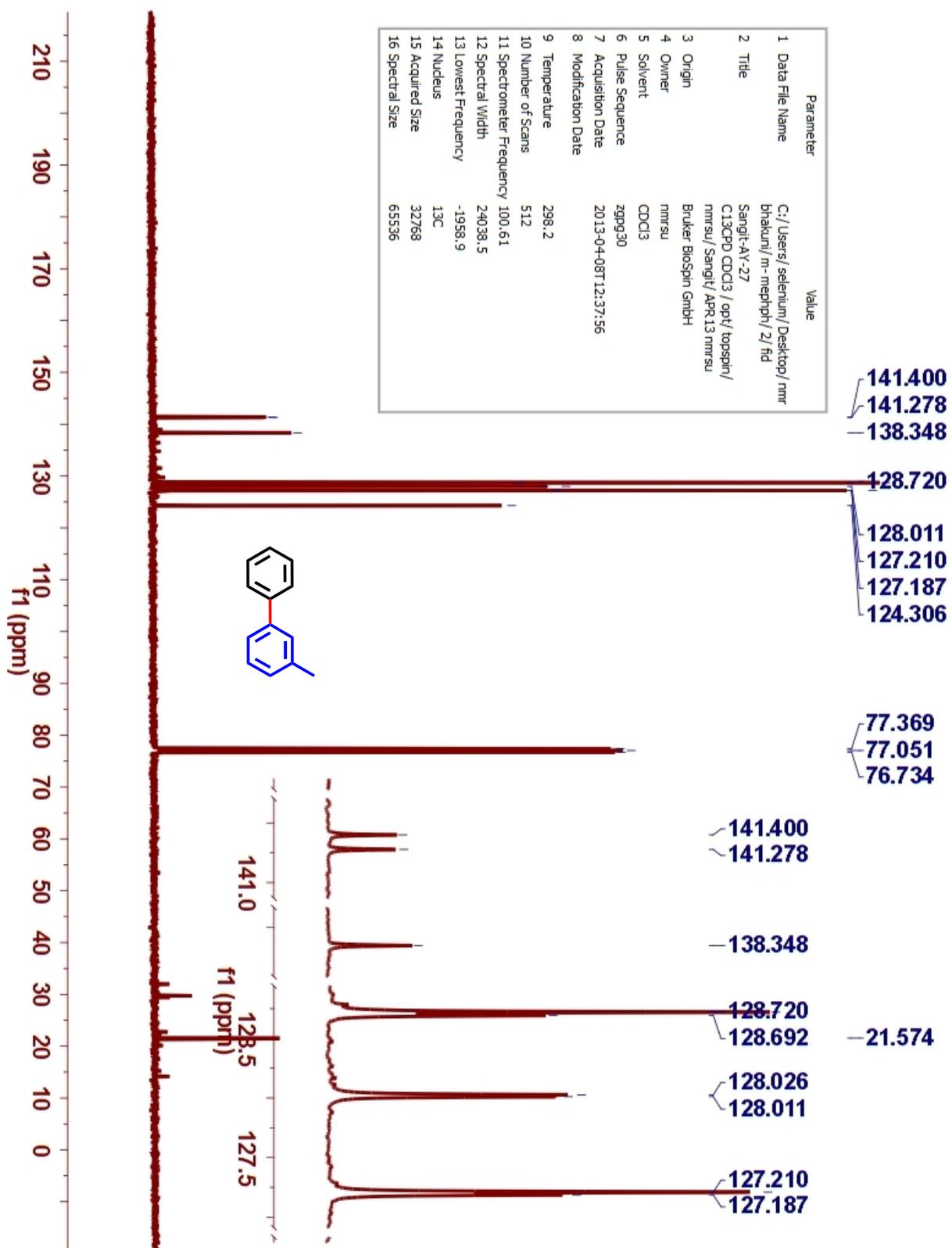


Figure S24  $^{13}\text{C}$  NMR DEPT-135 of 7

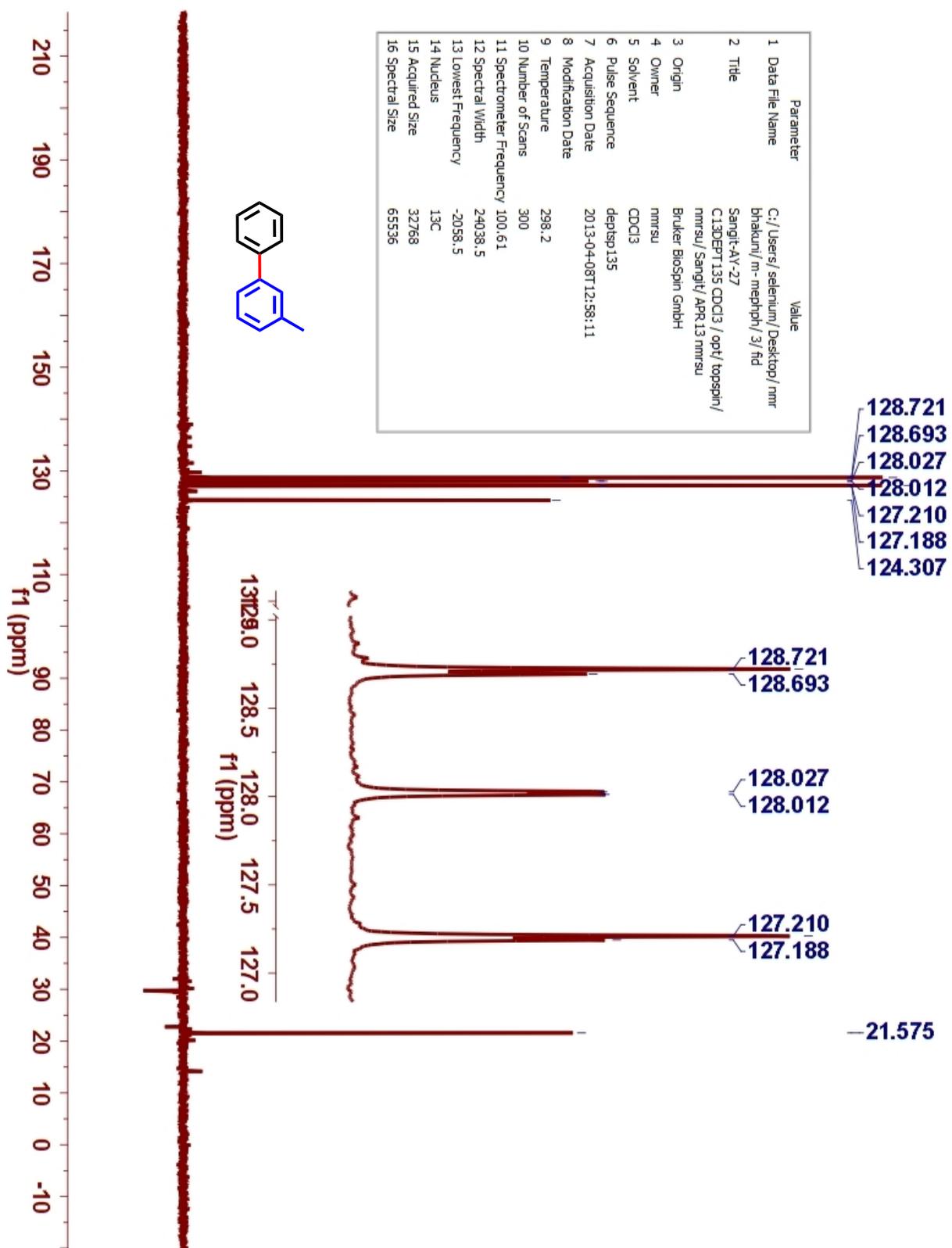


Figure S25 <sup>1</sup>H NMR of **8**

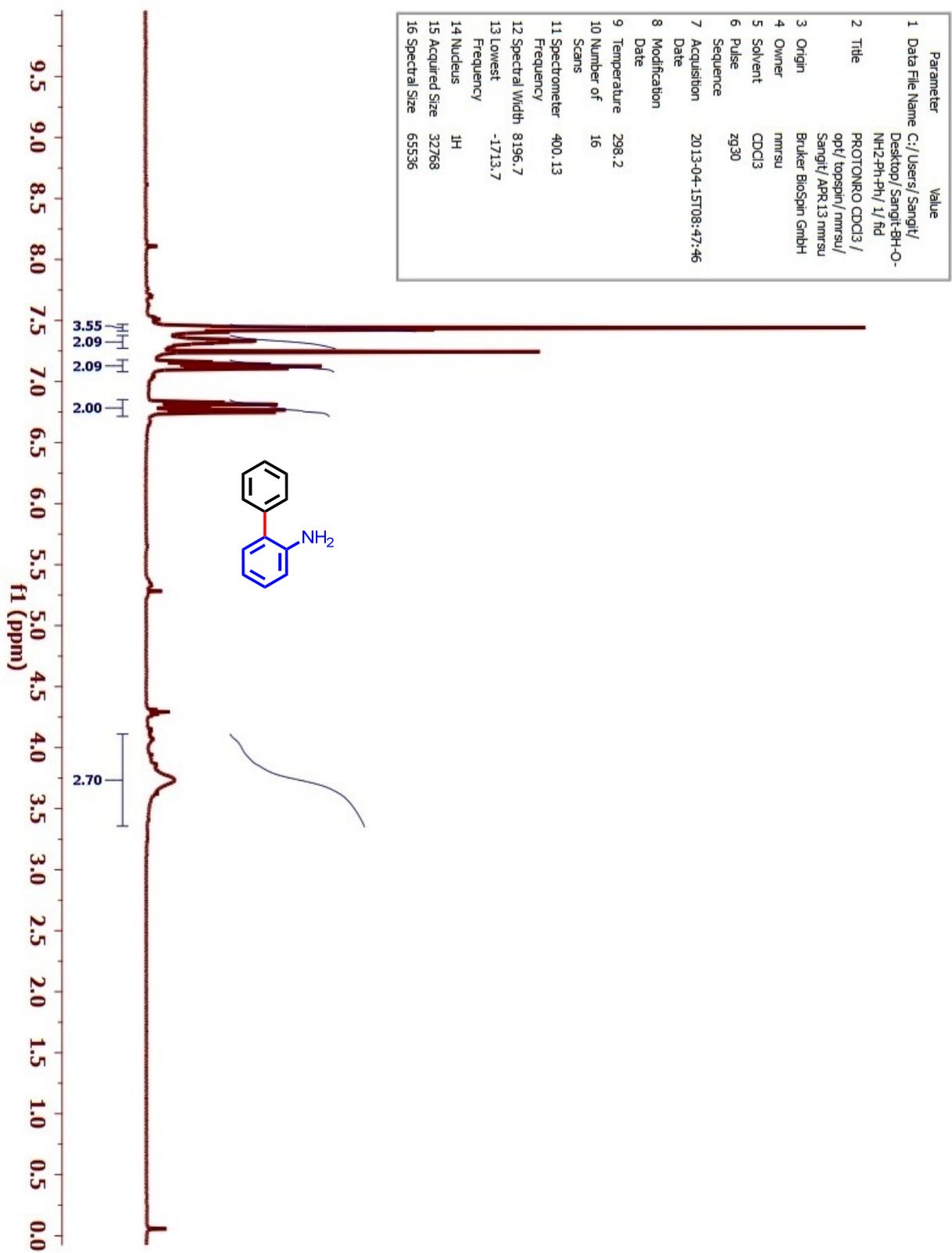


Figure S26  $^{13}\text{C}$  NMR spectrum of **8**

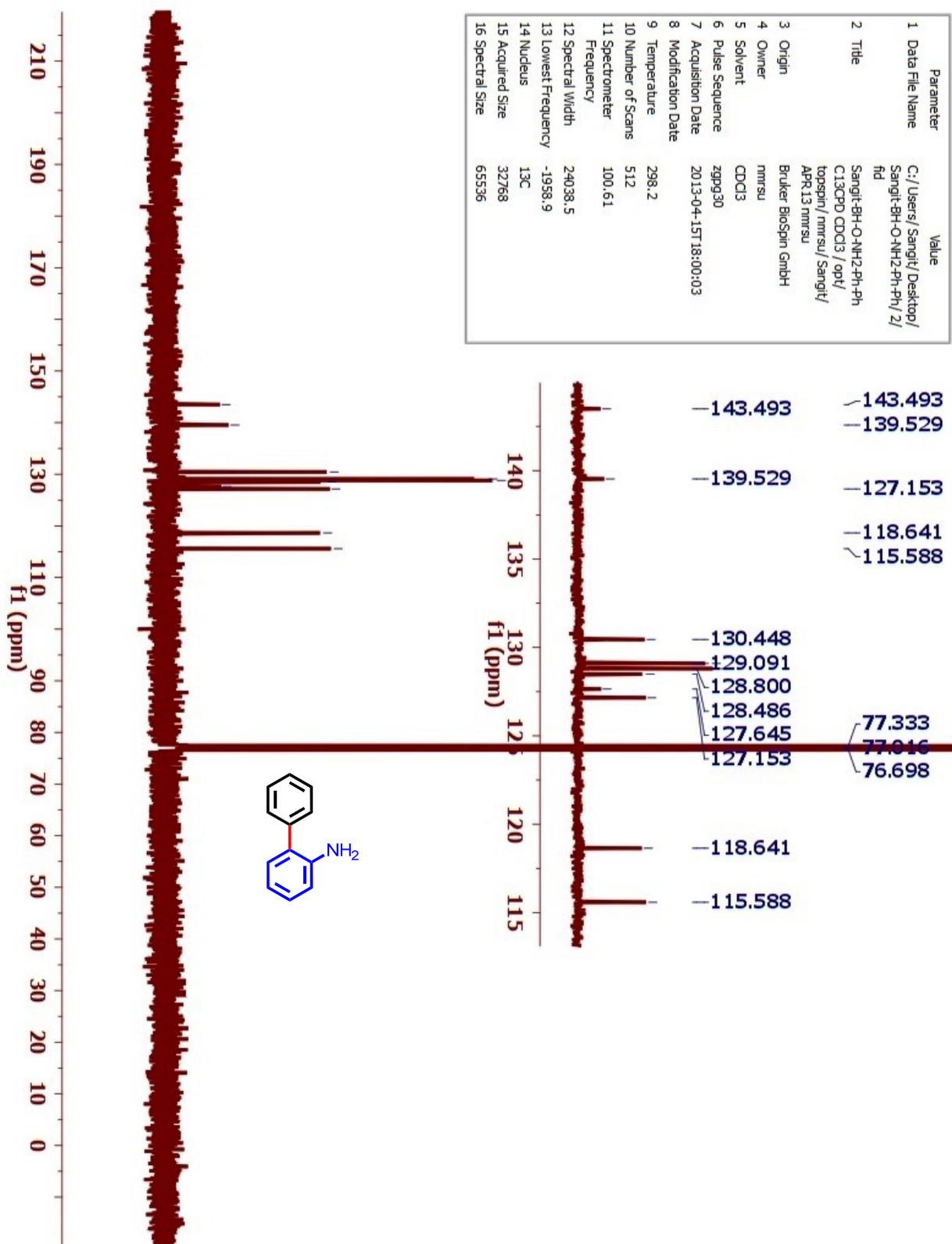


Figure S27  $^{13}\text{C}$  NMR DEPT-135 of **8**

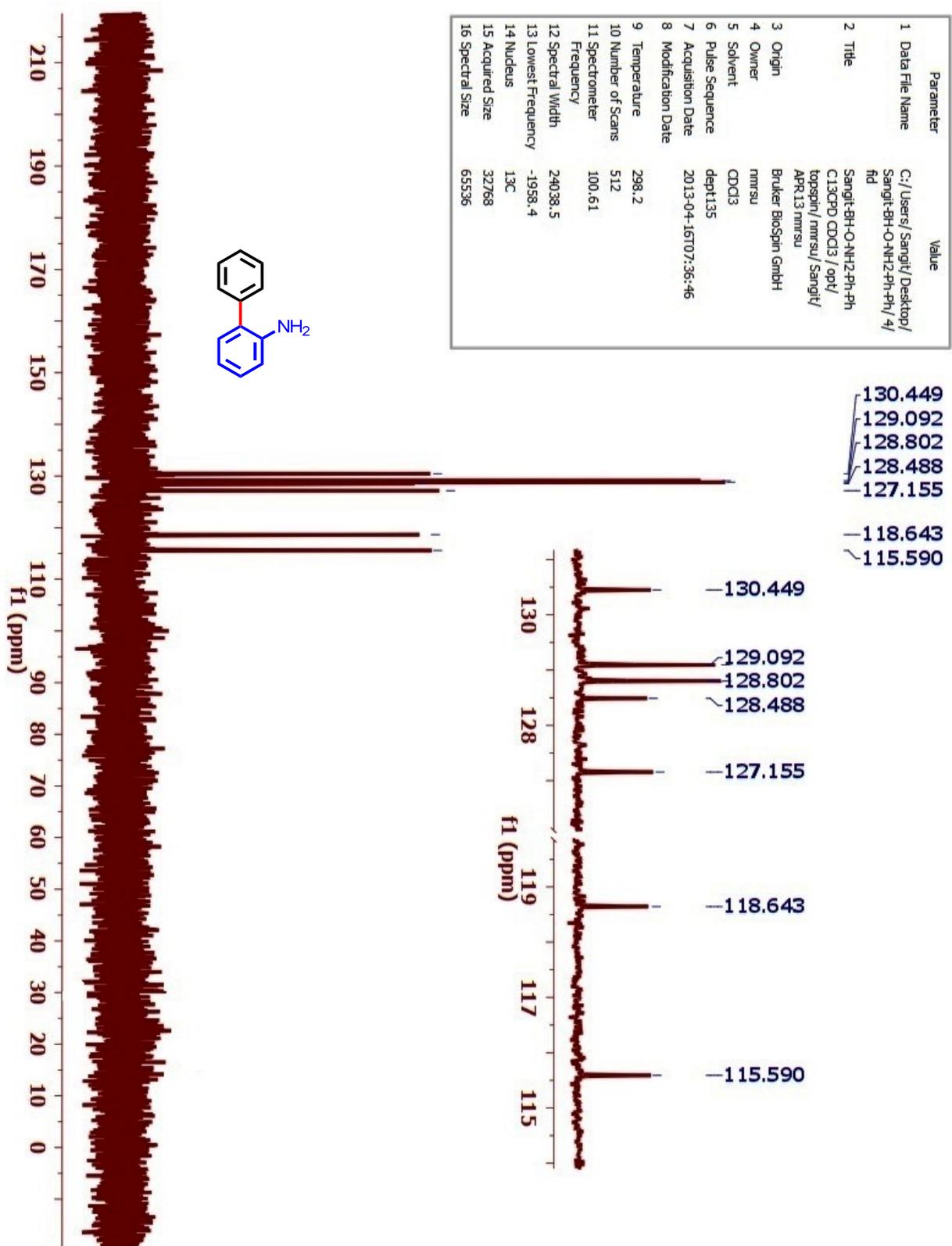


Figure S28 <sup>1</sup>H NMR of **9**

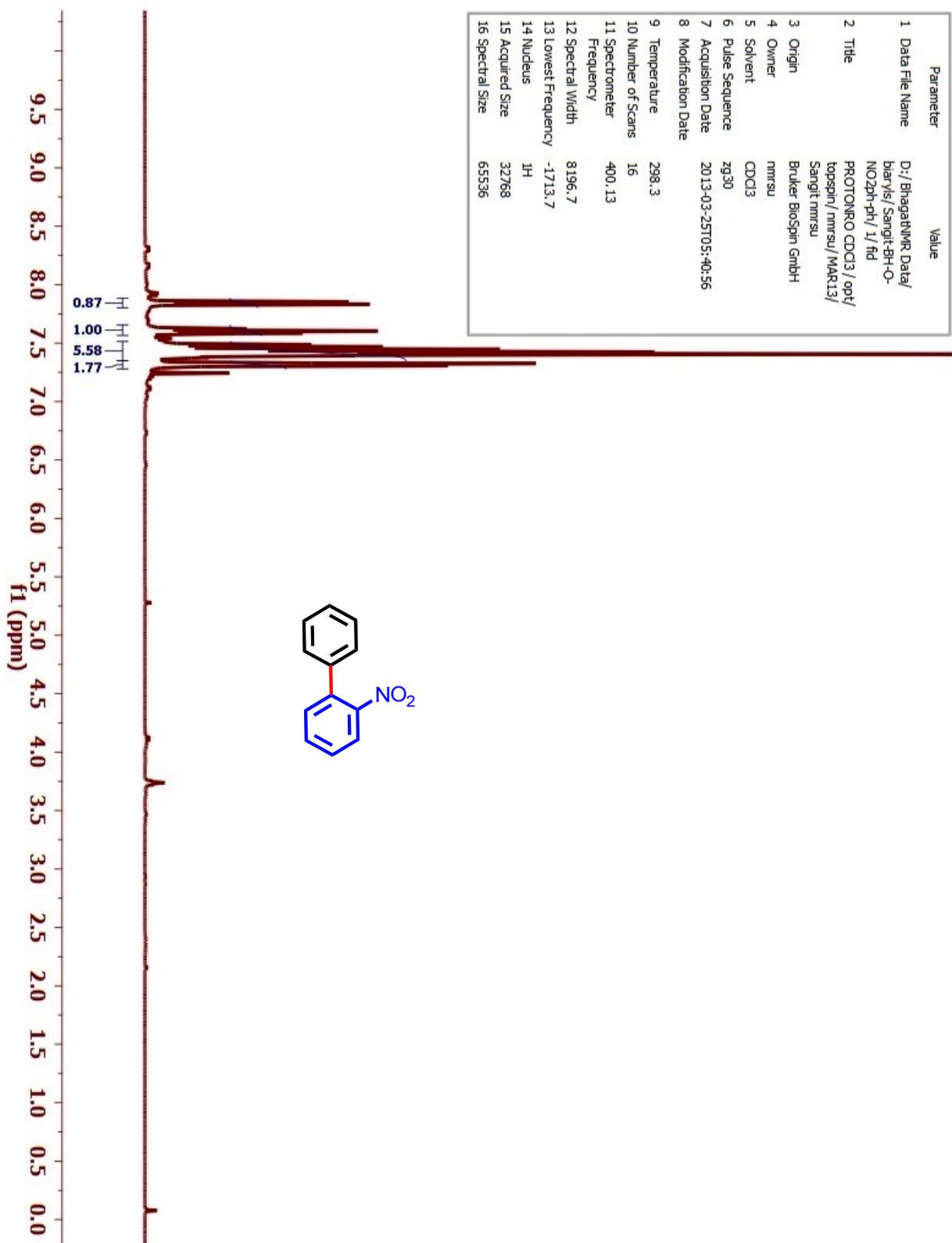


Figure S29  $^{13}\text{C}$  NMR spectrum of **9**

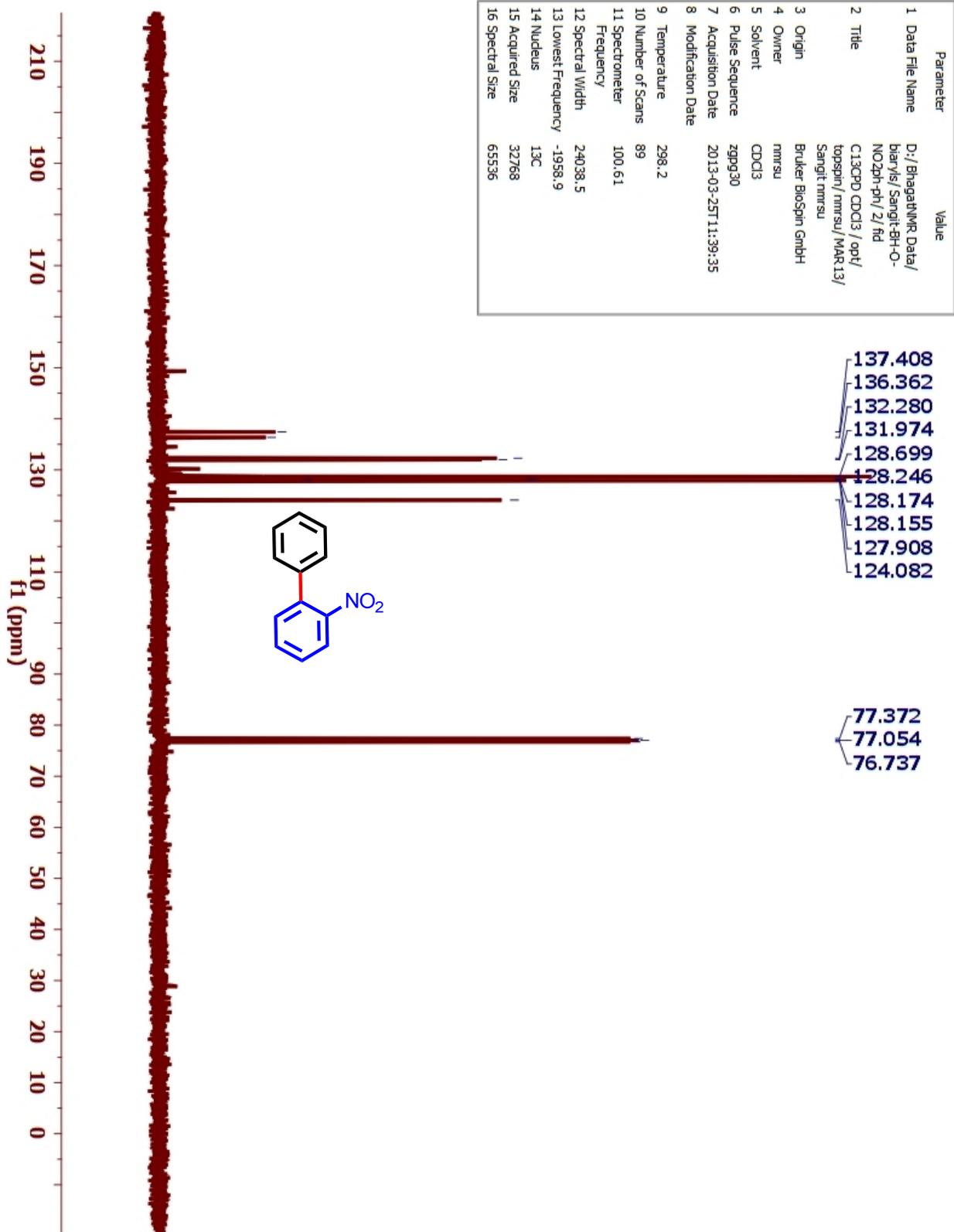


Figure S30  $^{13}\text{C}$  NMR DEPT-135 of **9**

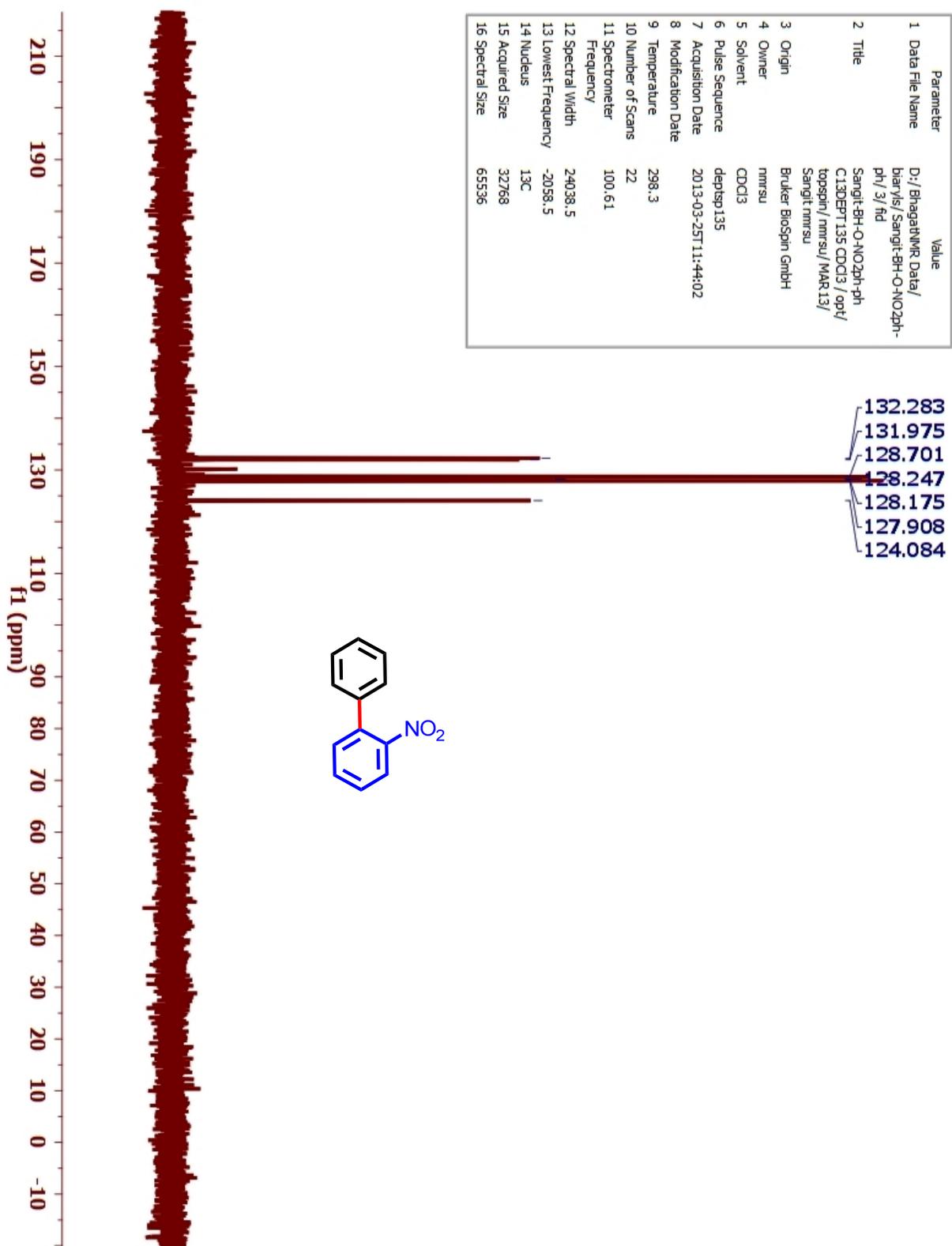


Figure S31 <sup>1</sup>H NMR of **10**

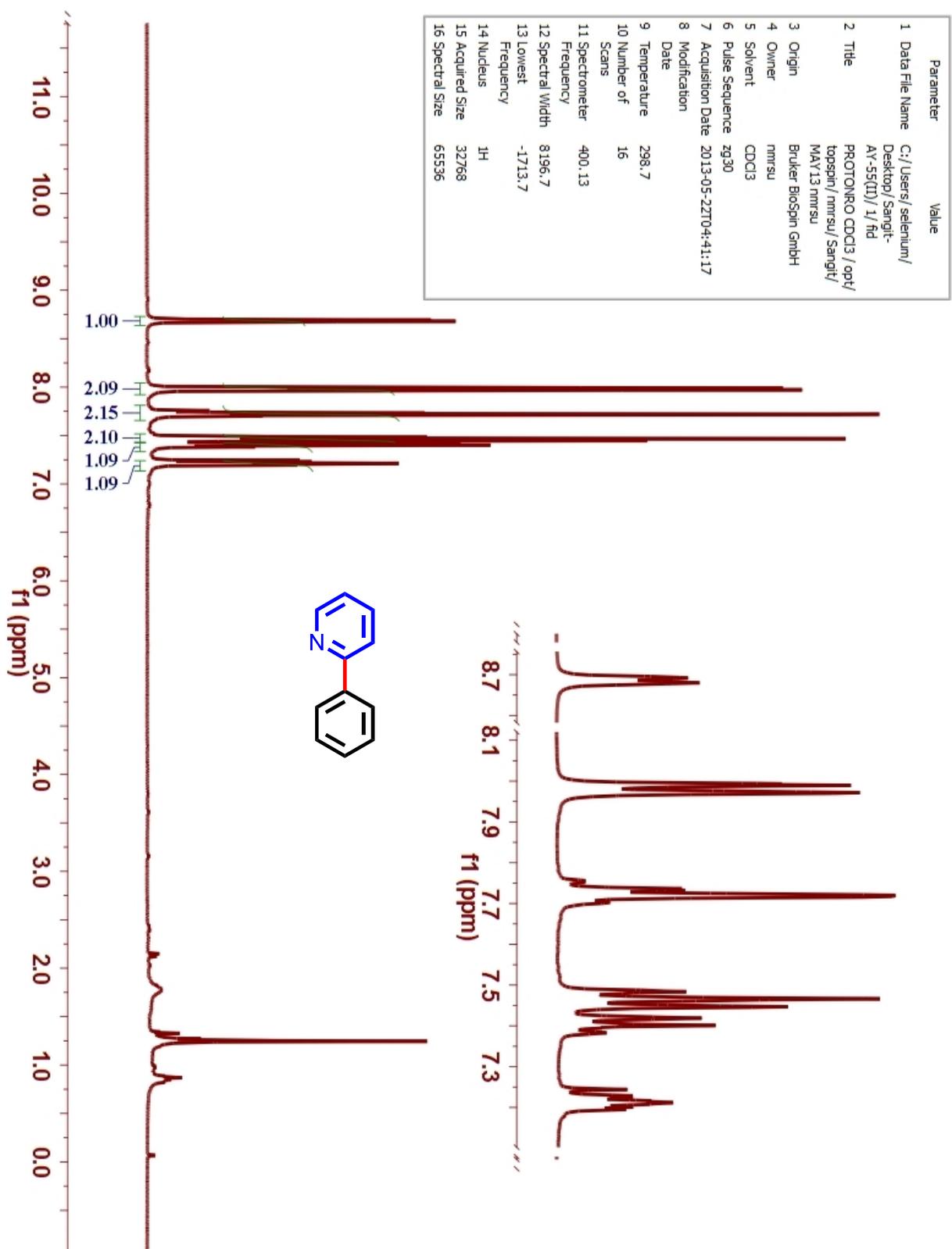


Figure S32  $^{13}\text{C}$  NMR spectrum of **10**

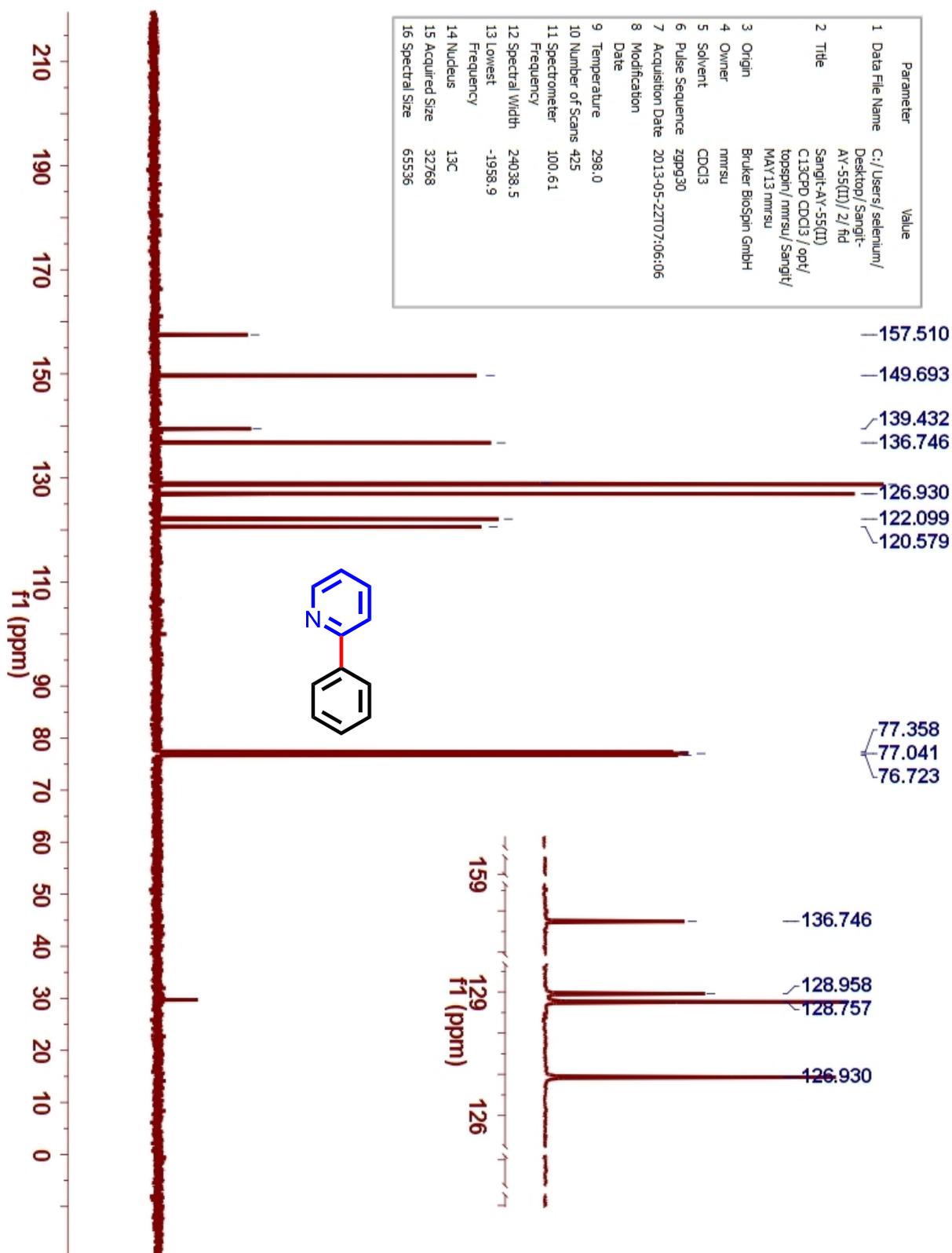


Figure S33  $^{13}\text{C}$  NMR DEPT-135 of **10**

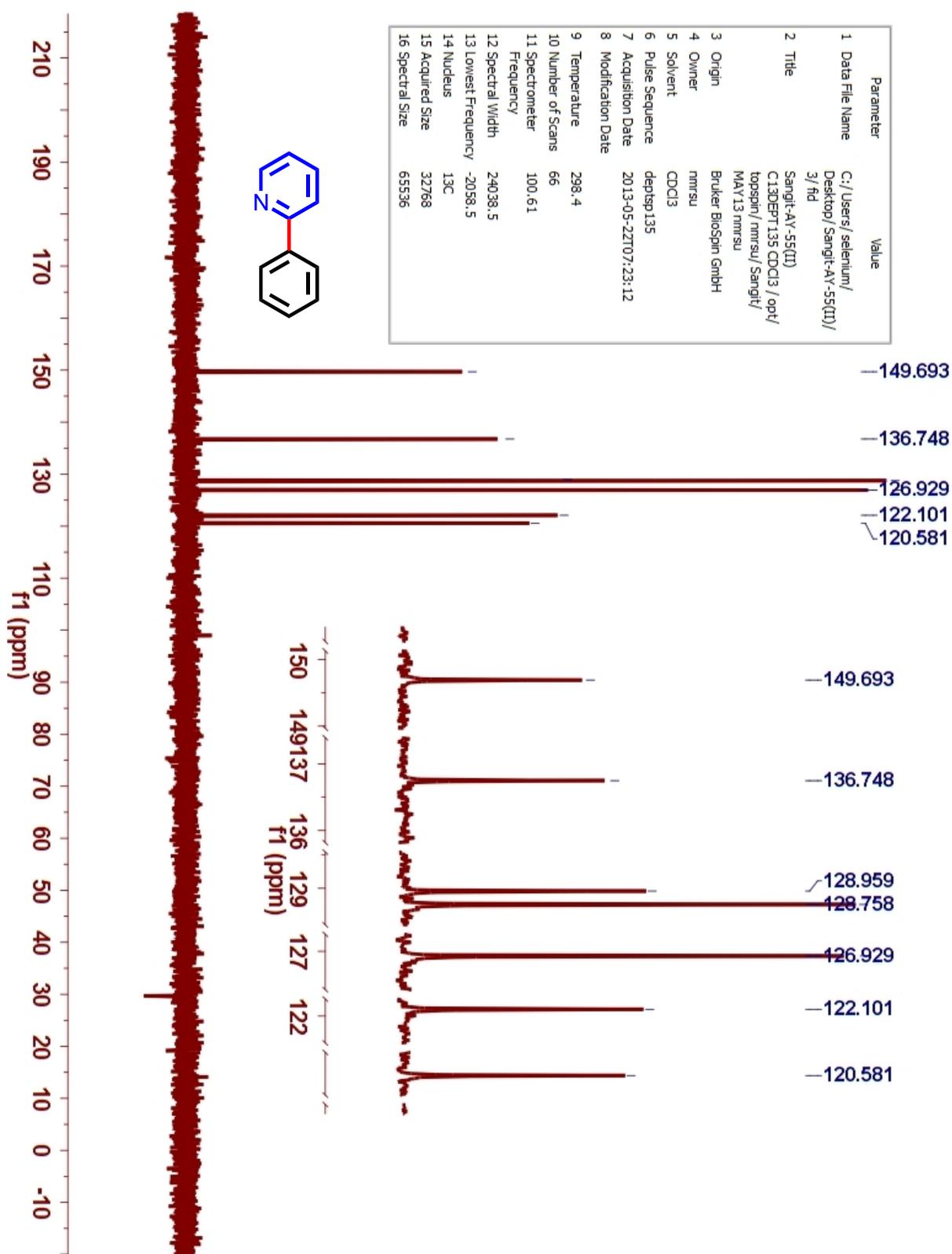


Figure S34  $^1\text{H}$  NMR of **11**

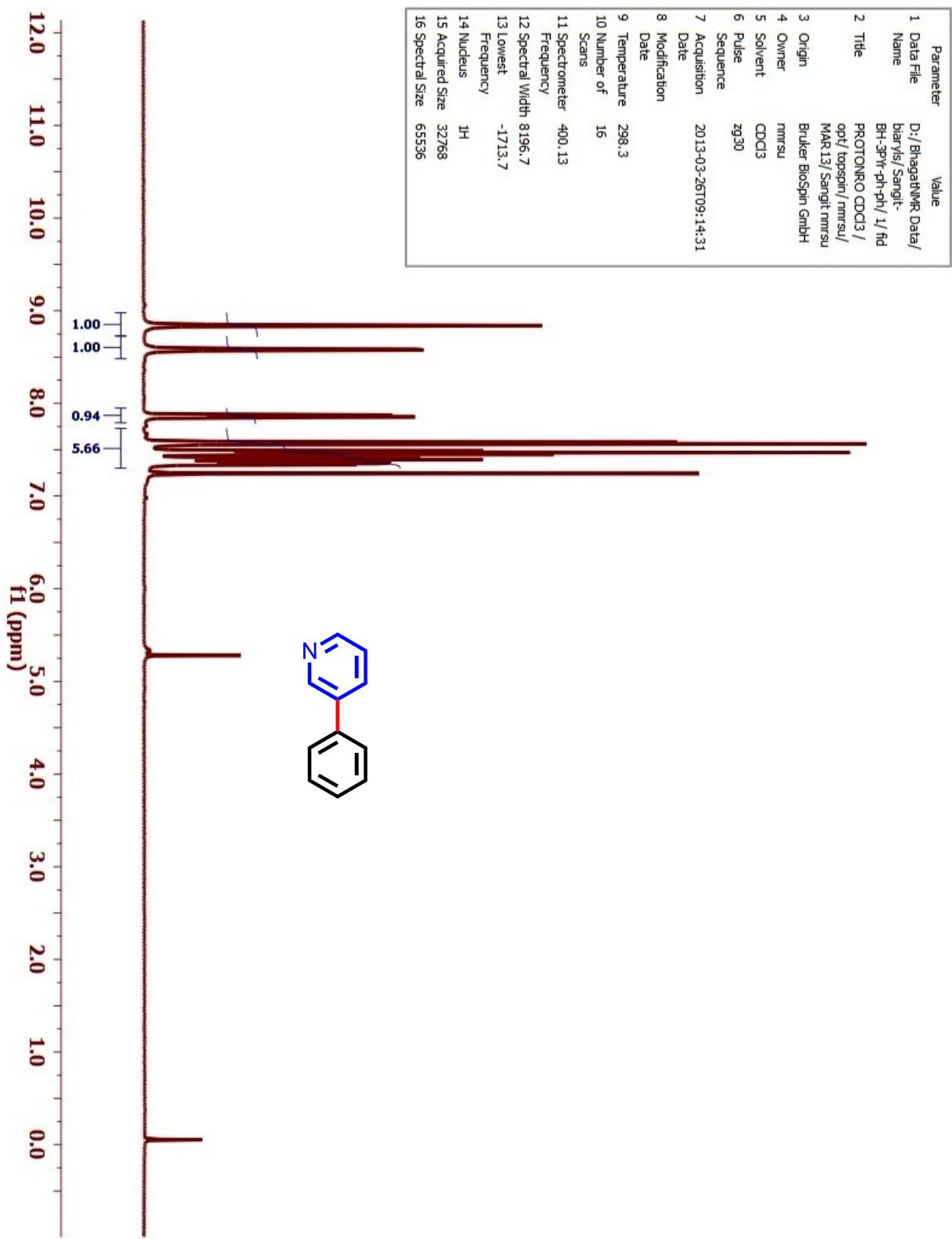


Figure S35  $^{13}\text{C}$  NMR spectrum of **11**

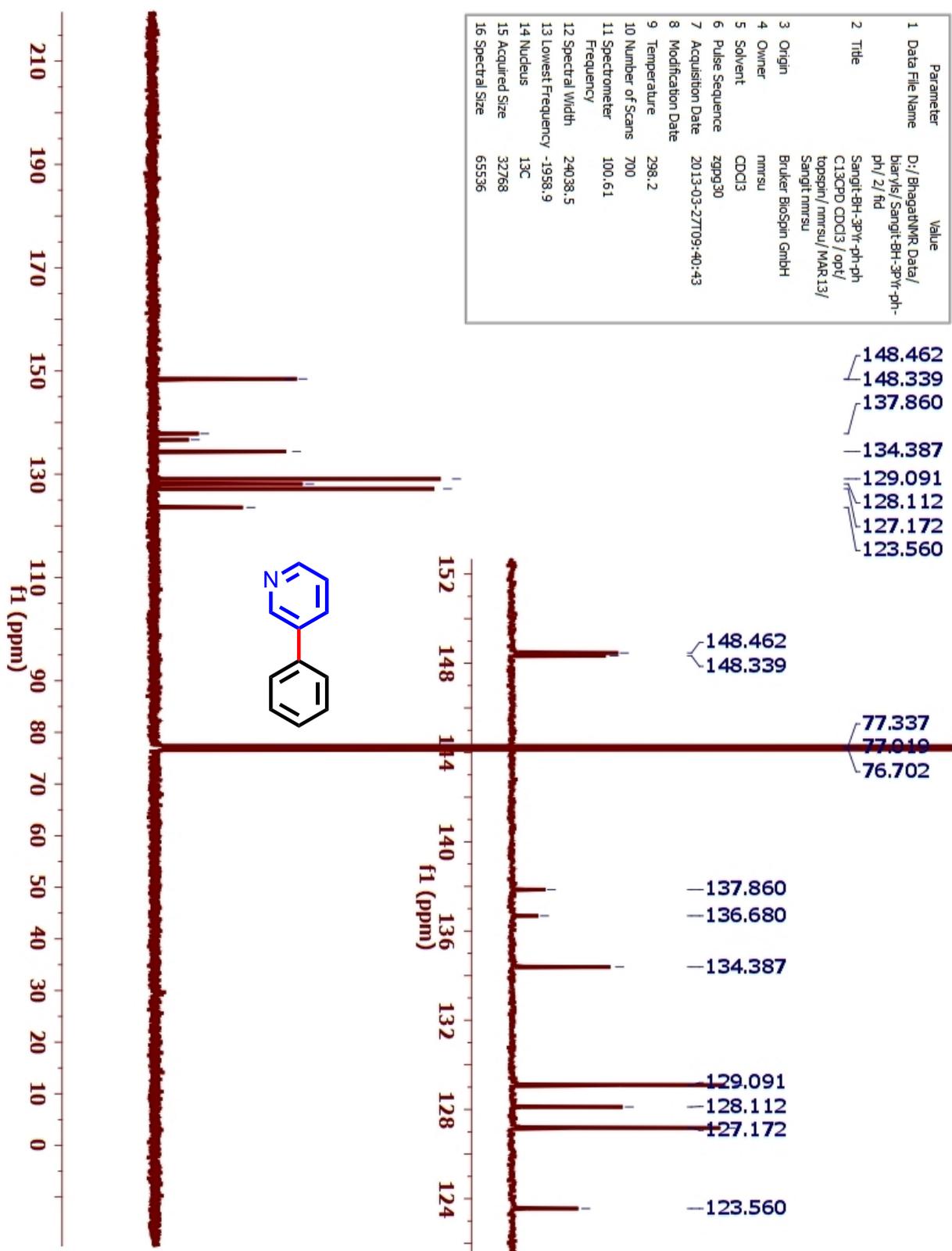


Figure S36  $^{13}\text{C}$  NMR DEPT-135 of **11**

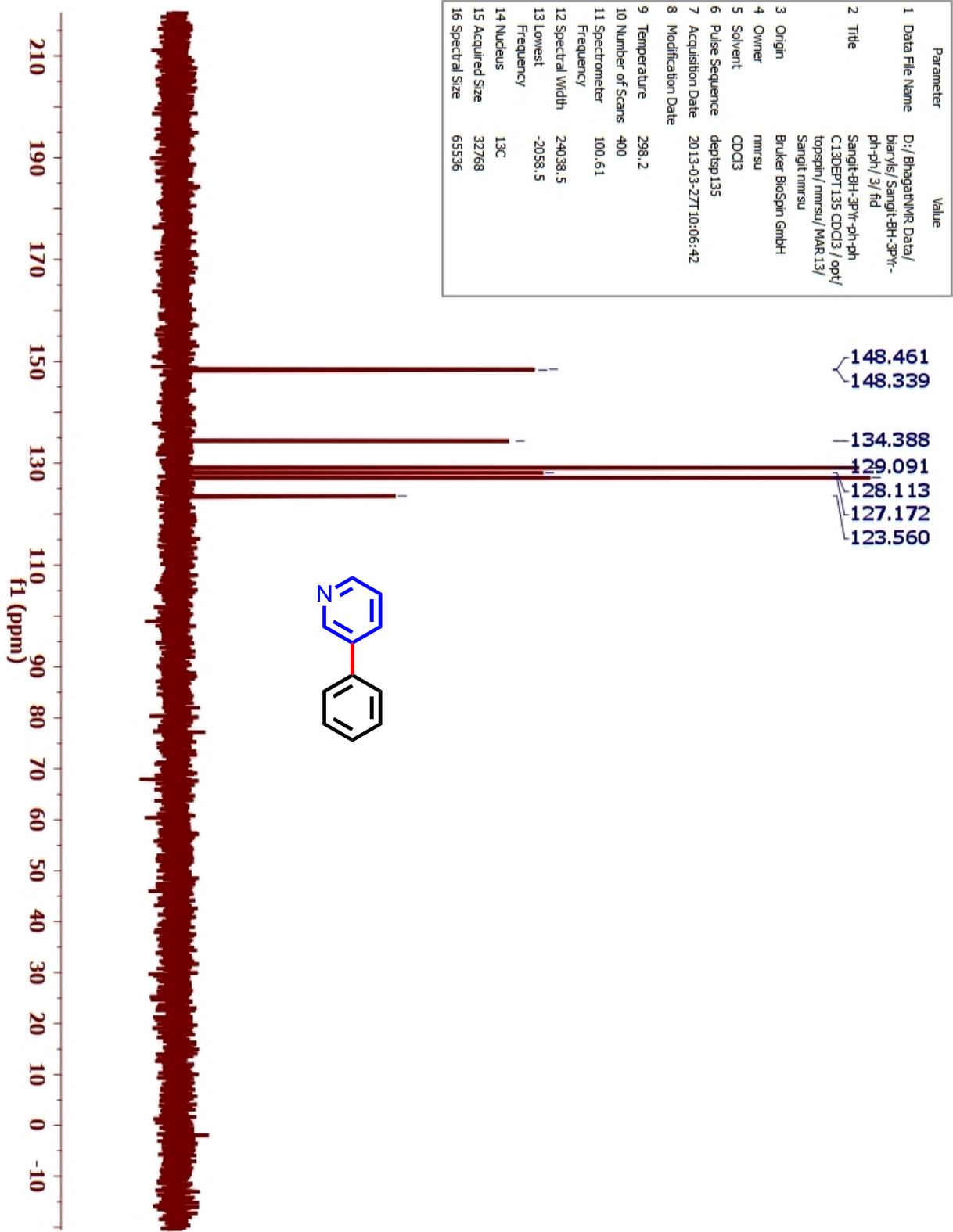


Figure S37  $^1\text{H}$  NMR of **12**

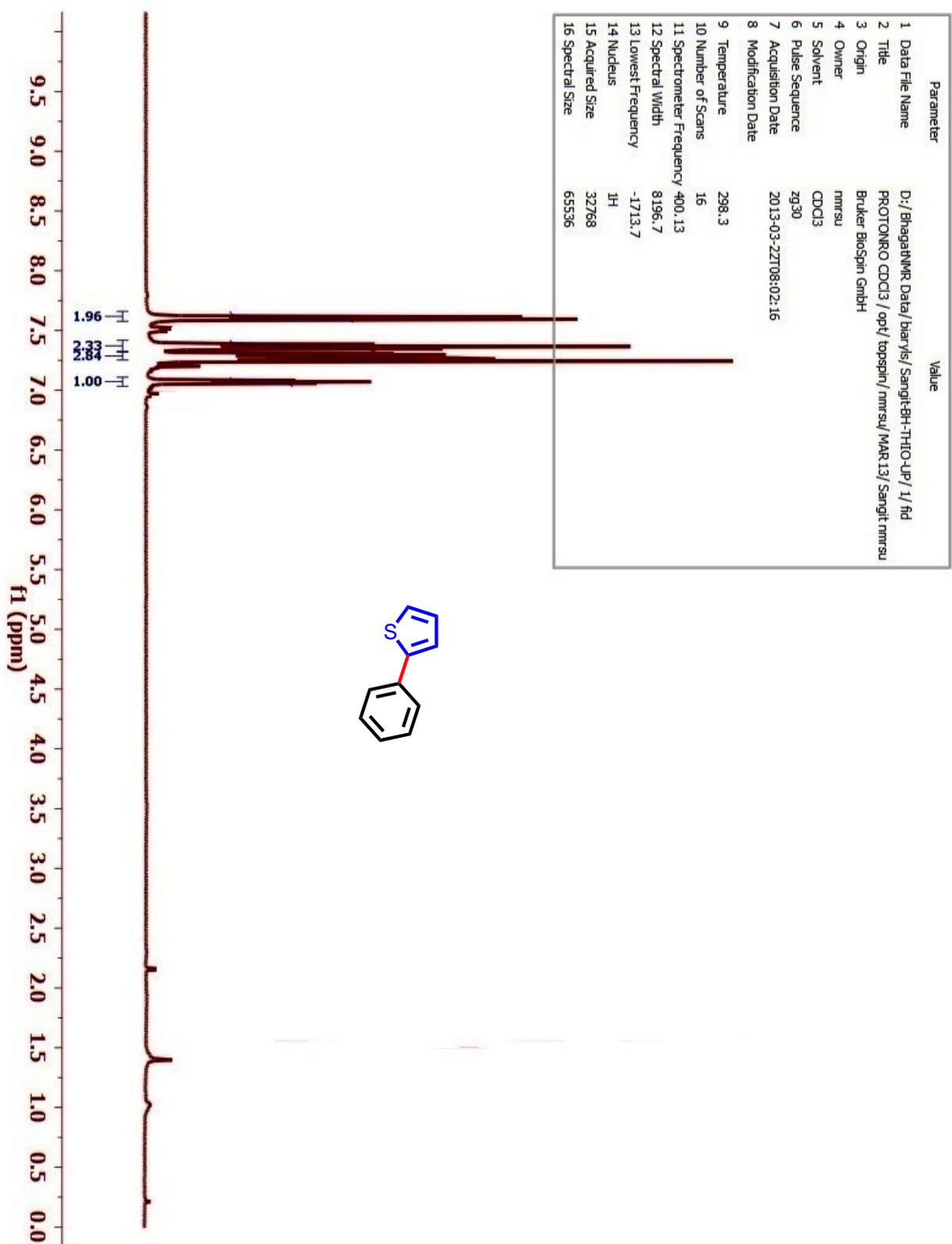


Figure S38  $^{13}\text{C}$  NMR spectrum of **12**

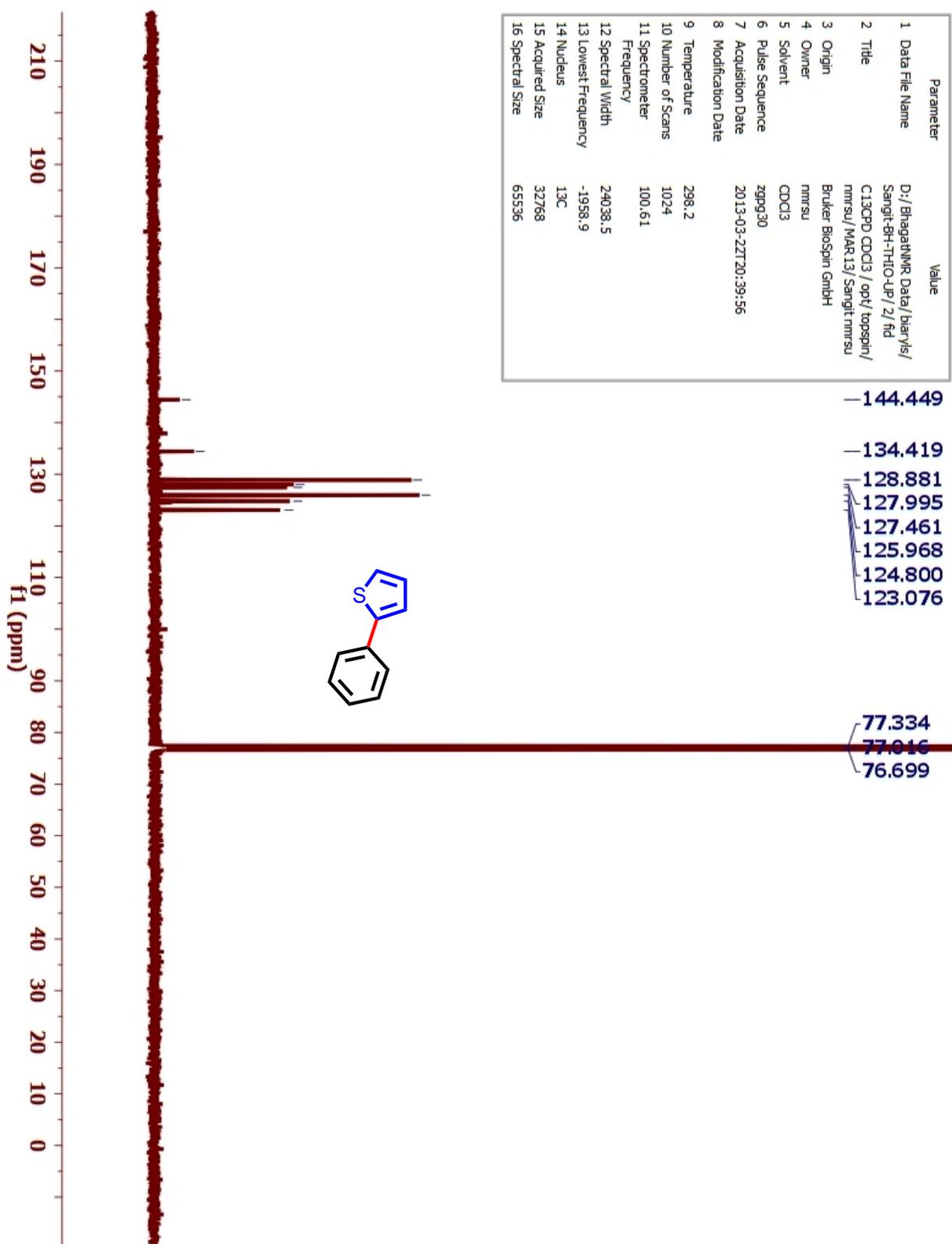


Figure S39  $^{13}\text{C}$  NMR DEPT-135 of **12**

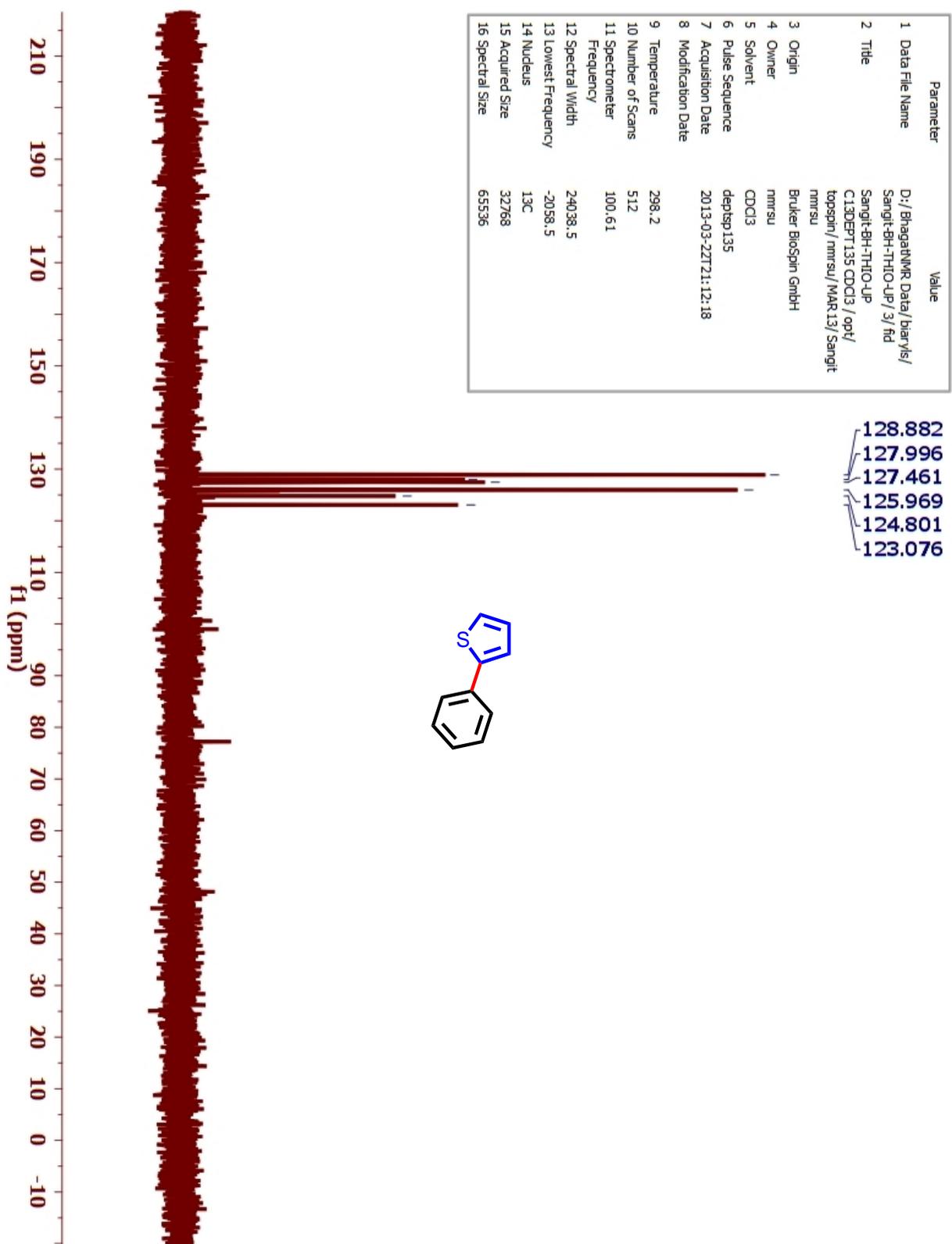


Figure S40  $^1\text{H}$  NMR of **13**

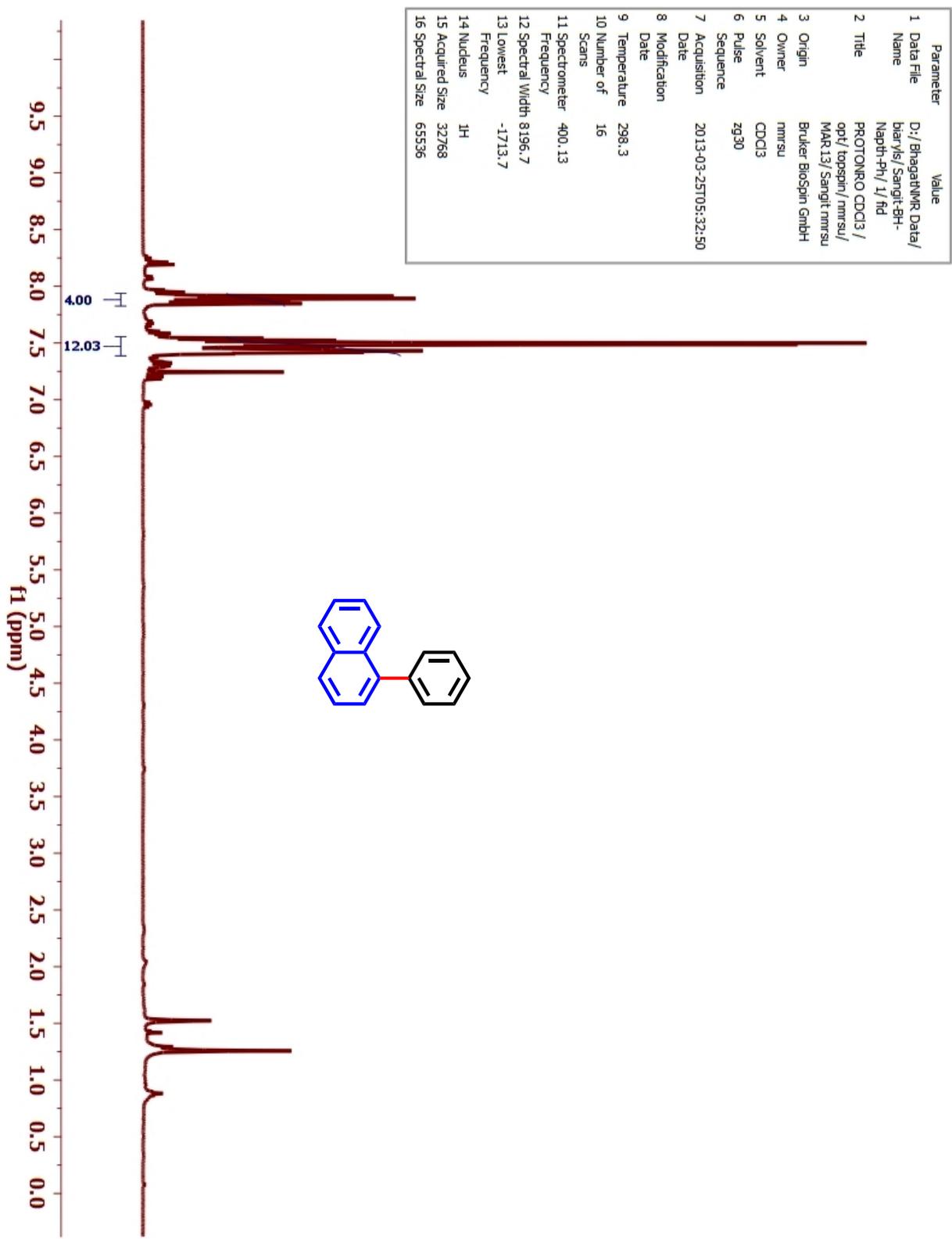


Figure S41  $^{13}\text{C}$  NMR spectrum of **13**

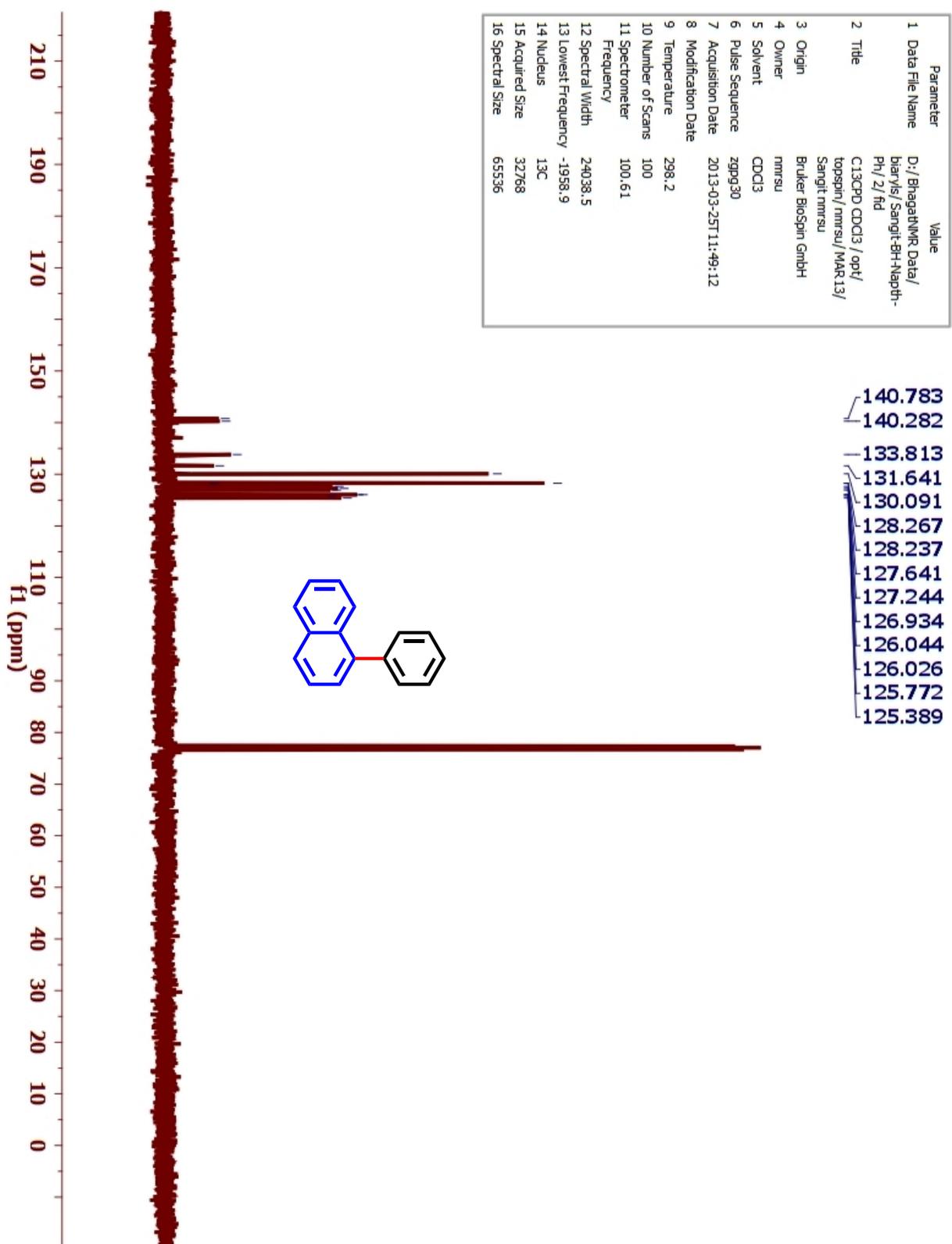


Figure S42  $^{13}\text{C}$  NMR DEPT-135 of **13**

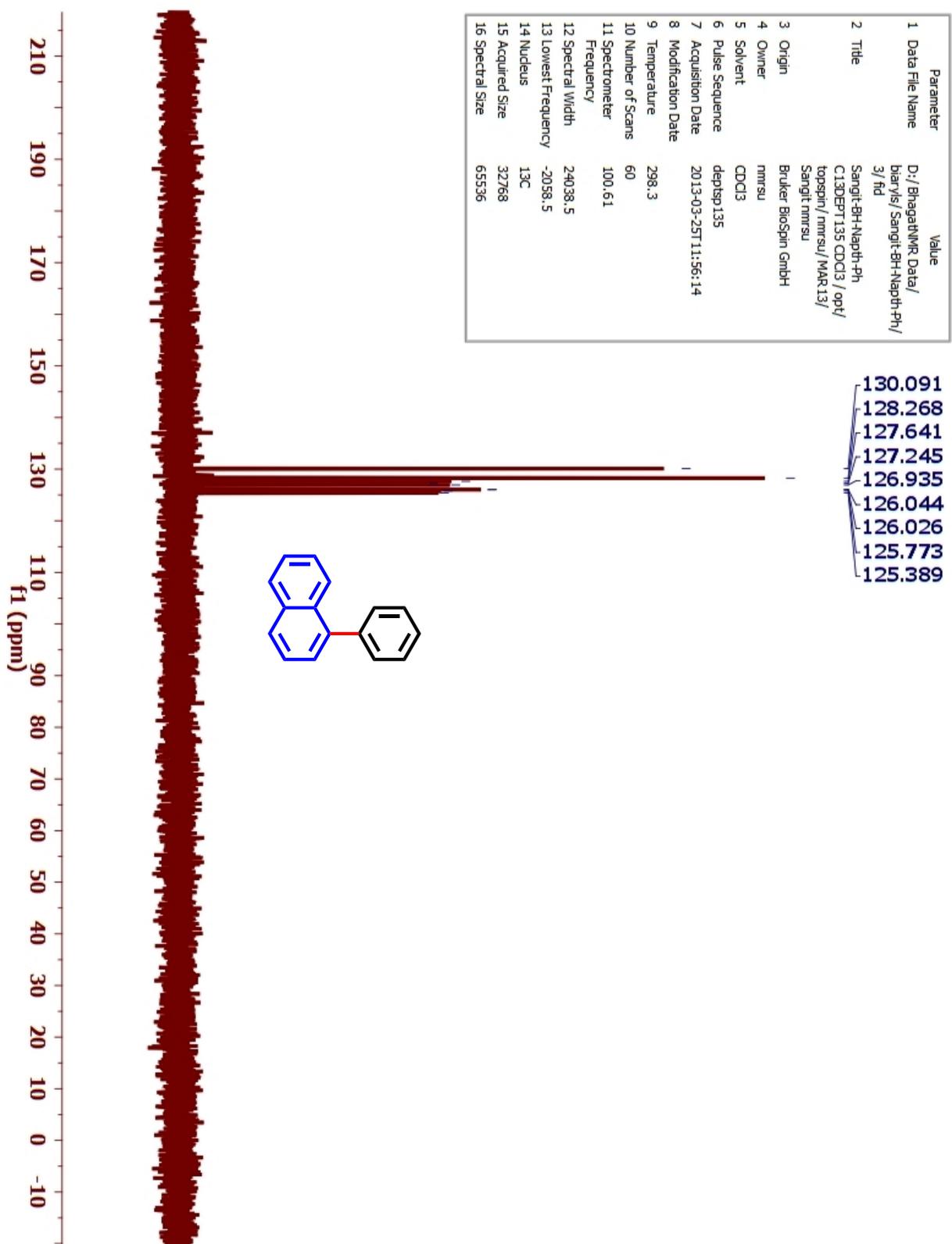


Figure S43 <sup>1</sup>H NMR of **14**

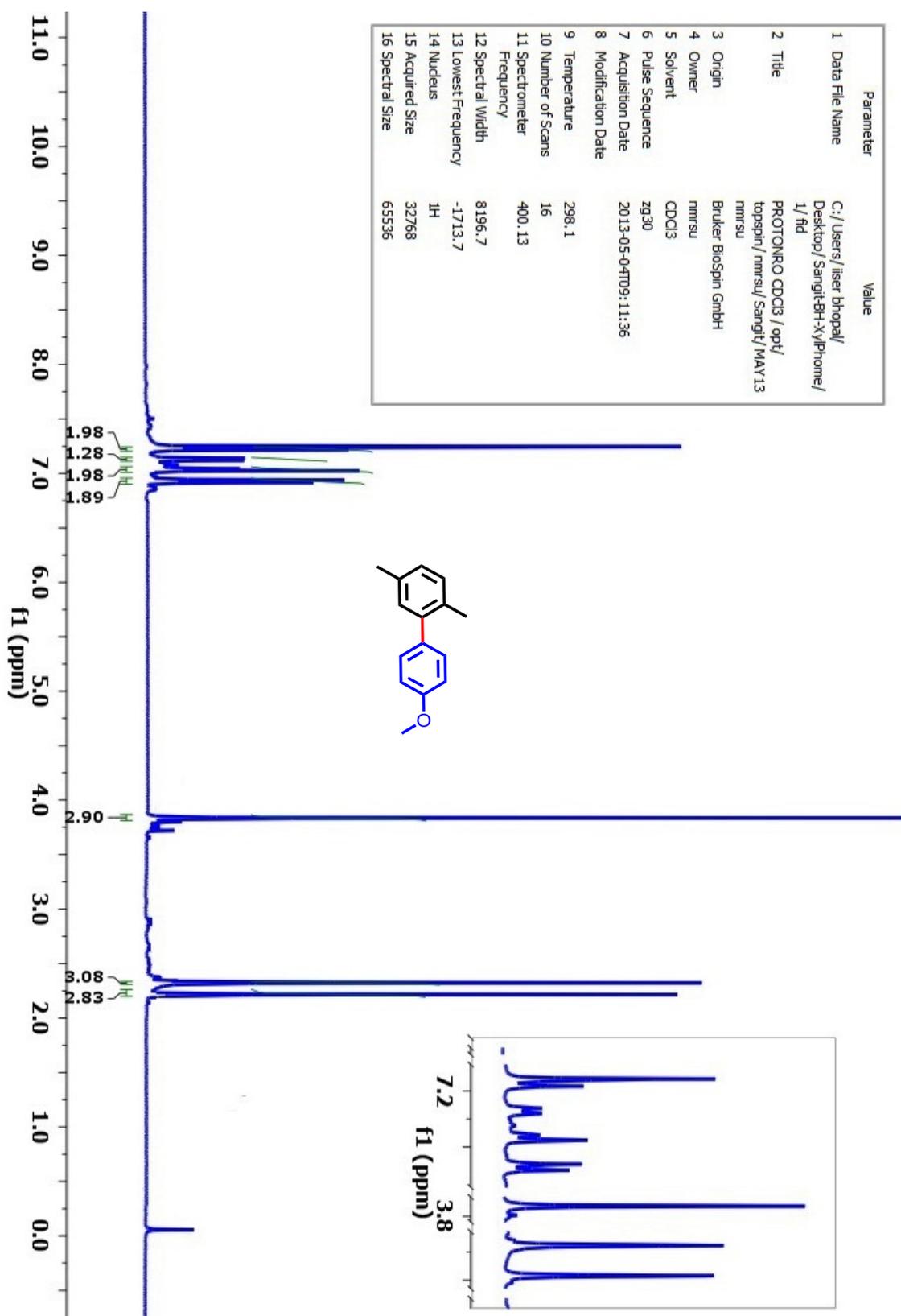


Figure S44  $^{13}\text{C}$  NMR spectrum of **14**

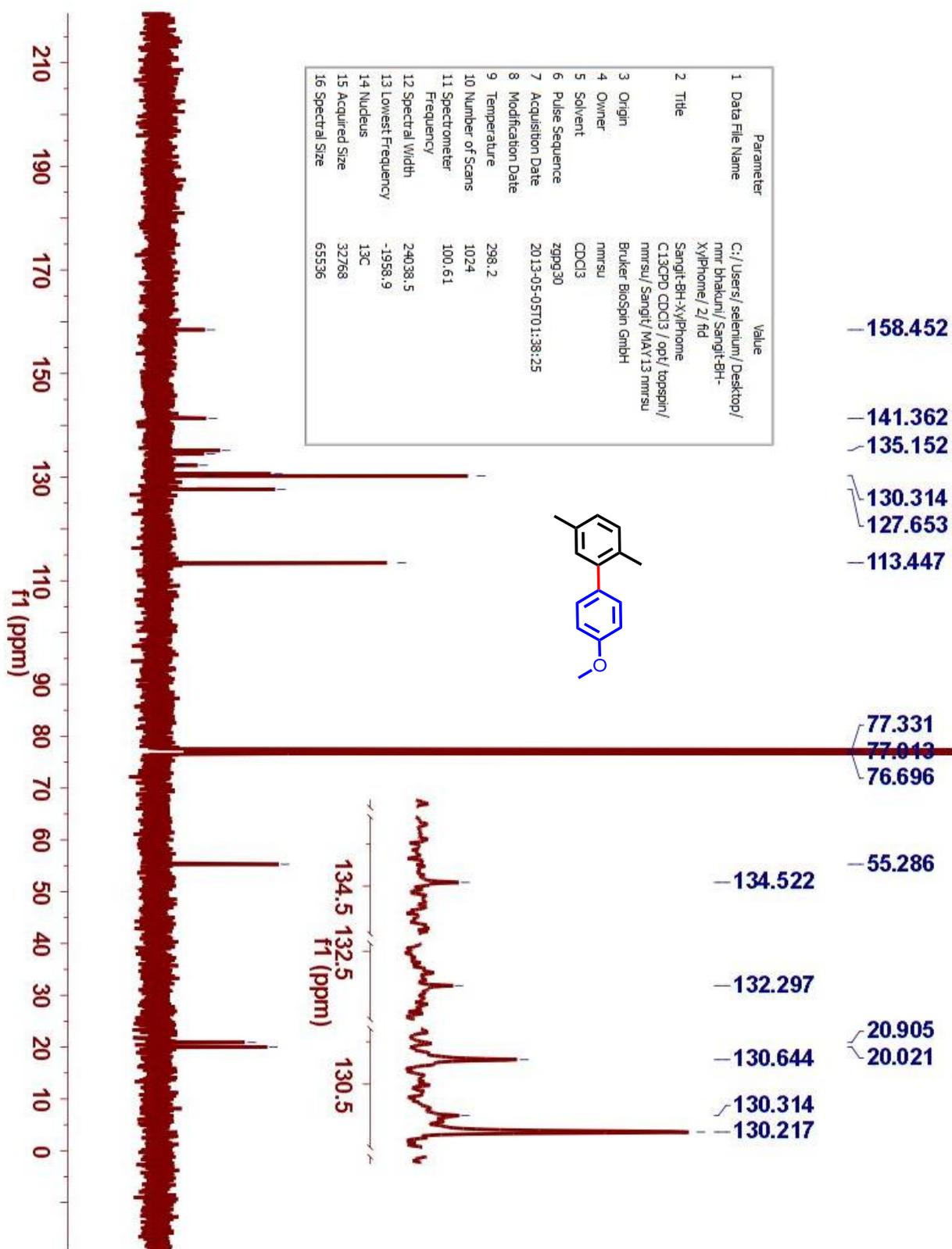


Figure S45  $^{13}\text{C}$  NMR DEPT-135 of **14**

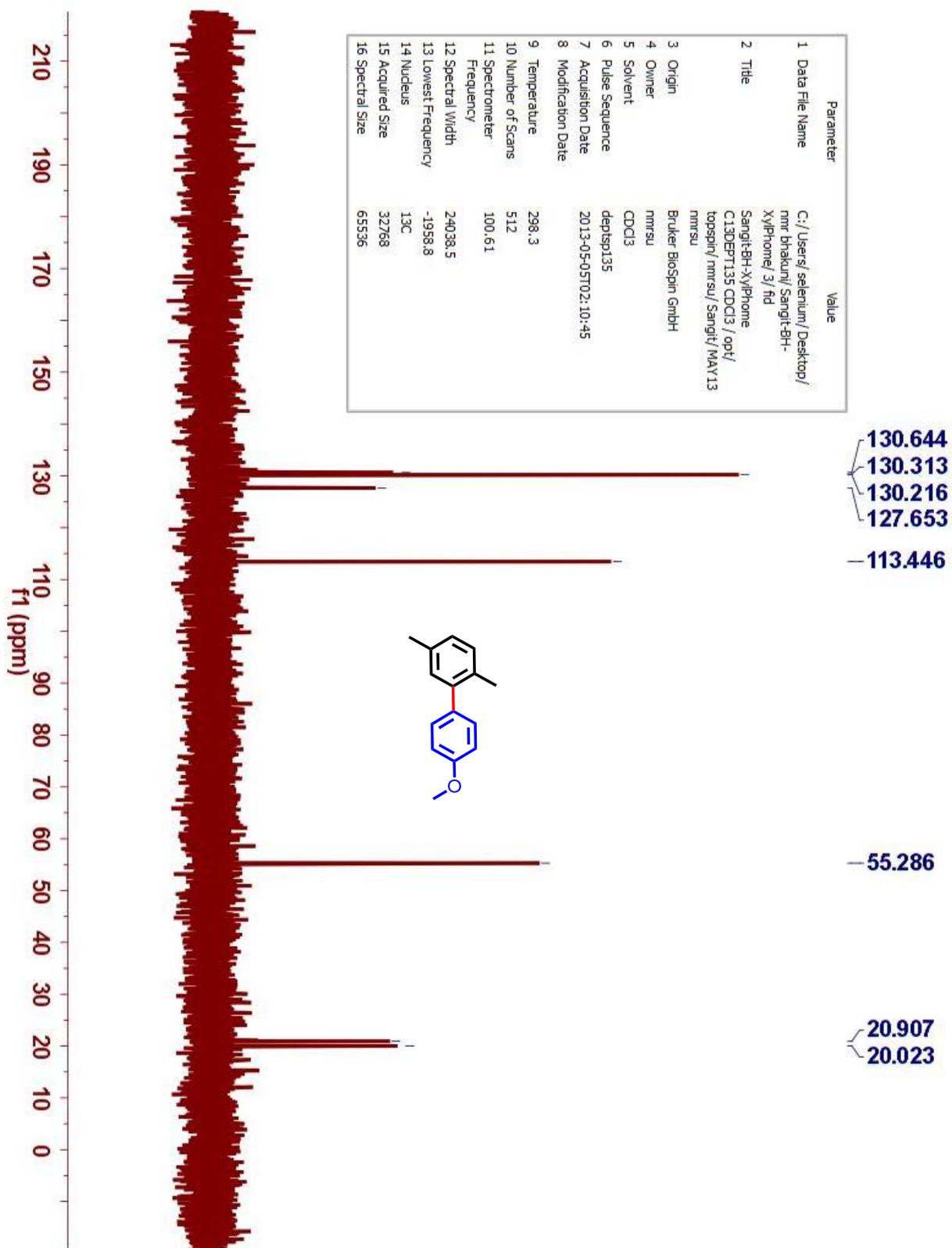


Figure S46 <sup>1</sup>H NMR of **15**

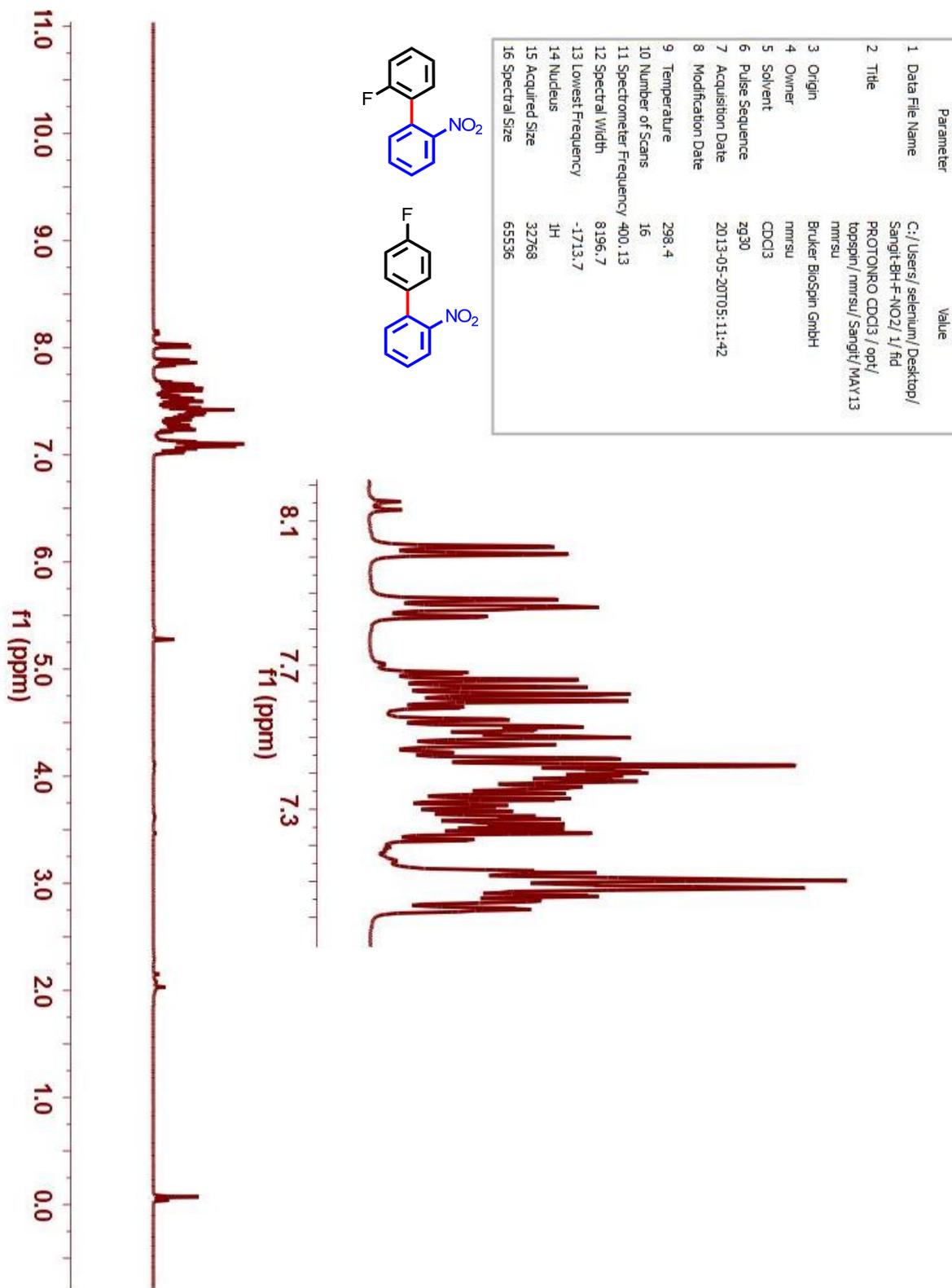


Figure S47 <sup>13</sup>C NMR spectrum of **15**

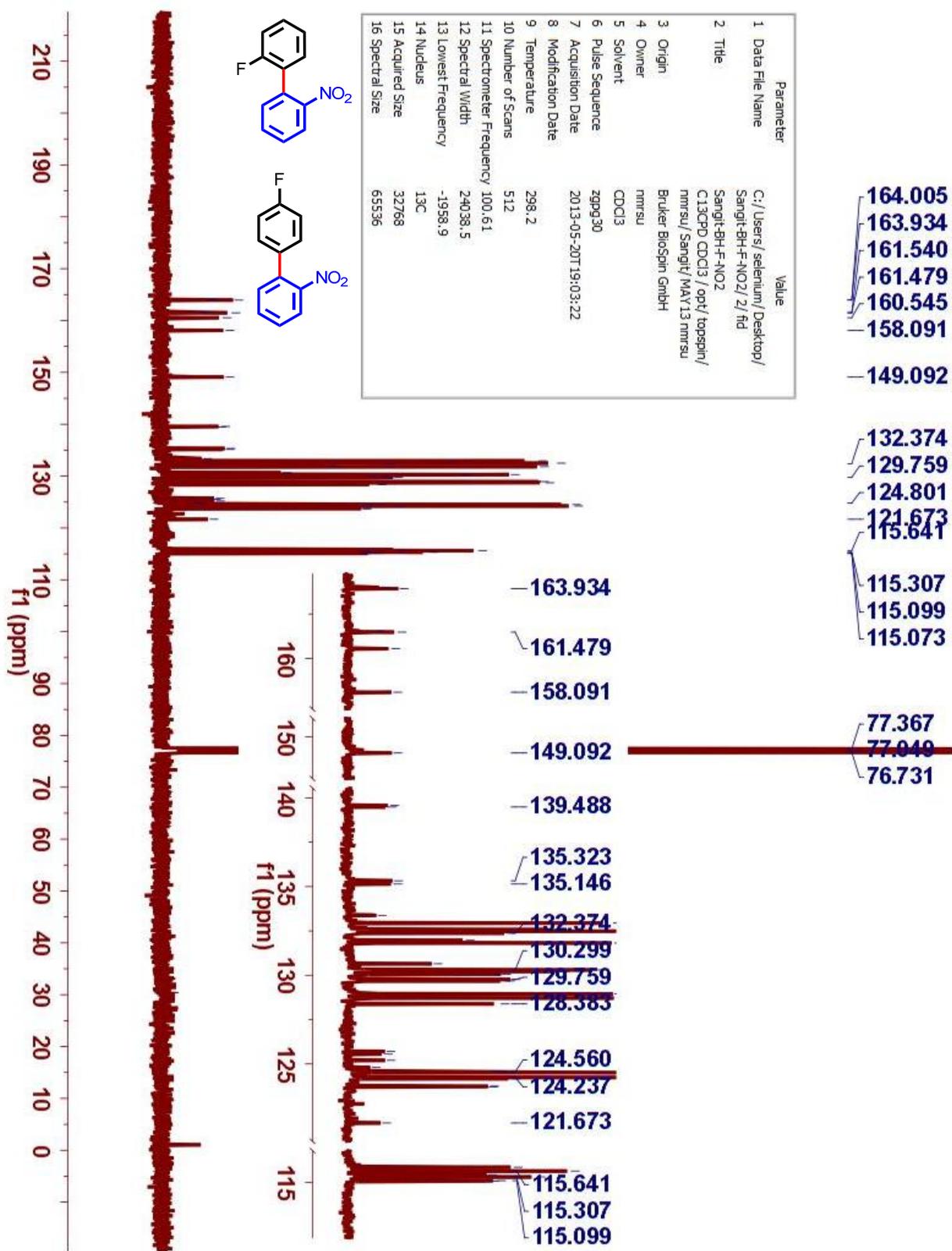


Figure S48 <sup>13</sup>C NMR DEPT-135 of **15**

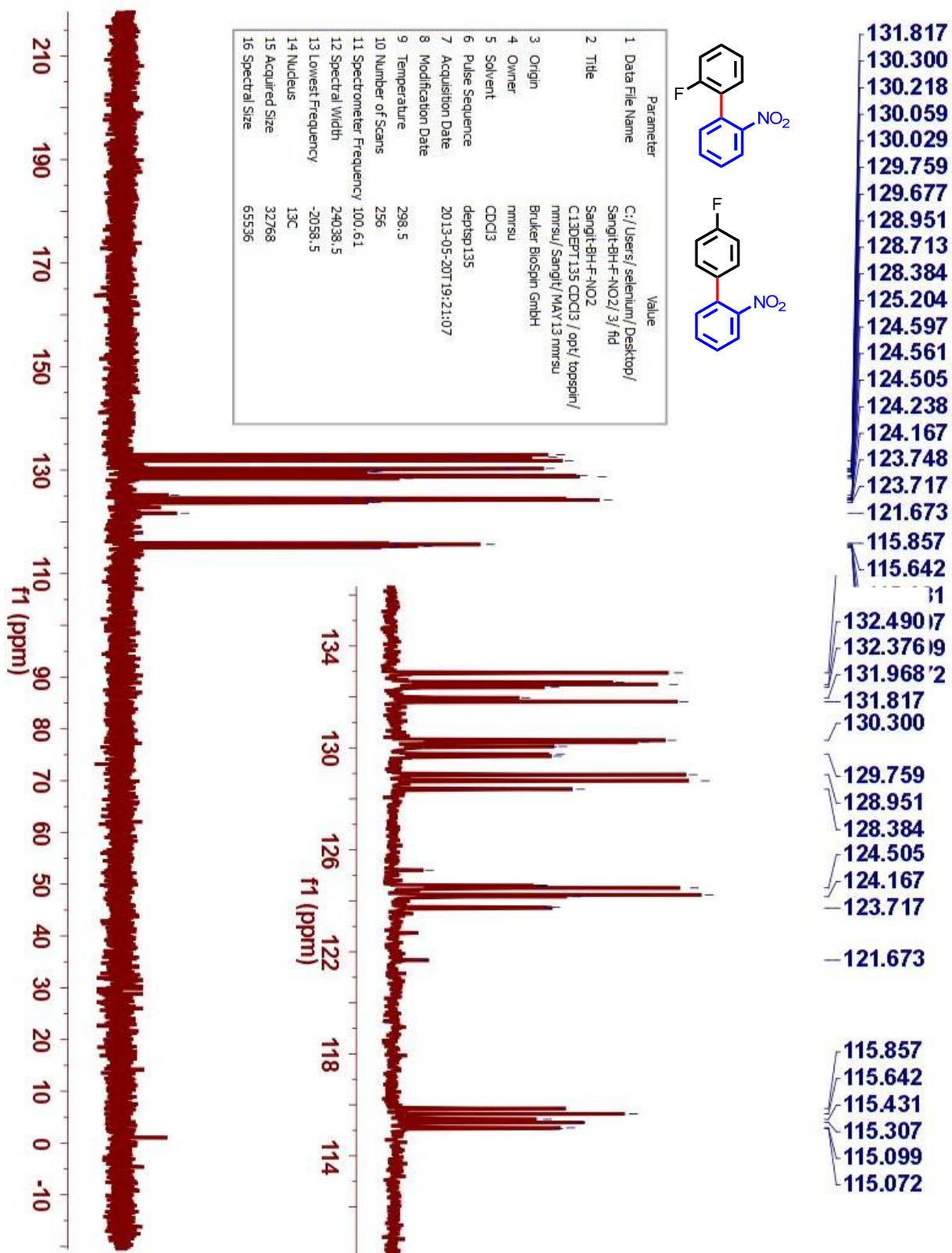


Figure S49  $^1\text{H}$  NMR of **16**

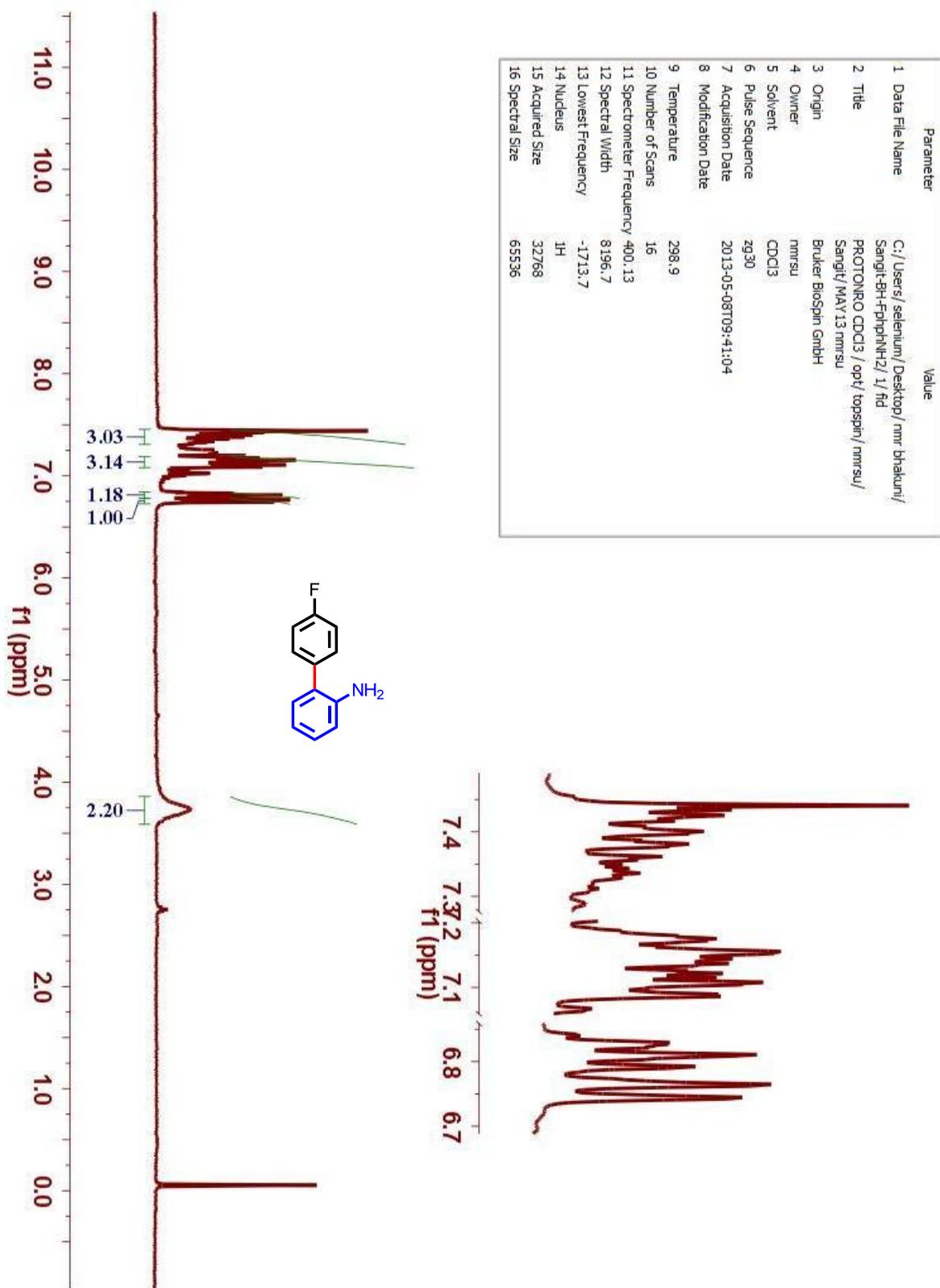


Figure S50  $^{13}\text{C}$  NMR spectrum of **16**

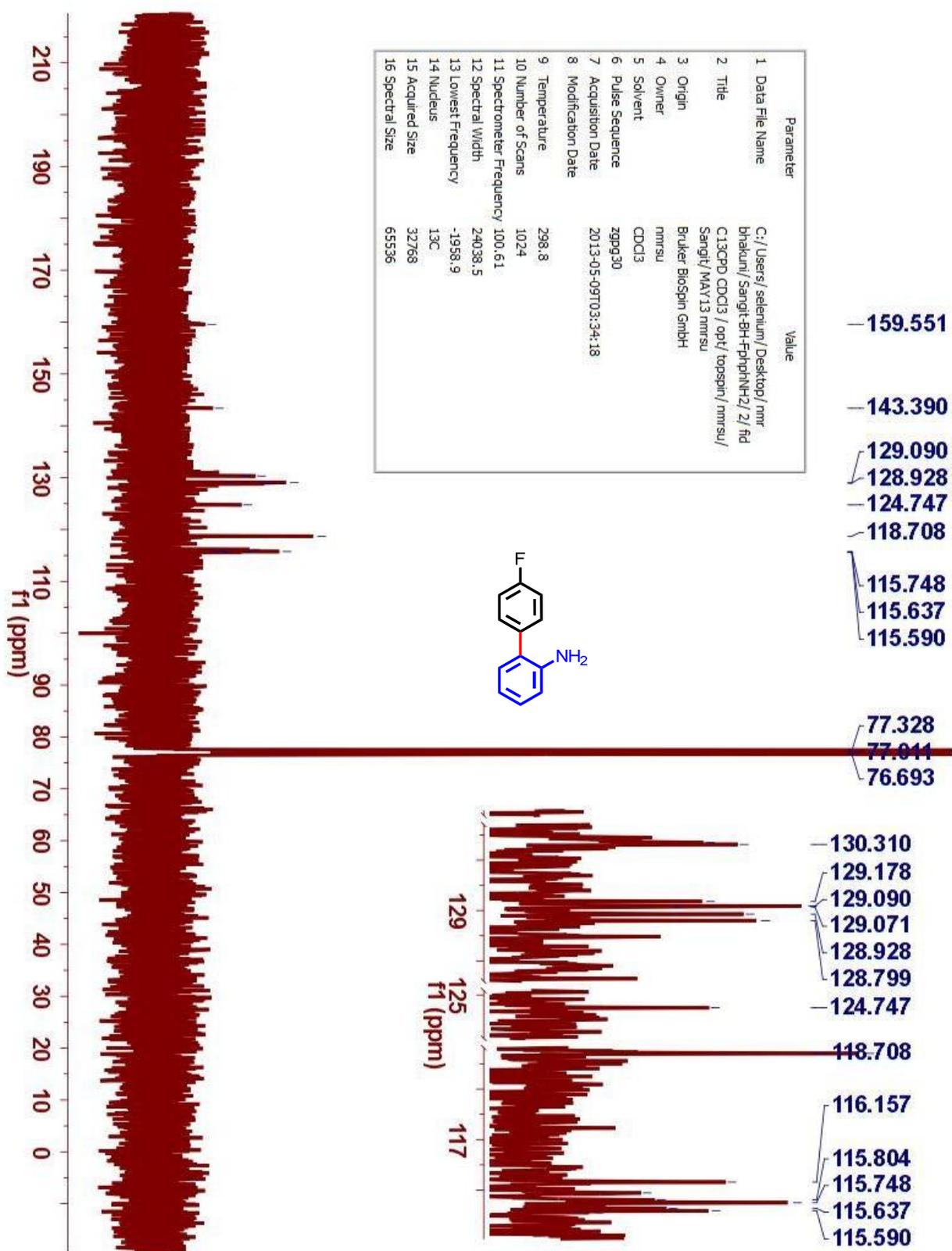


Figure S51  $^1\text{H}$  NMR of **17**

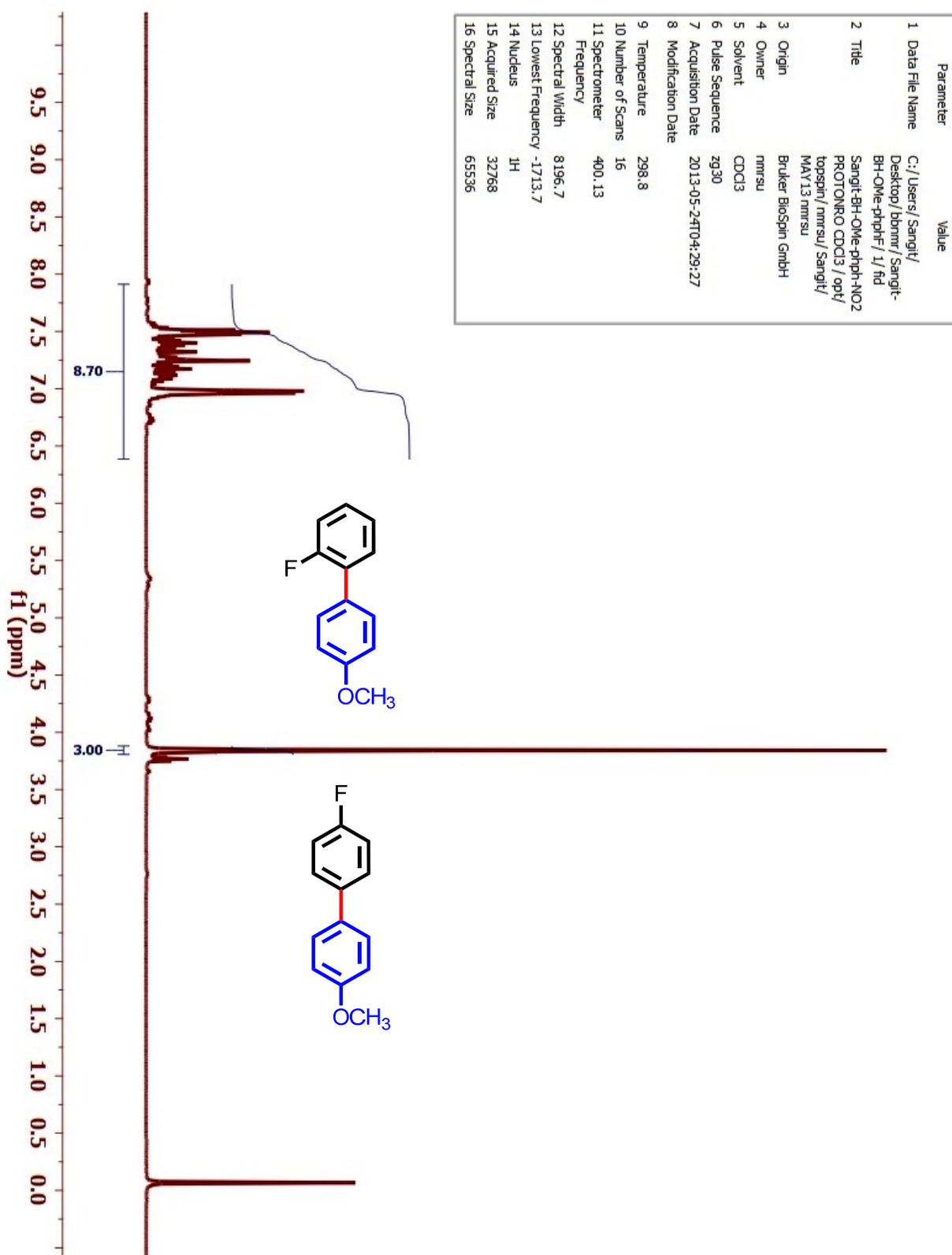


Figure S52 <sup>13</sup>C NMR spectrum of **17**

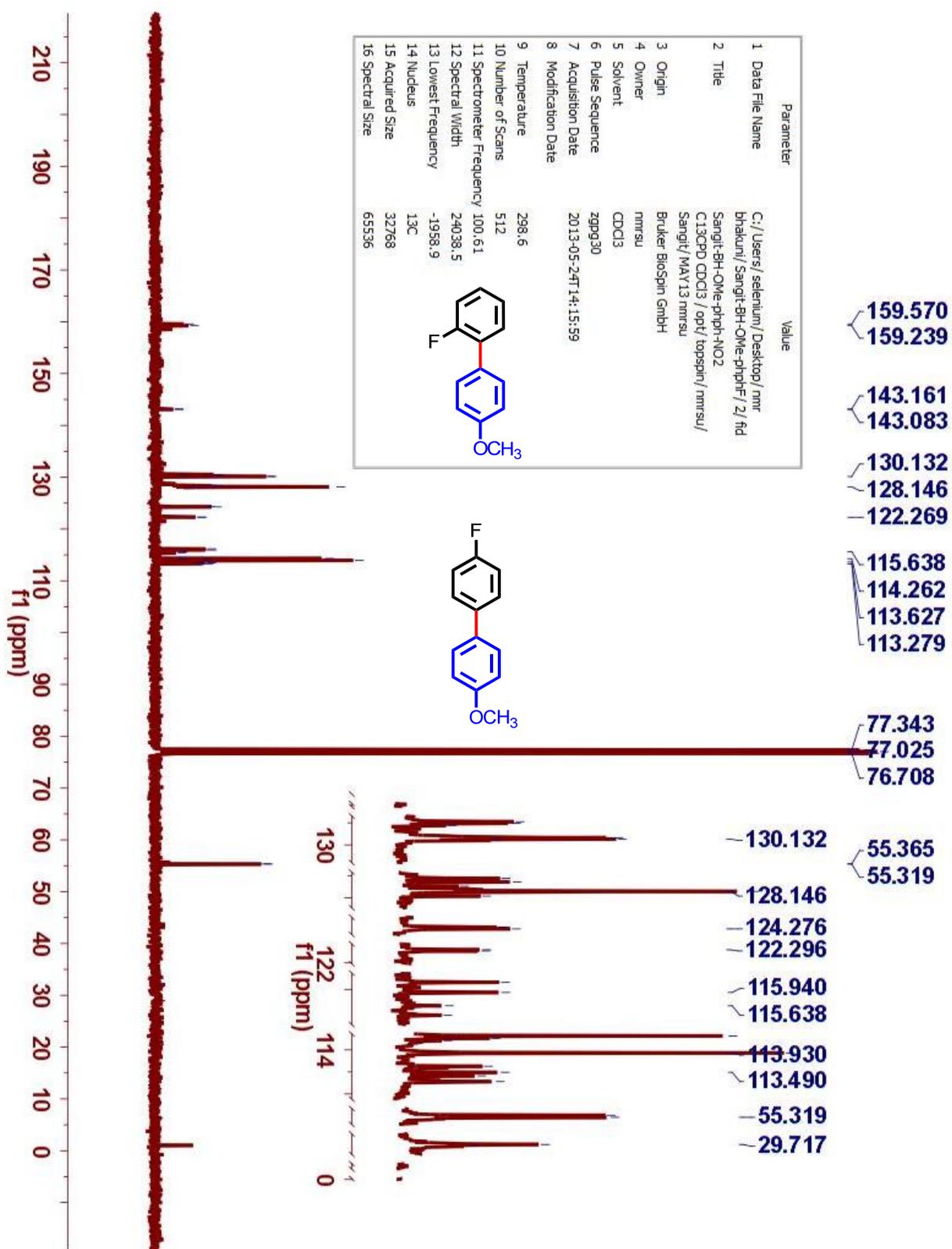


Figure S53 <sup>13</sup>C NMR DEPT-135 of **17**

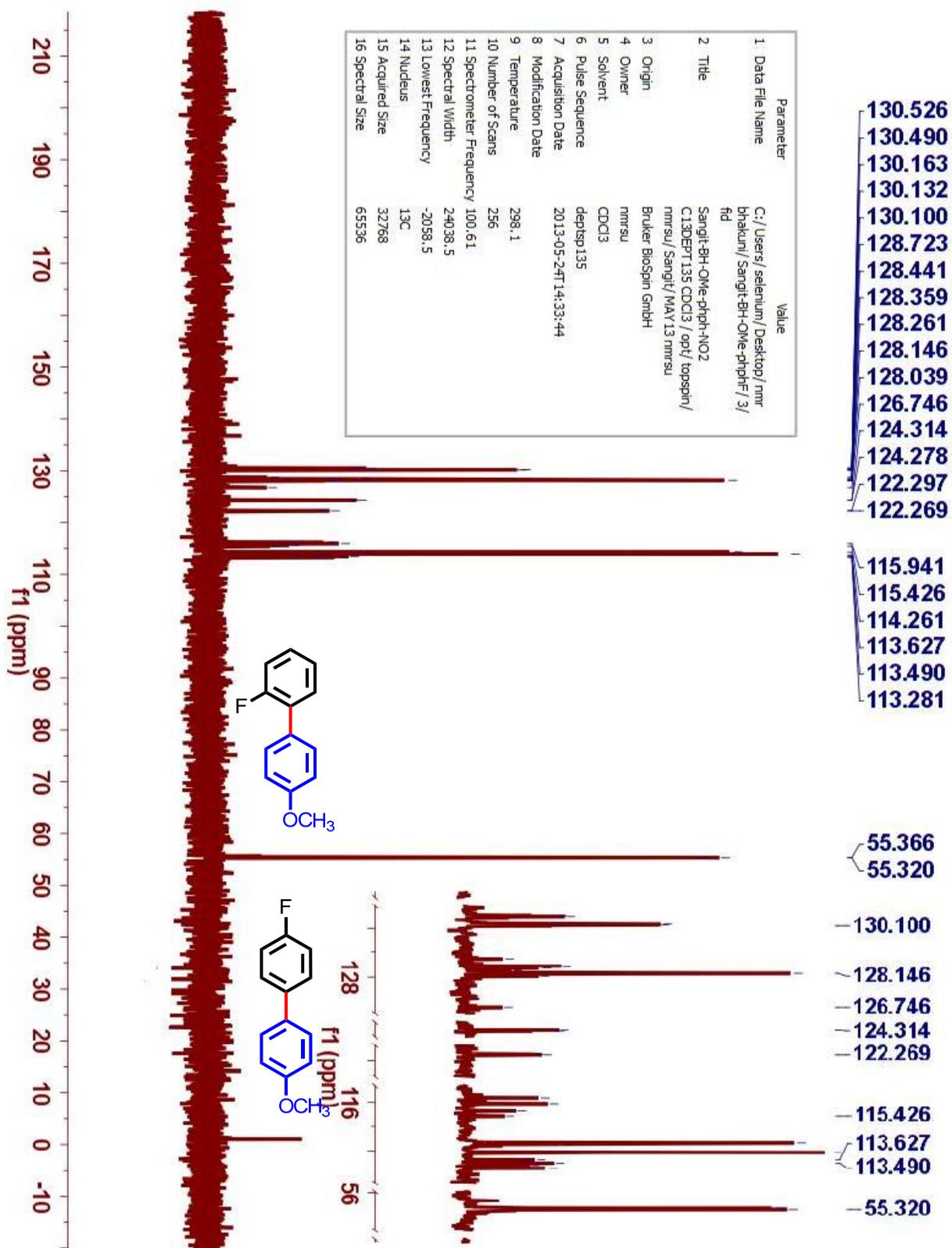


Figure S54 <sup>1</sup>H NMR of **18**

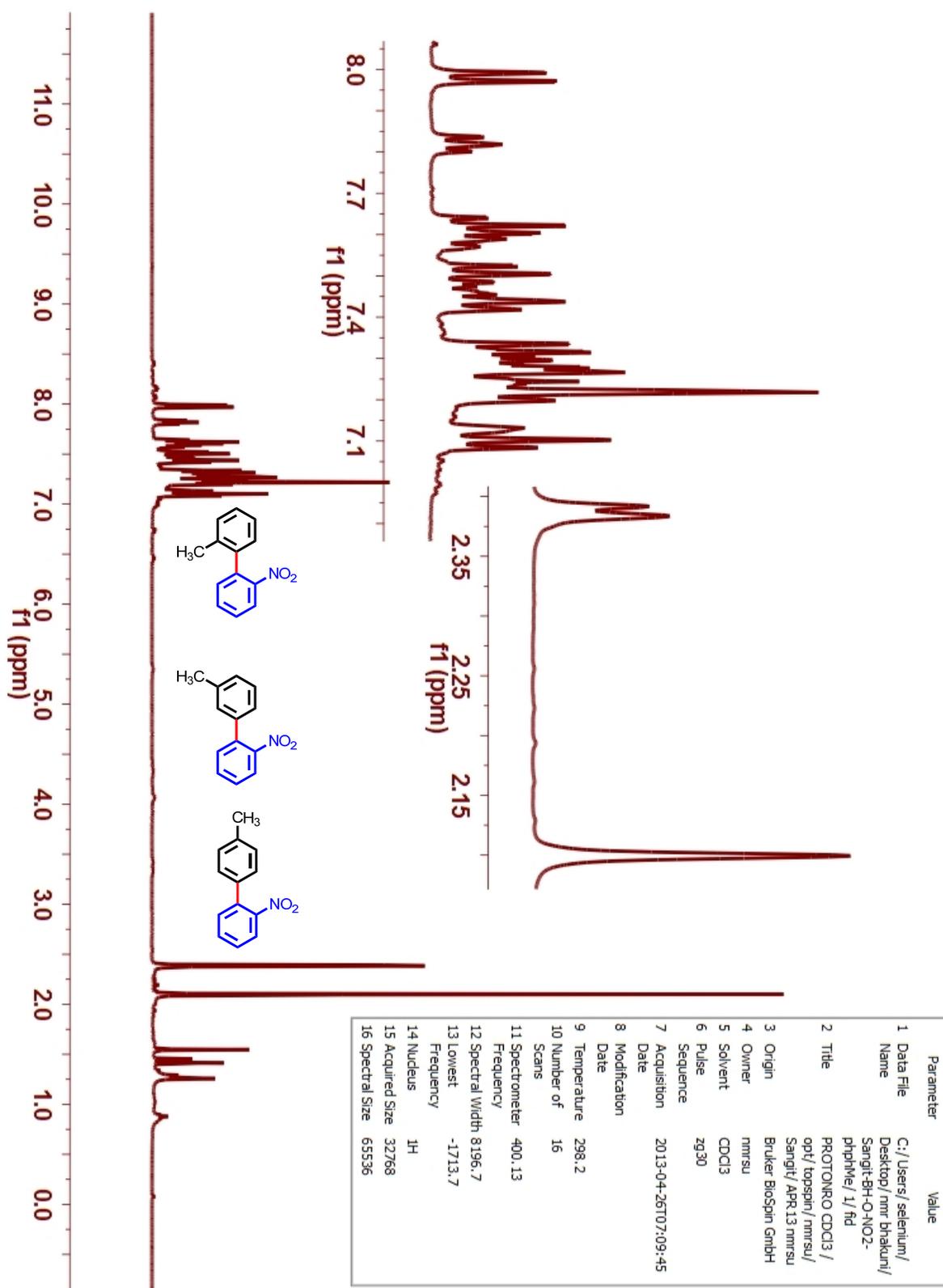


Figure S55 <sup>13</sup>C NMR spectrum of **18**

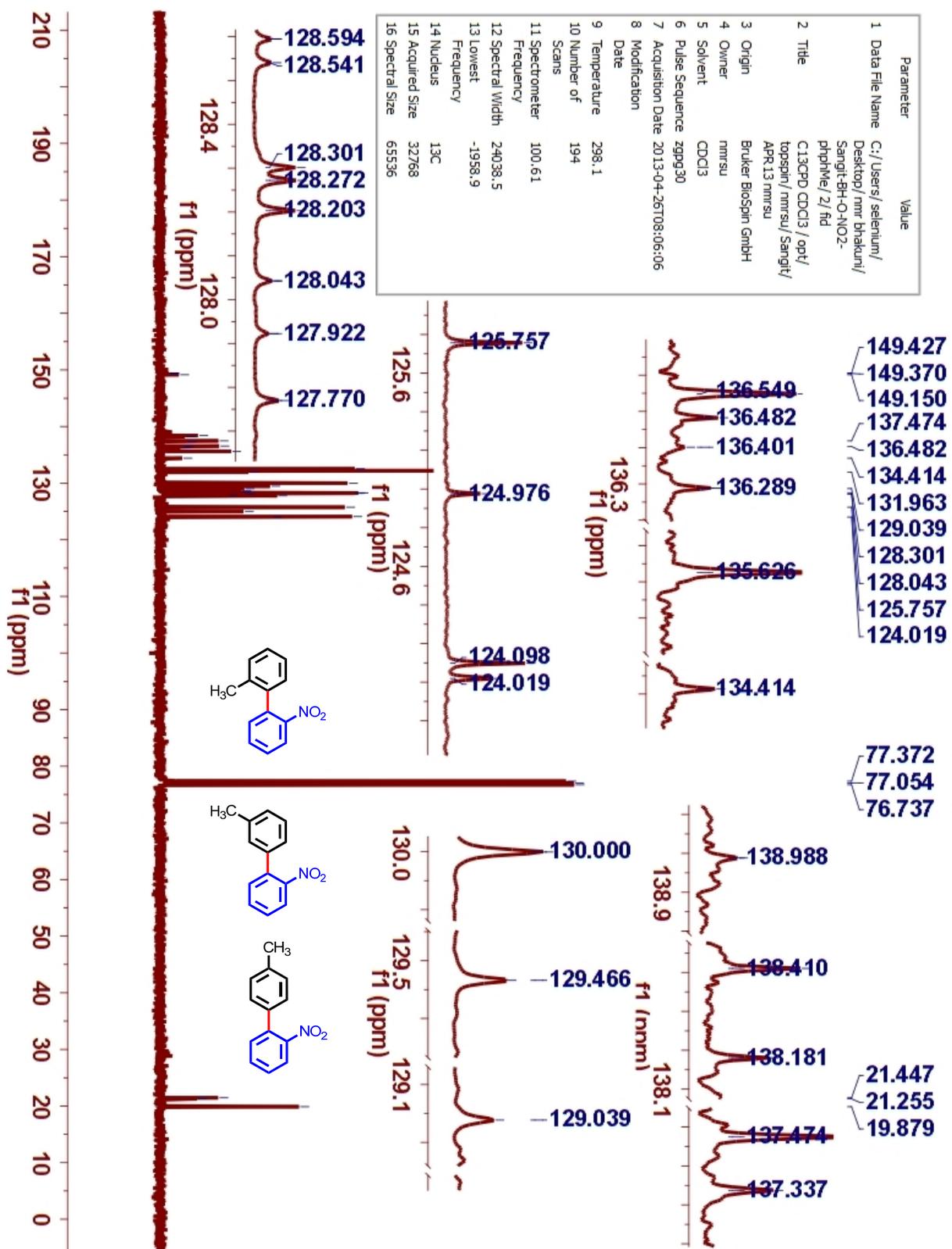


Figure S56  $^{13}\text{C}$  NMR DEPT-135 of **18**

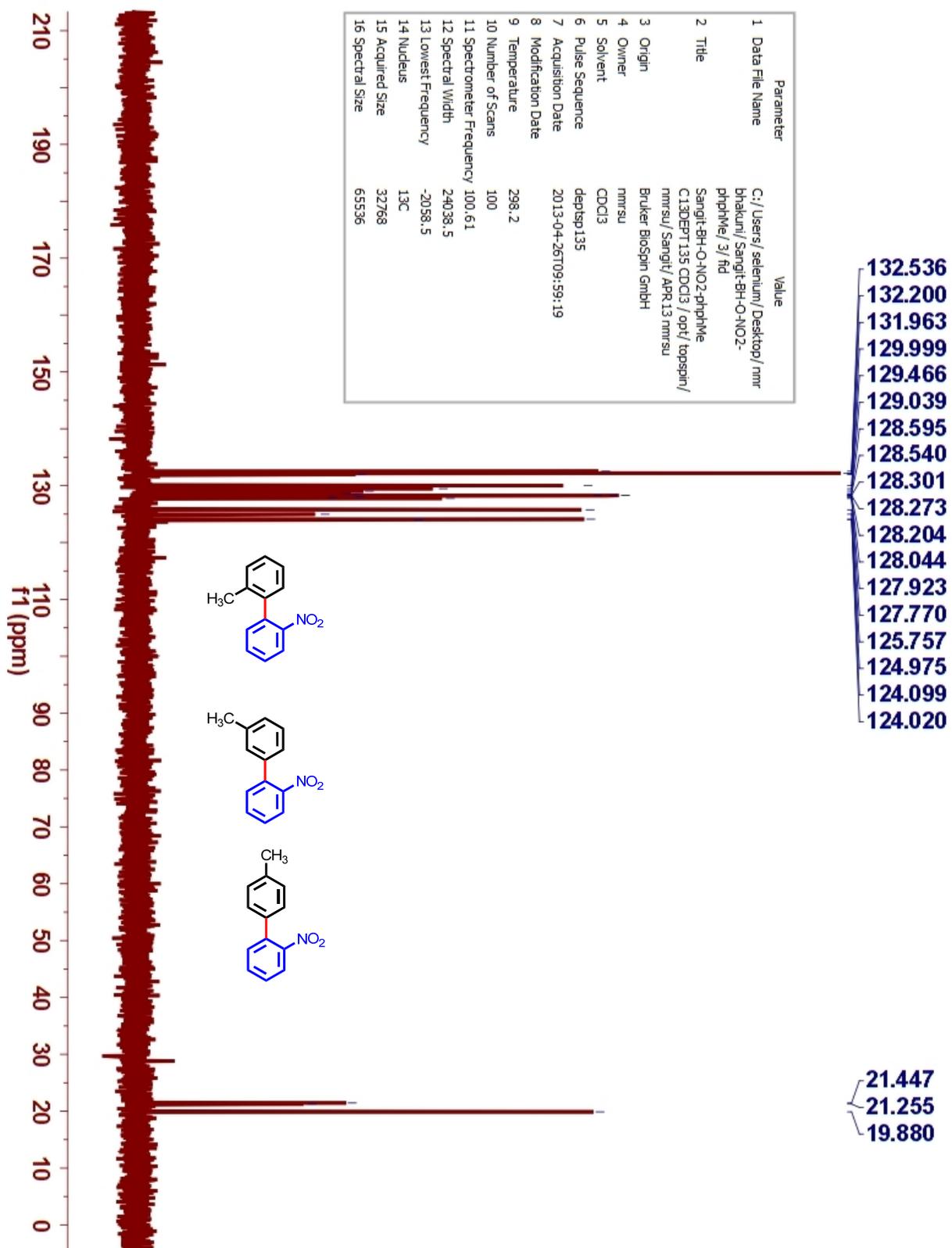


Figure S57  $^1\text{H}$  NMR of **19**

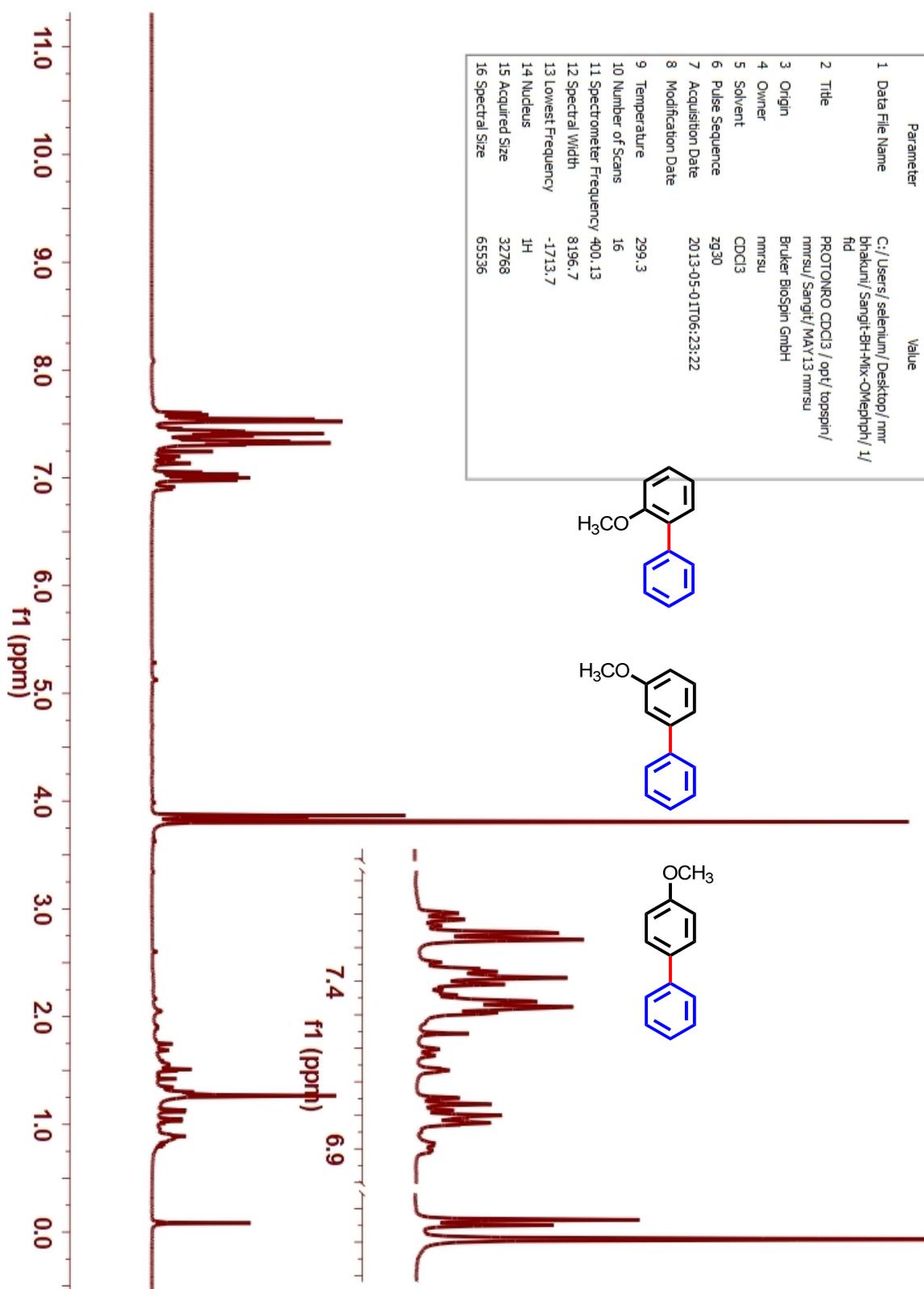


Figure S58 <sup>13</sup>C NMR spectrum of **19**

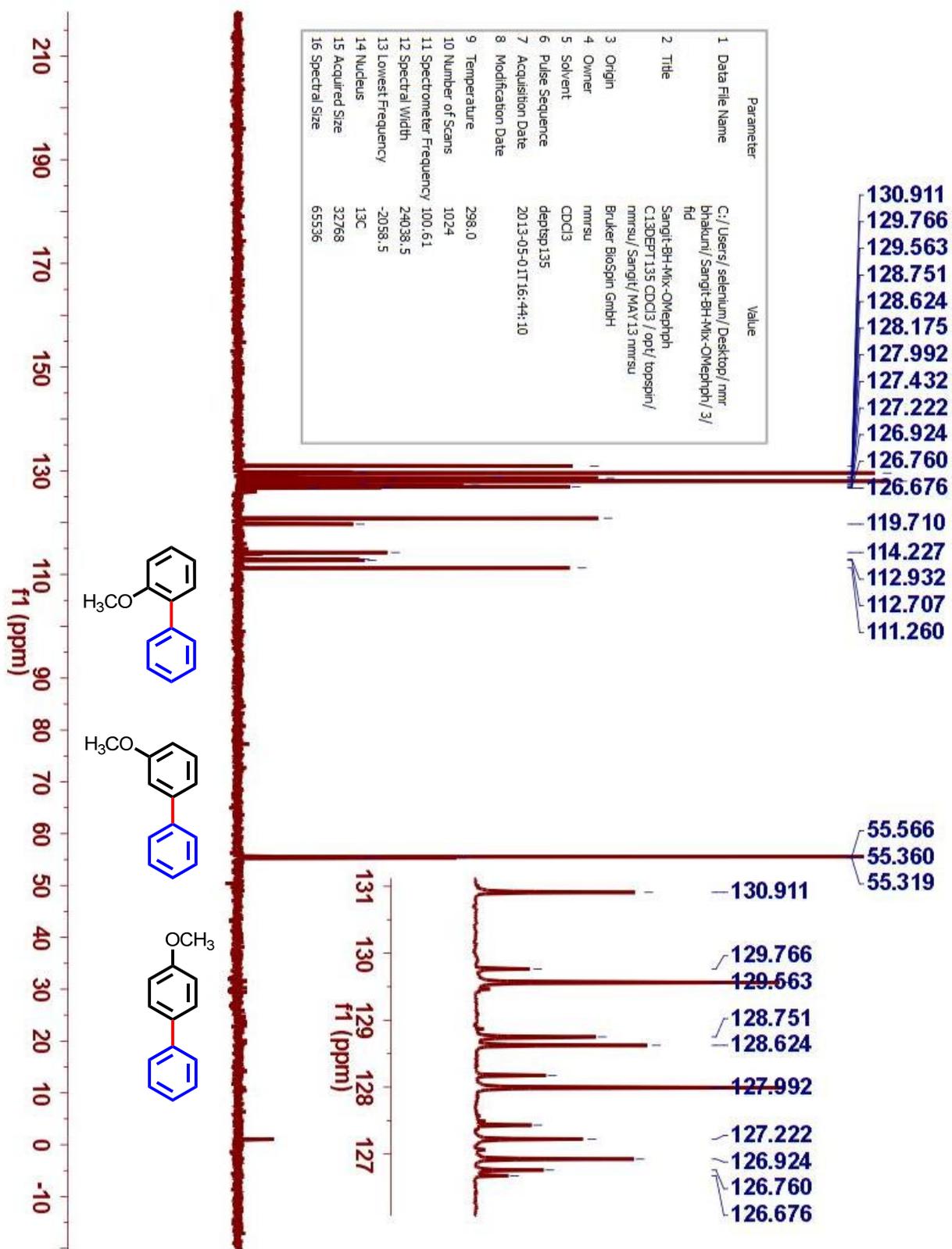


Figure S59 <sup>13</sup>C NMR DEPT-135 of **19**

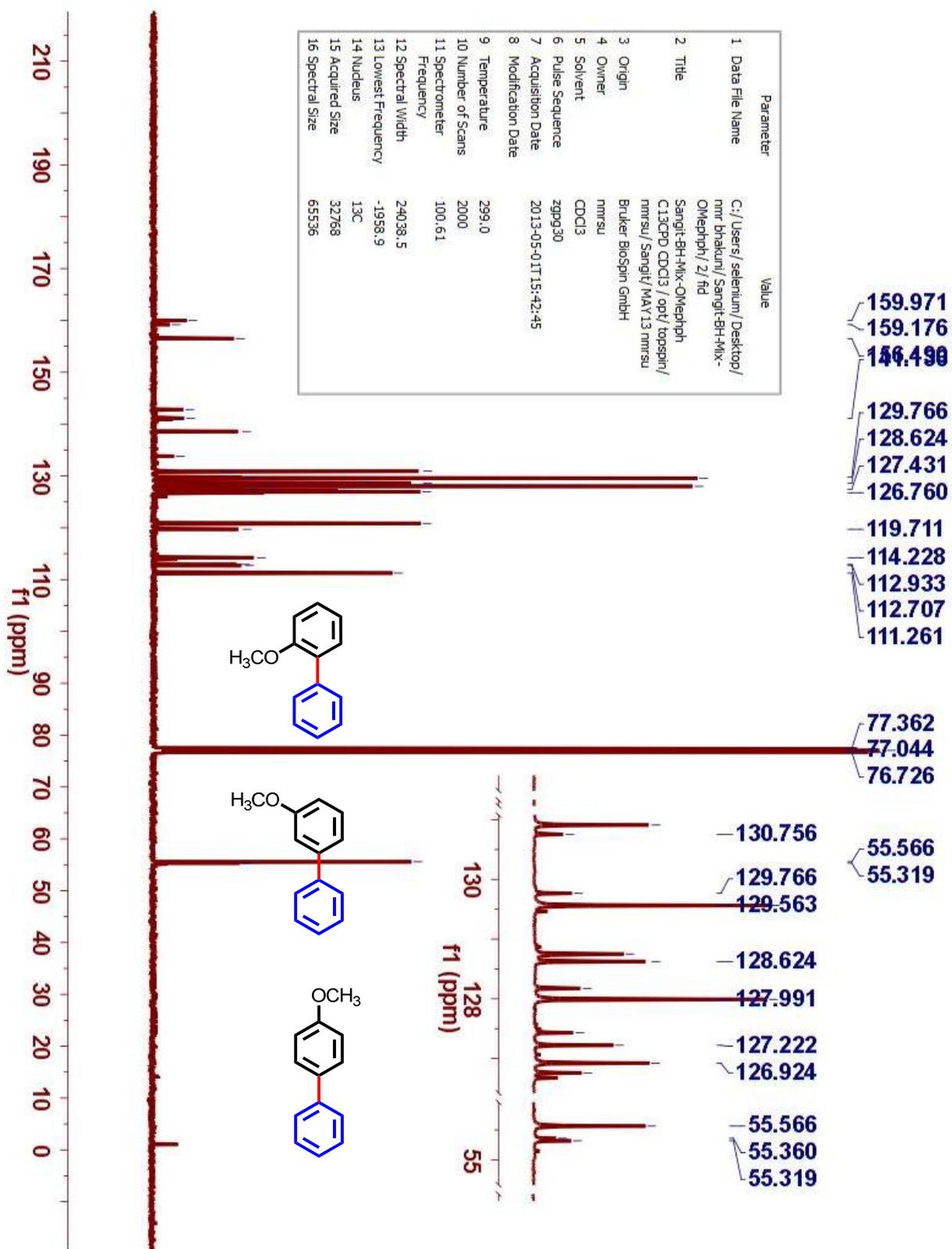


Figure S60  $^1\text{H}$  NMR of **20**

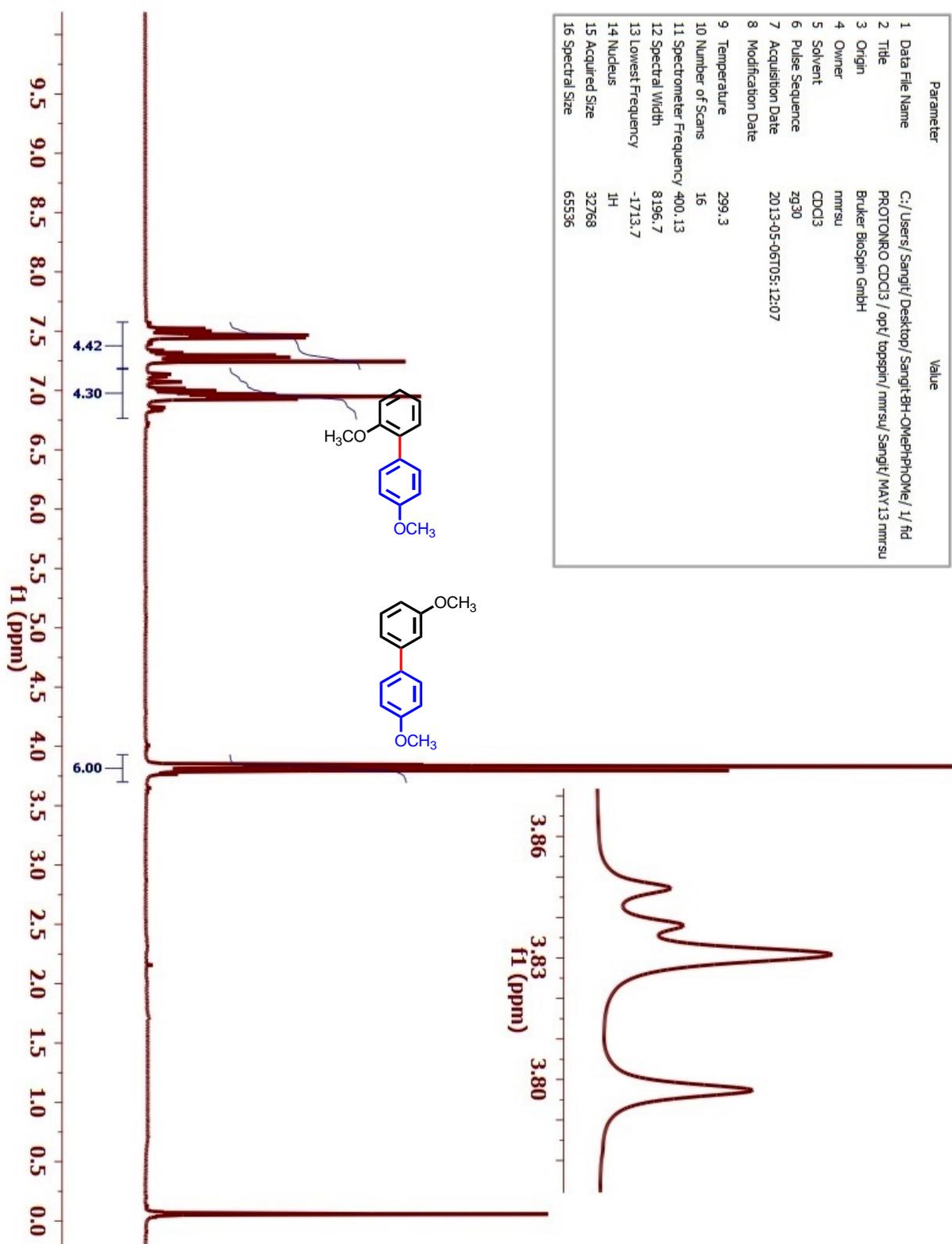


Figure S61  $^{13}\text{C}$  NMR spectrum of **20**

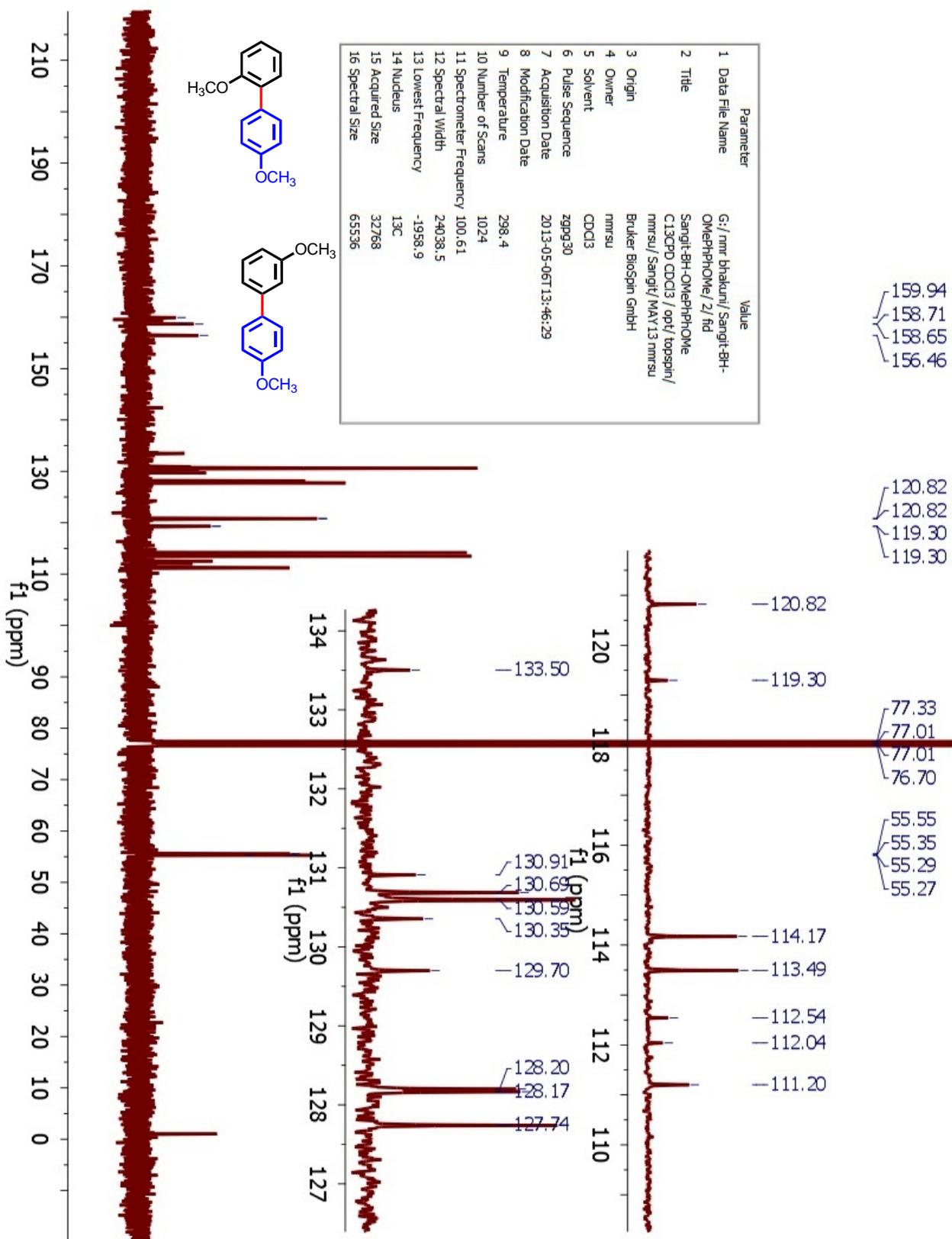


Figure S62 <sup>13</sup>C NMR DEPT-135 of 20

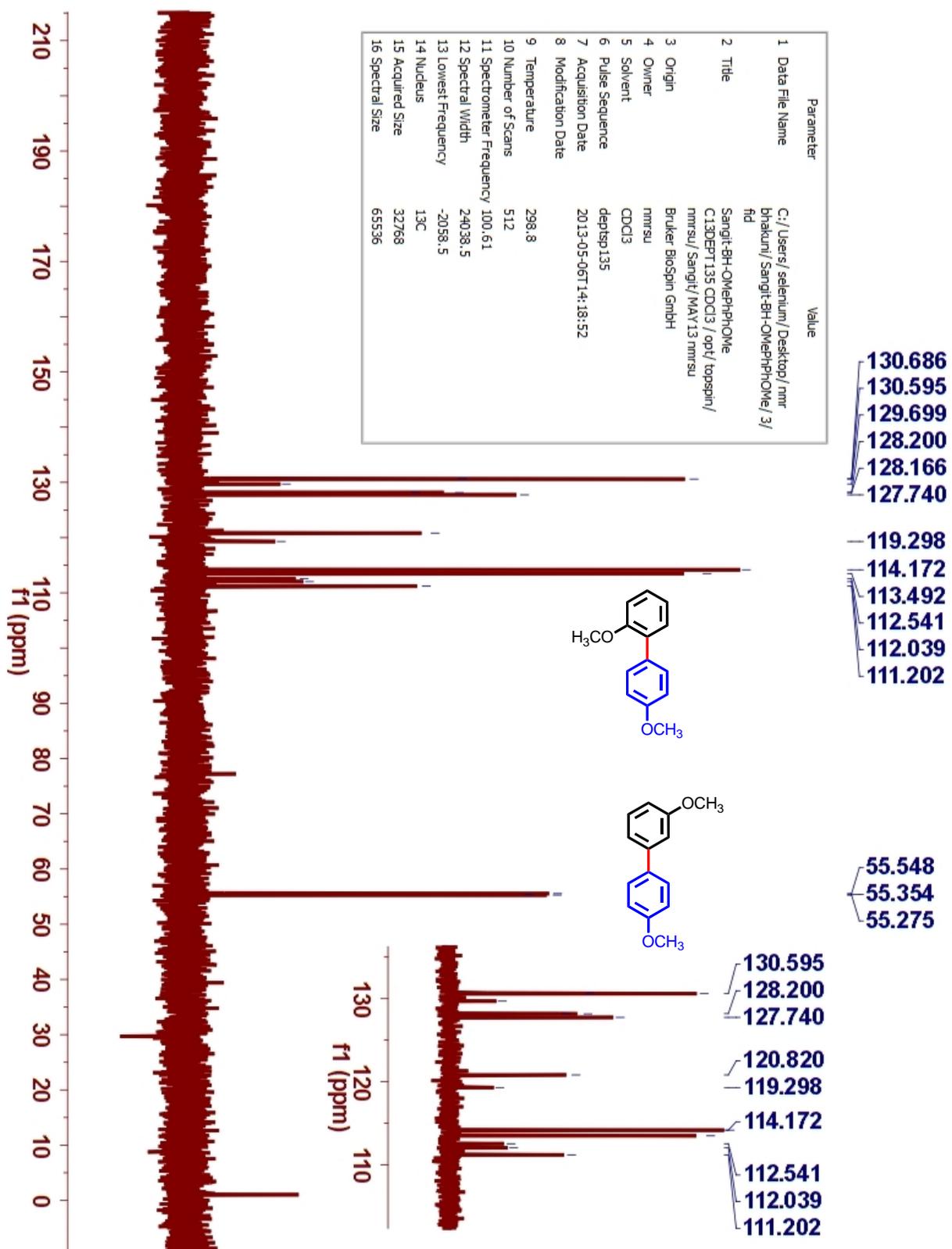


Figure S63  $^1\text{H}$  NMR of **20** obtained using aryl-diazo ligand **L3**

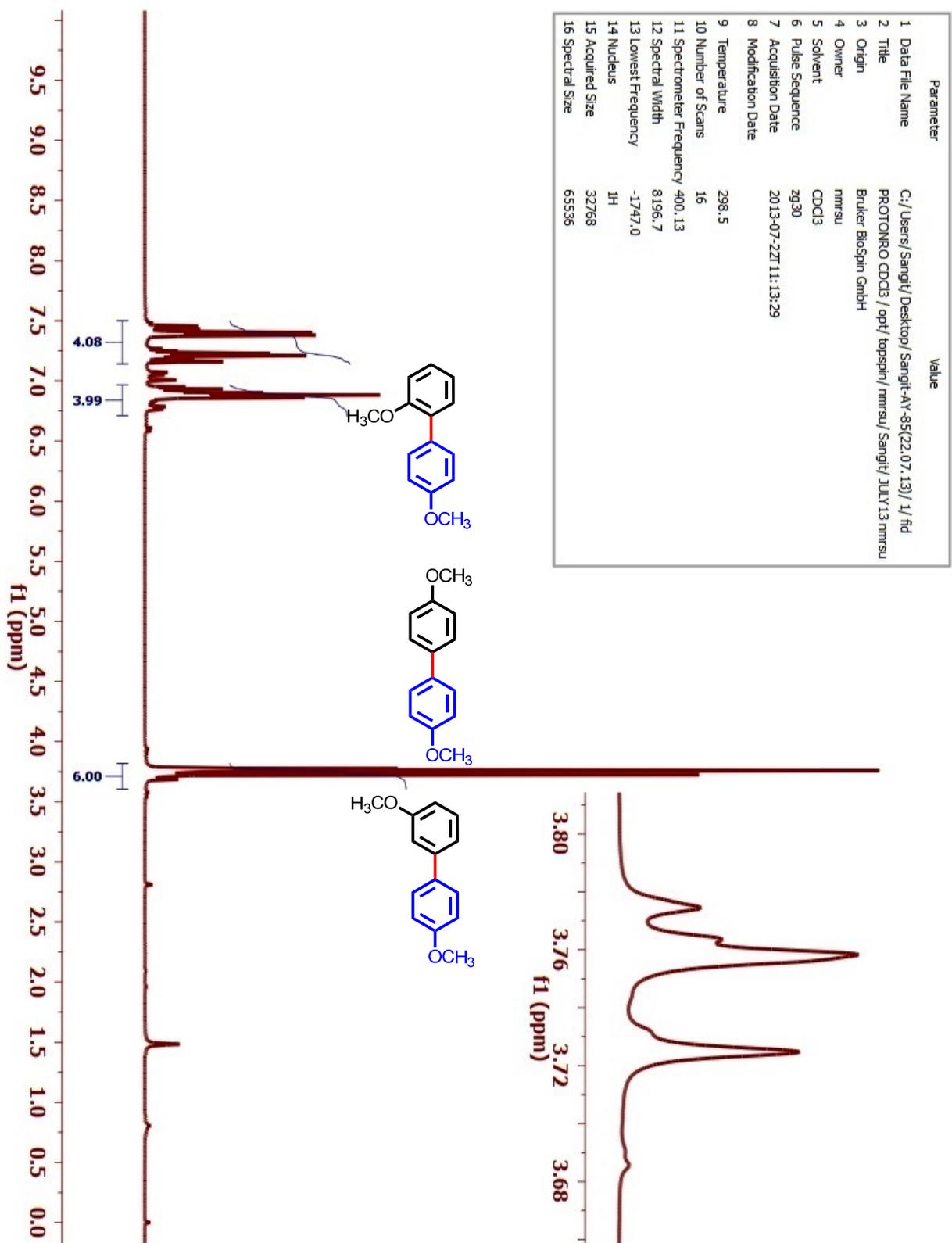


Figure S64  $^{13}\text{C}$  NMR spectrum of **20** obtained using aryl-diazo ligand **L3**

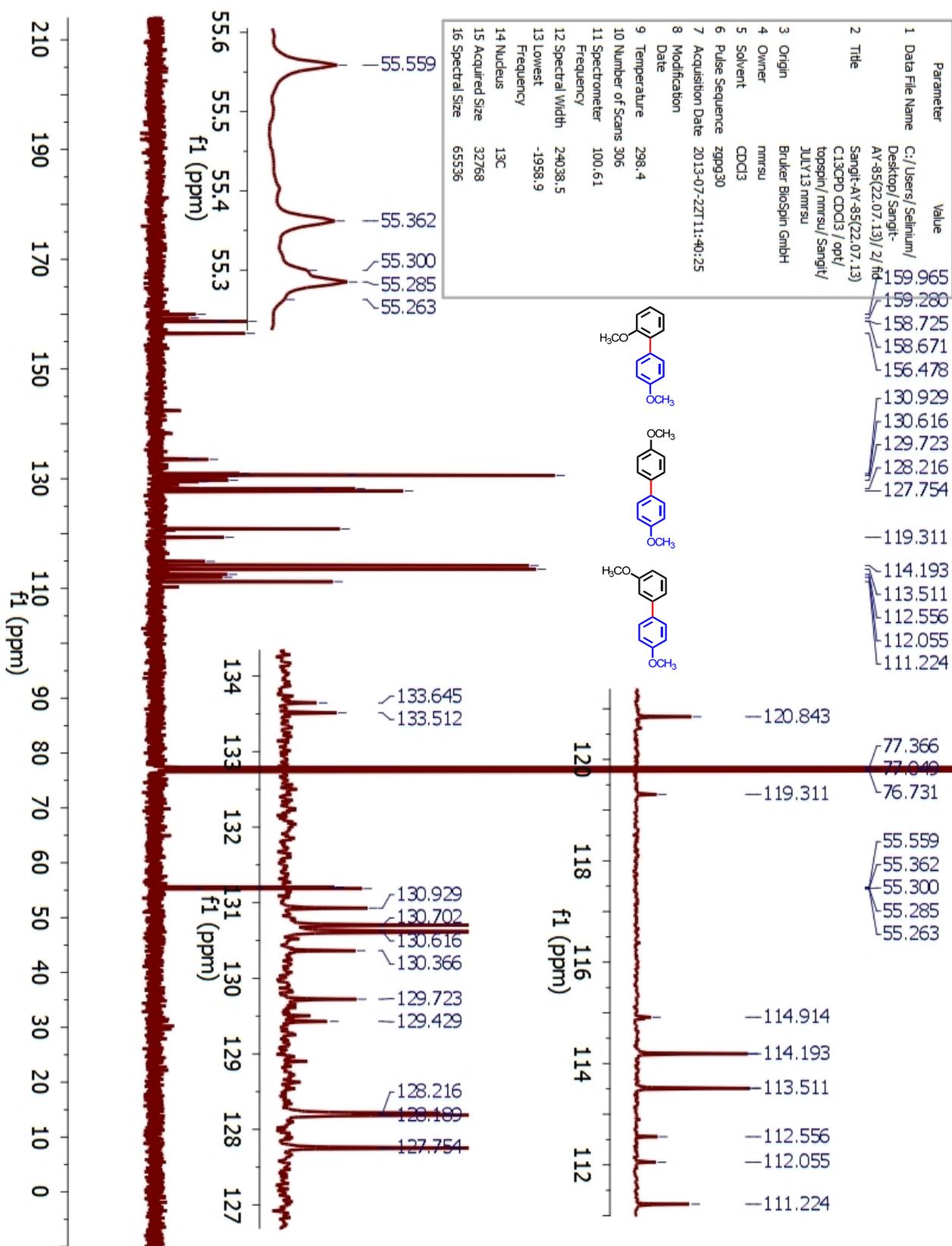


Figure S65  $^1\text{H}$  NMR of **21**

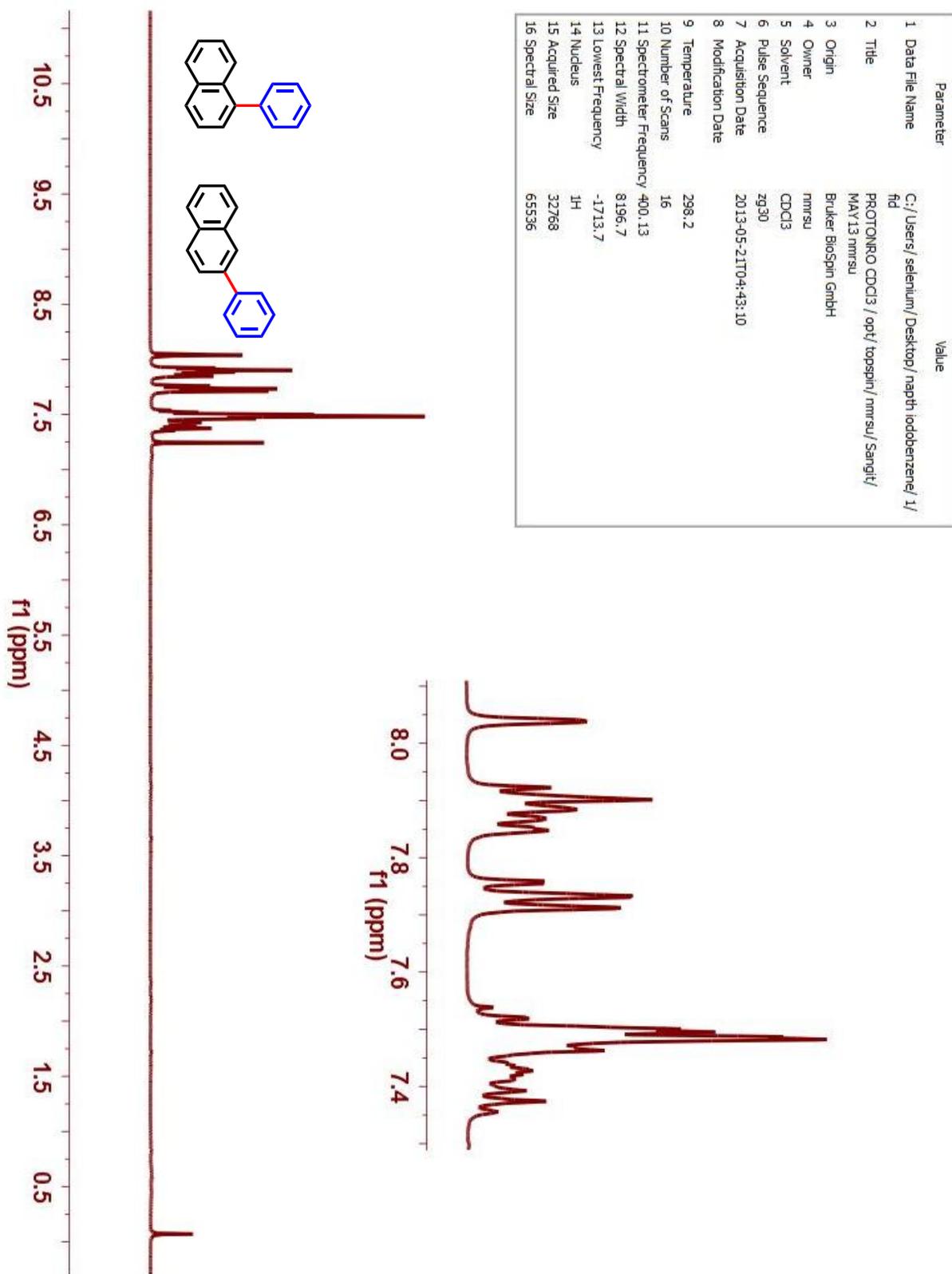


Figure S66 <sup>13</sup>C NMR spectrum of **21**

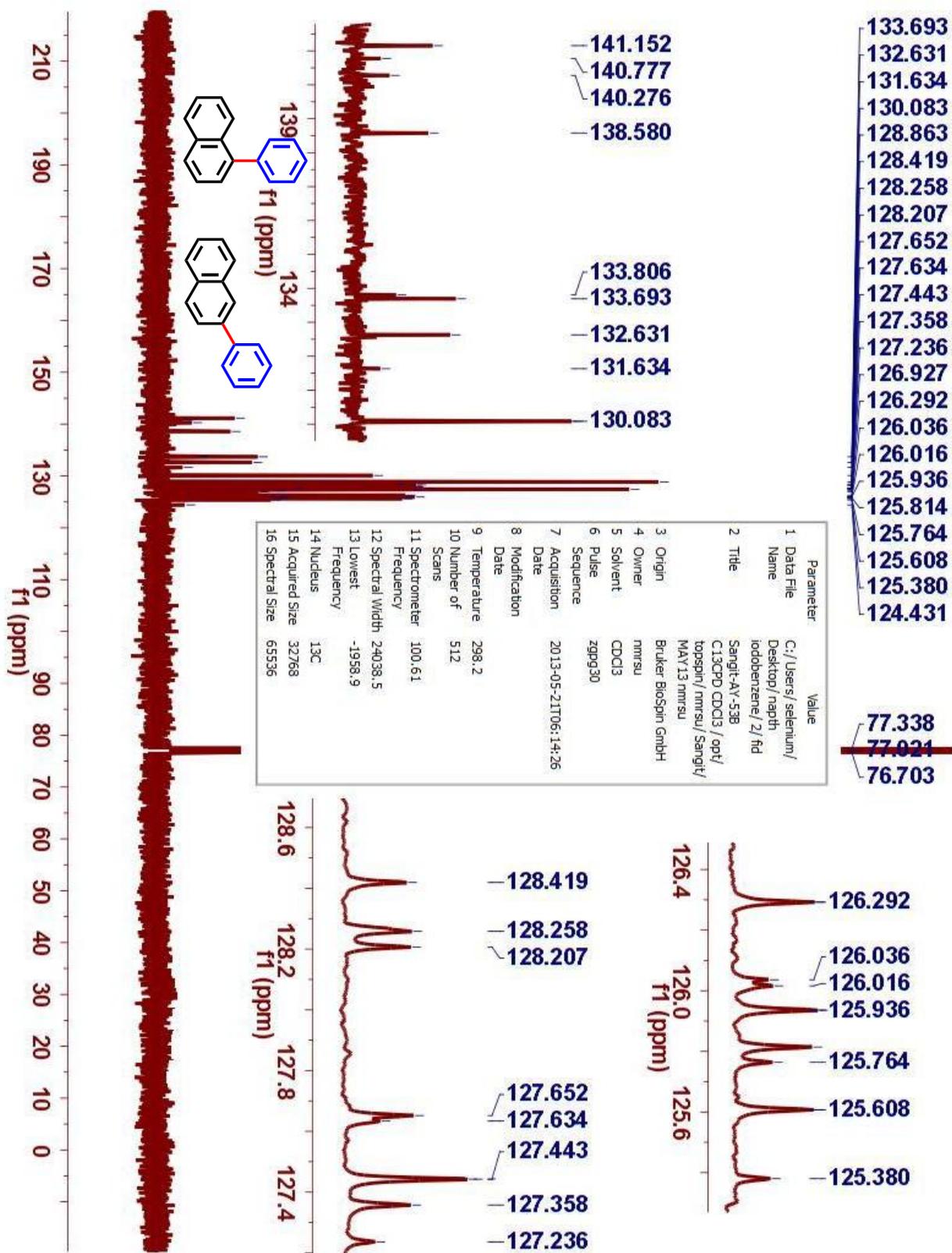


Figure S67 <sup>13</sup>C NMR DEPT-135 of **21**

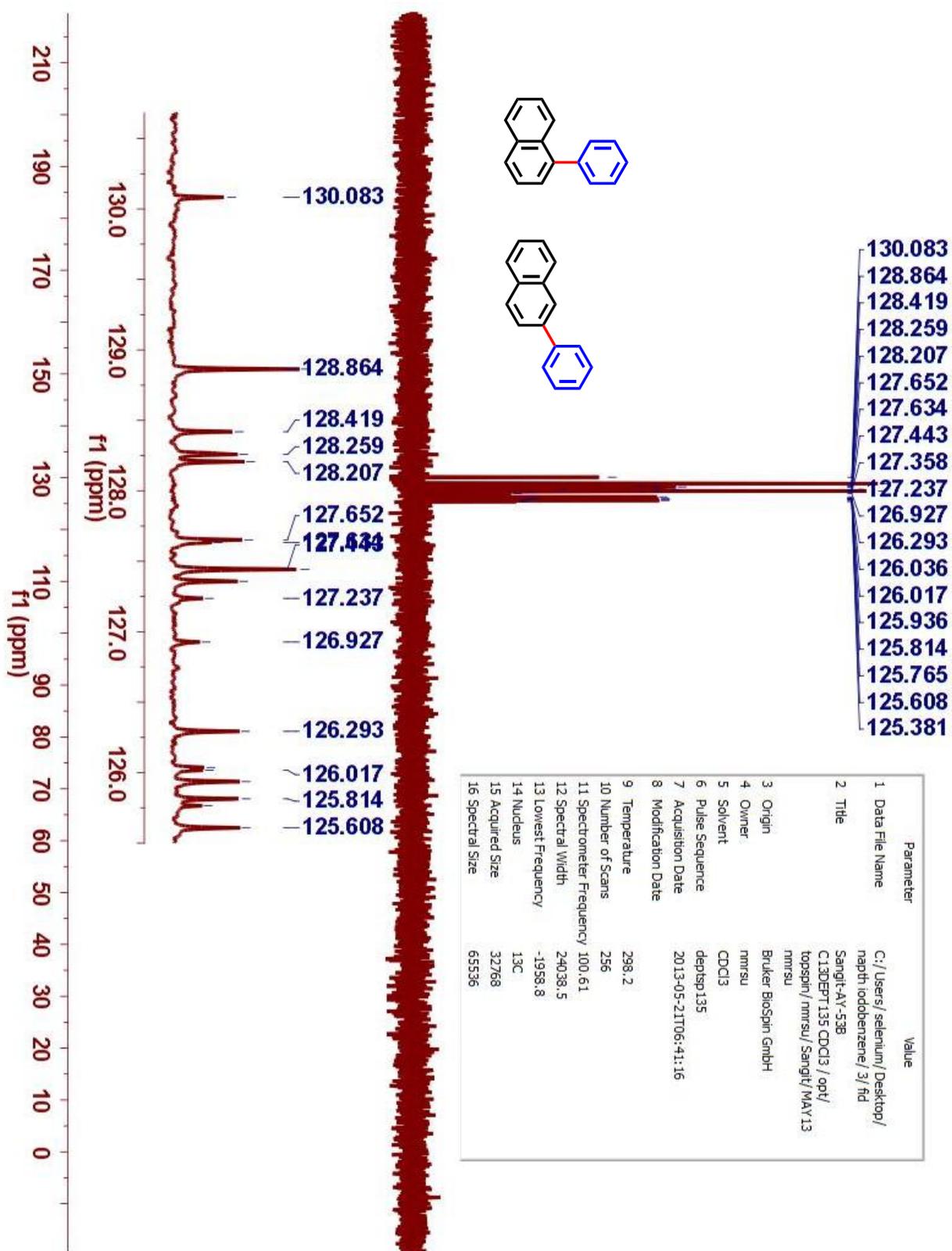


Figure S68  $^1\text{H}$  NMR of **22**

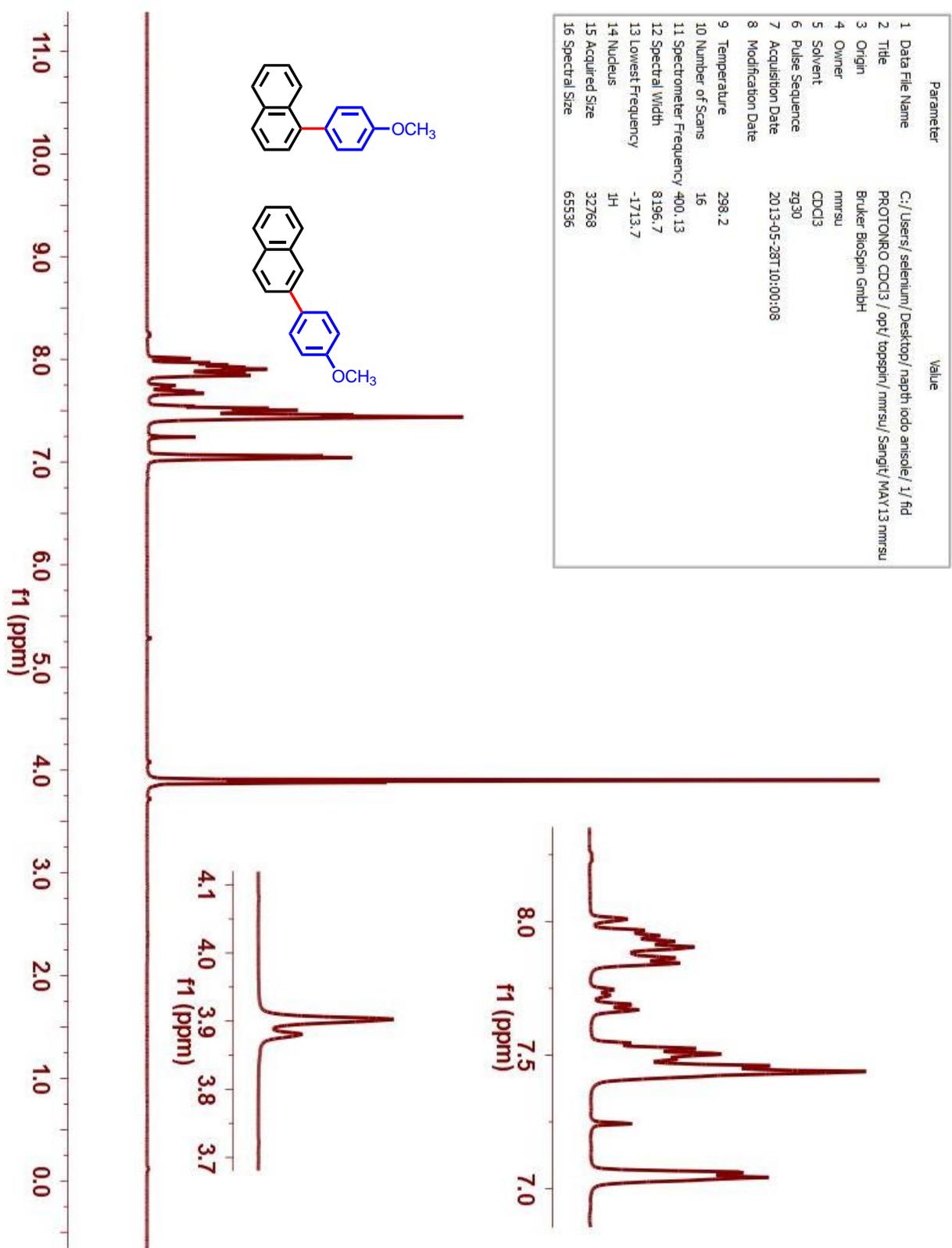


Figure S69 <sup>13</sup>C NMR spectrum of **22**

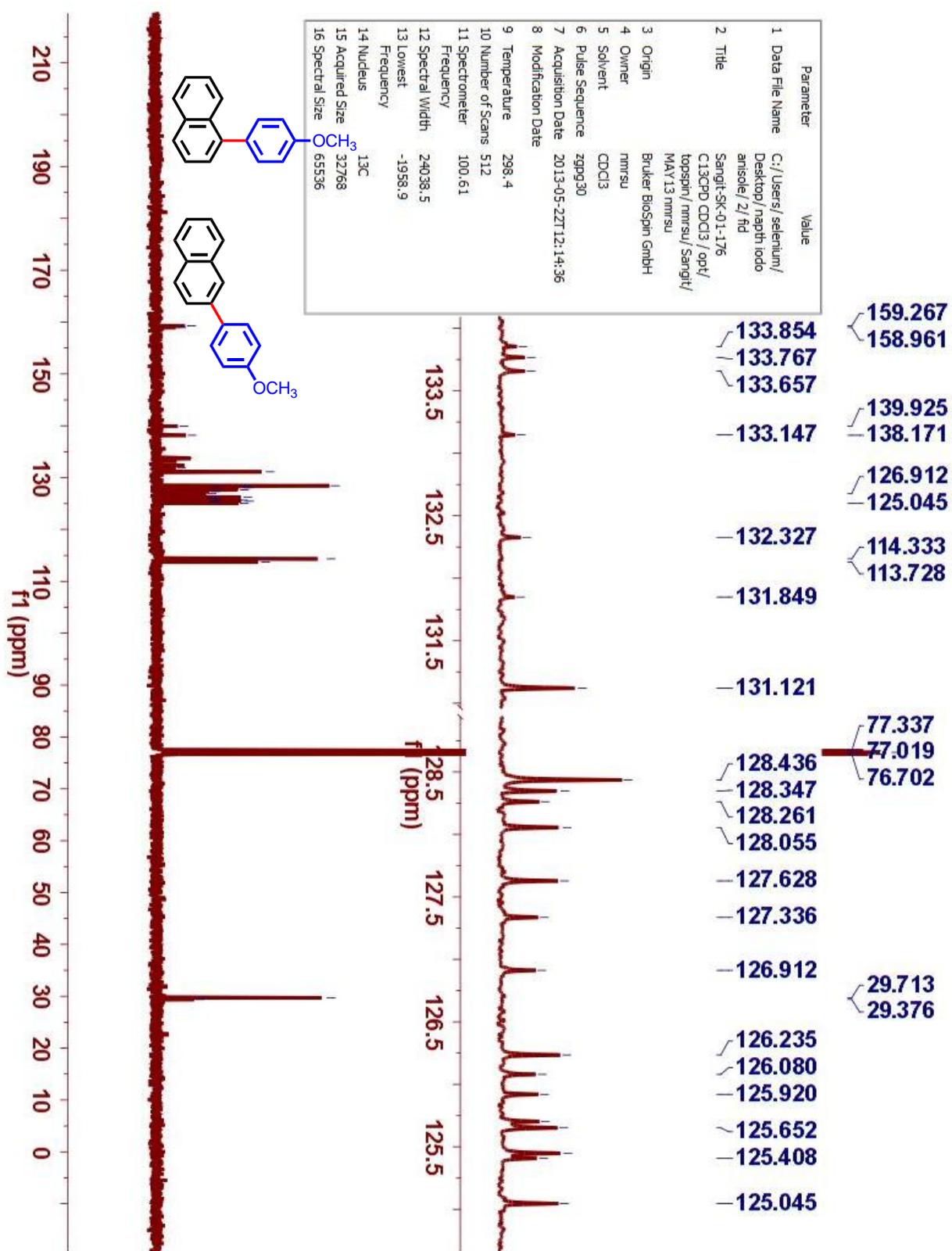


Figure S70  $^{13}\text{C}$  NMR DEPT-135 of **22**

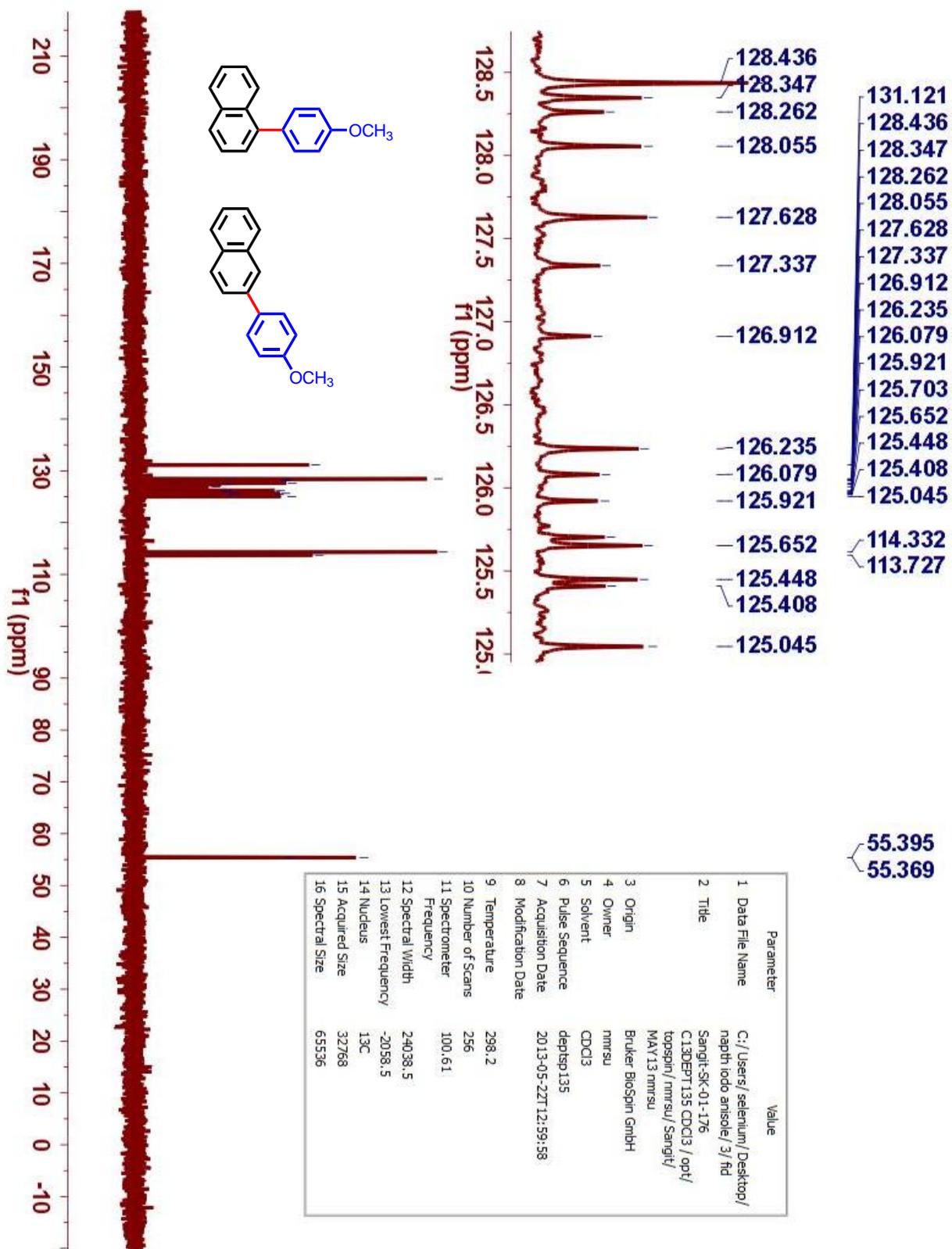


Figure S71  $^1\text{H}$  NMR of **10** obtained from pyridine

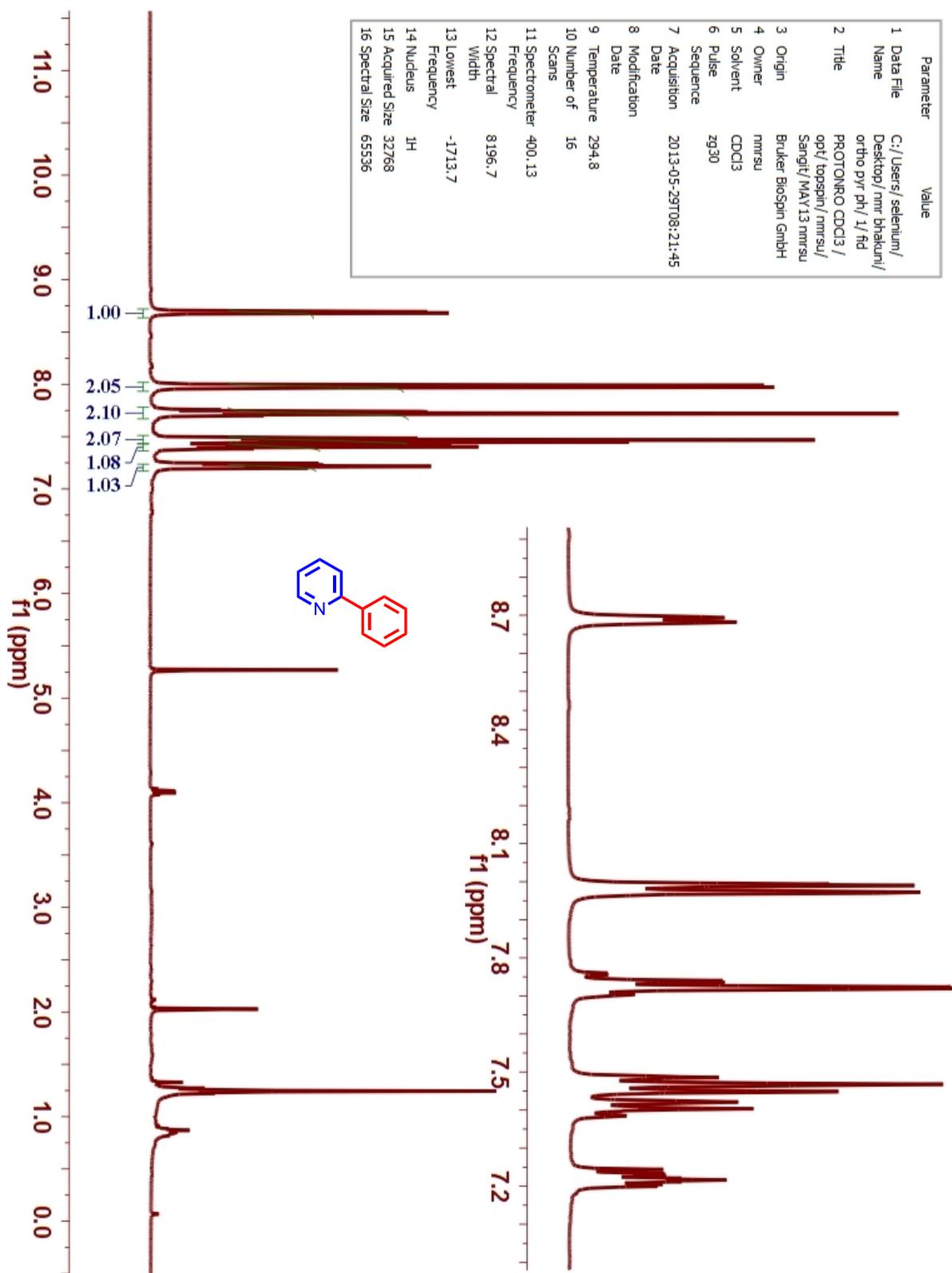


Figure S72  $^{13}\text{C}$  NMR spectrum of **10** obtained from pyridine

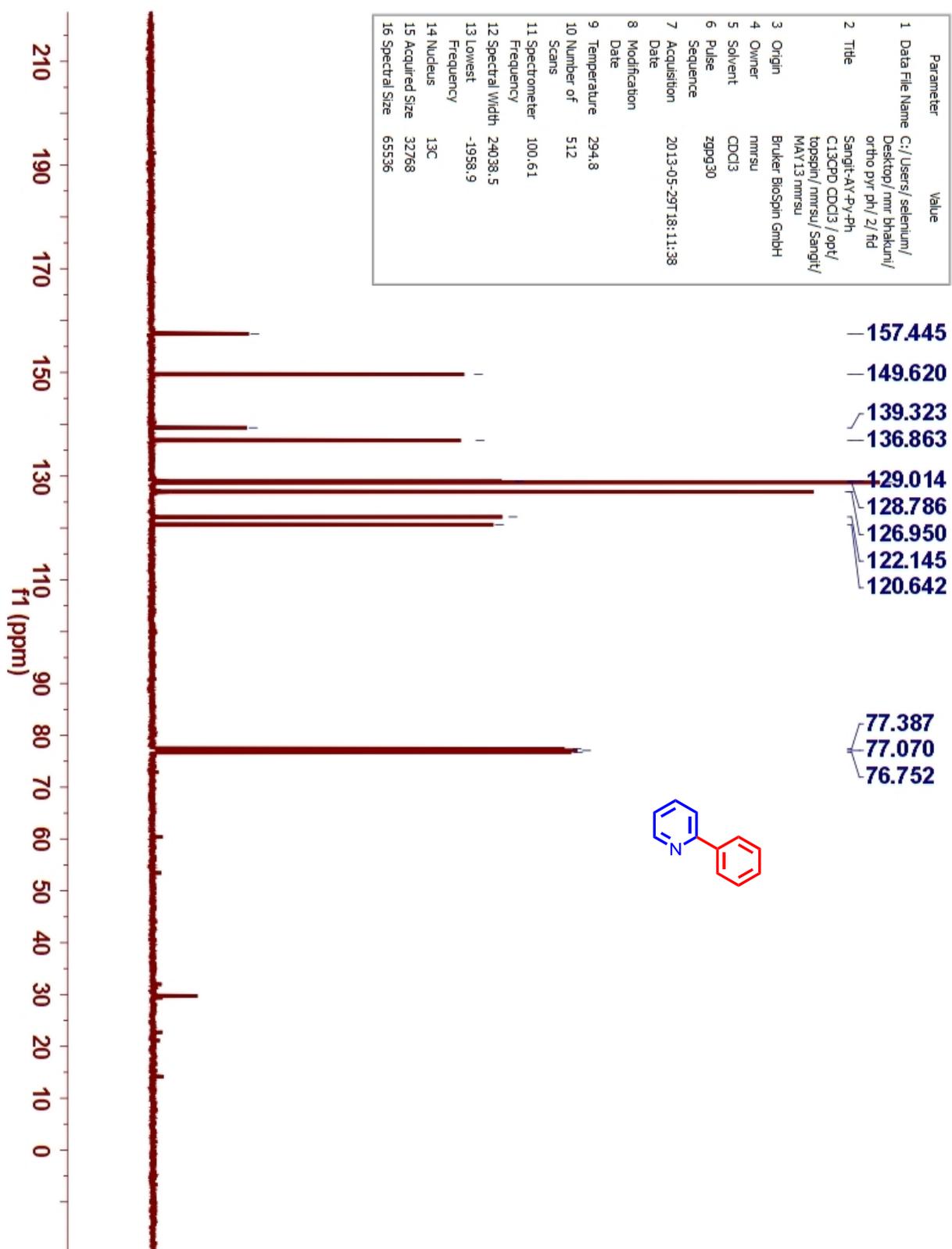


Figure S73  $^{13}\text{C}$  NMR DEPT-135 of **10** obtained from pyridine

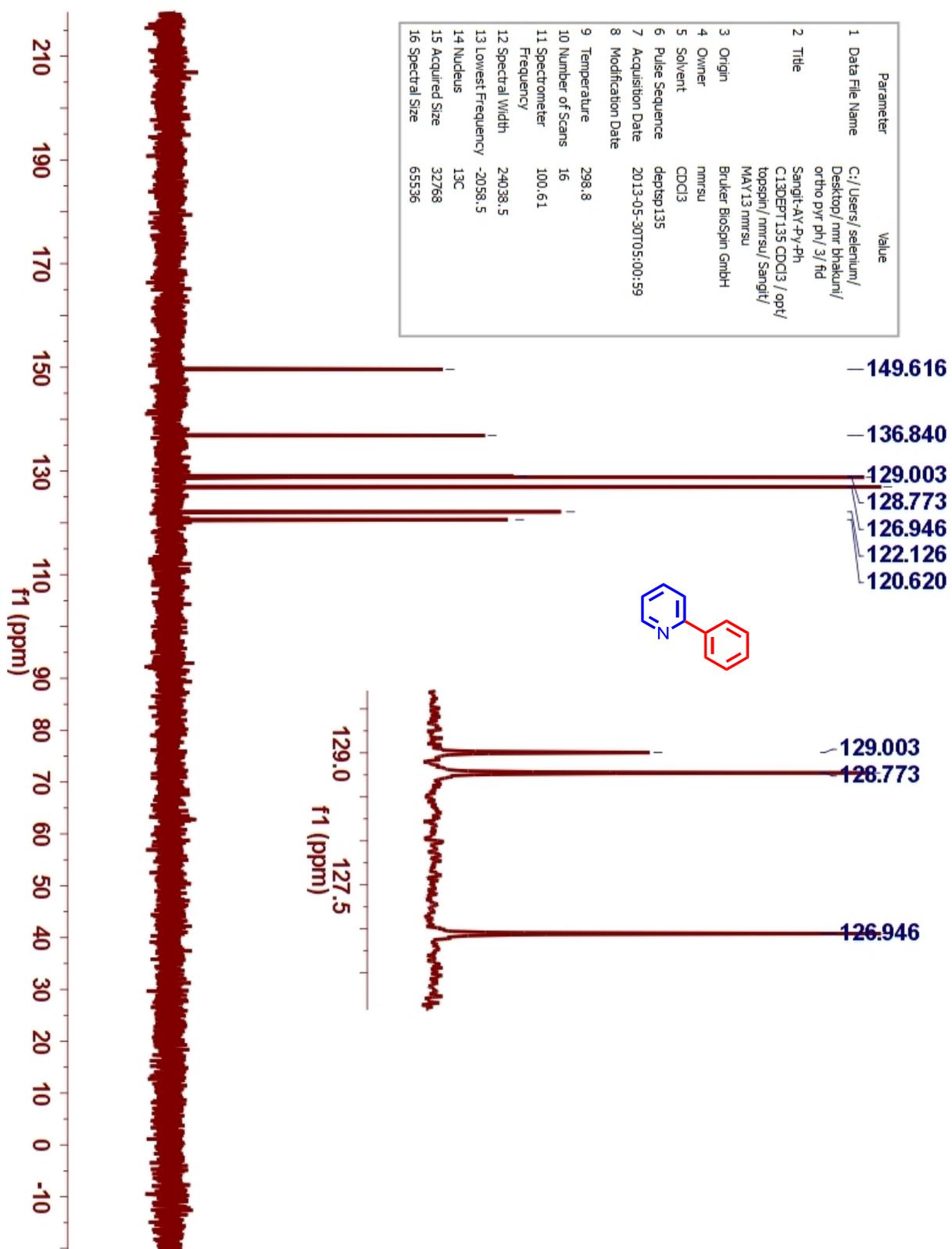


Figure S74 <sup>1</sup>H NMR of **11** obtained using pyridine substrate

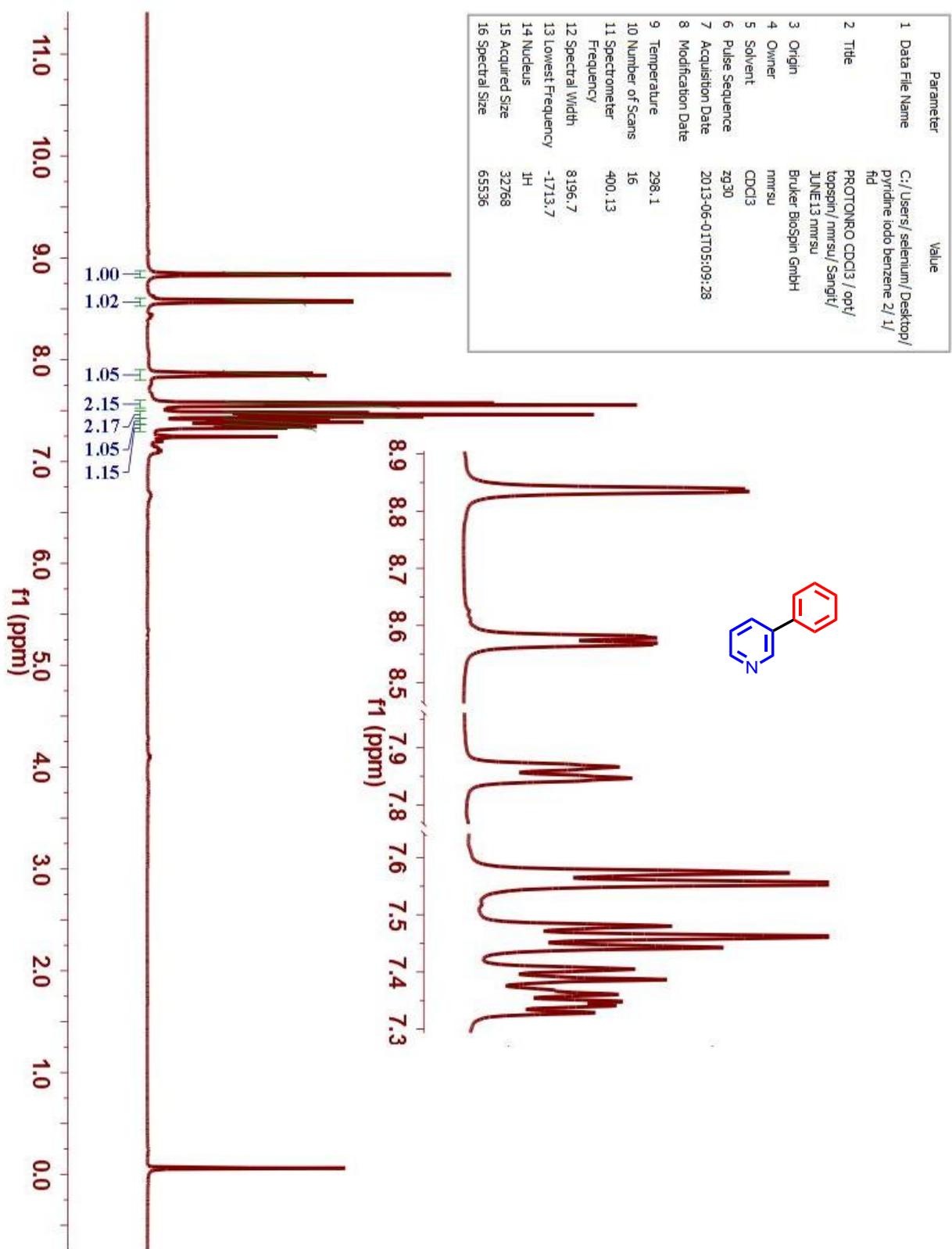


Figure S75  $^{13}\text{C}$  NMR DEPT-135 of **11** obtained using pyridine substrate

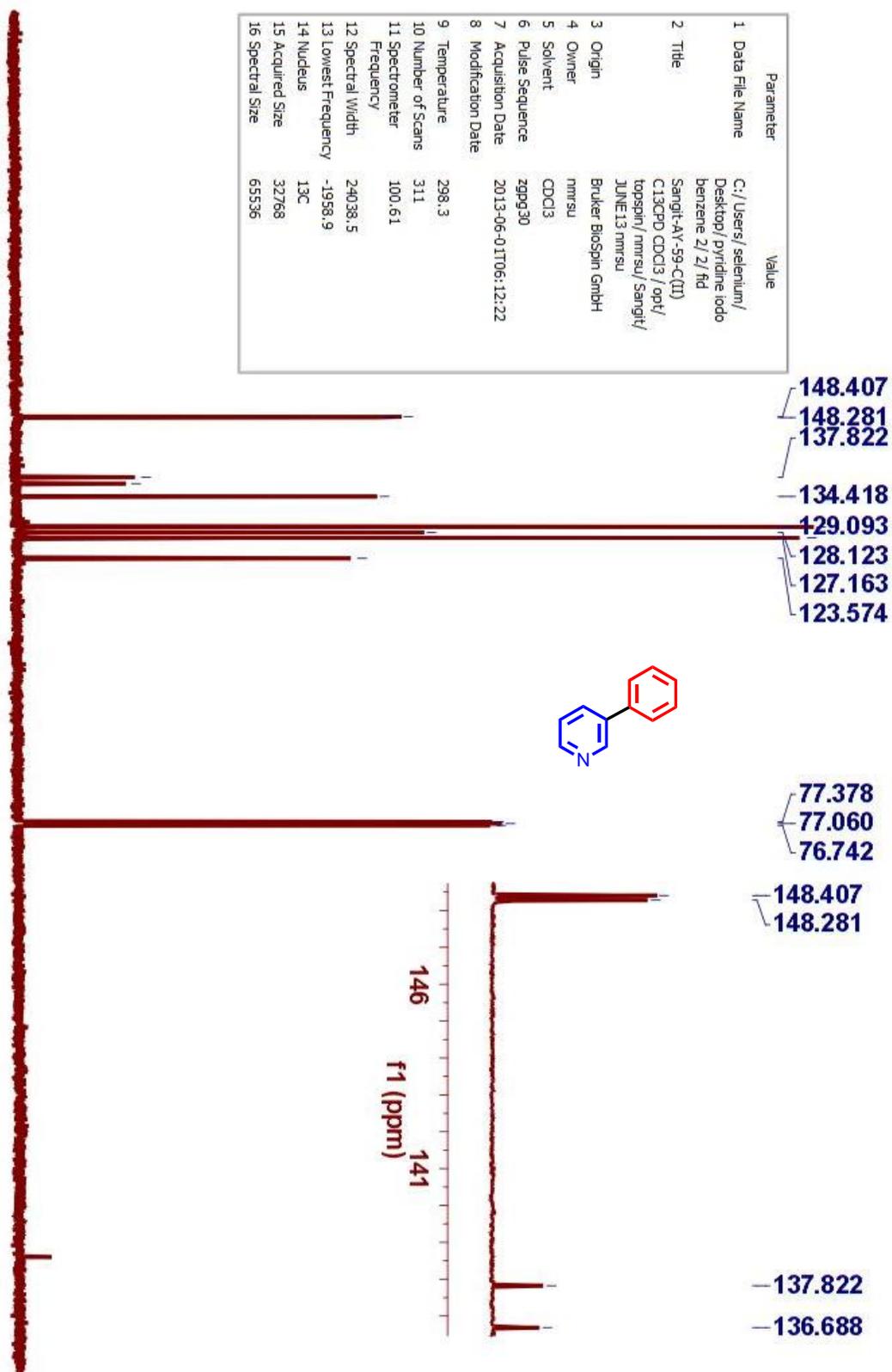


Figure S76  $^{13}\text{C}$  NMR DEPT-135 of **11** obtained using pyridine substrate

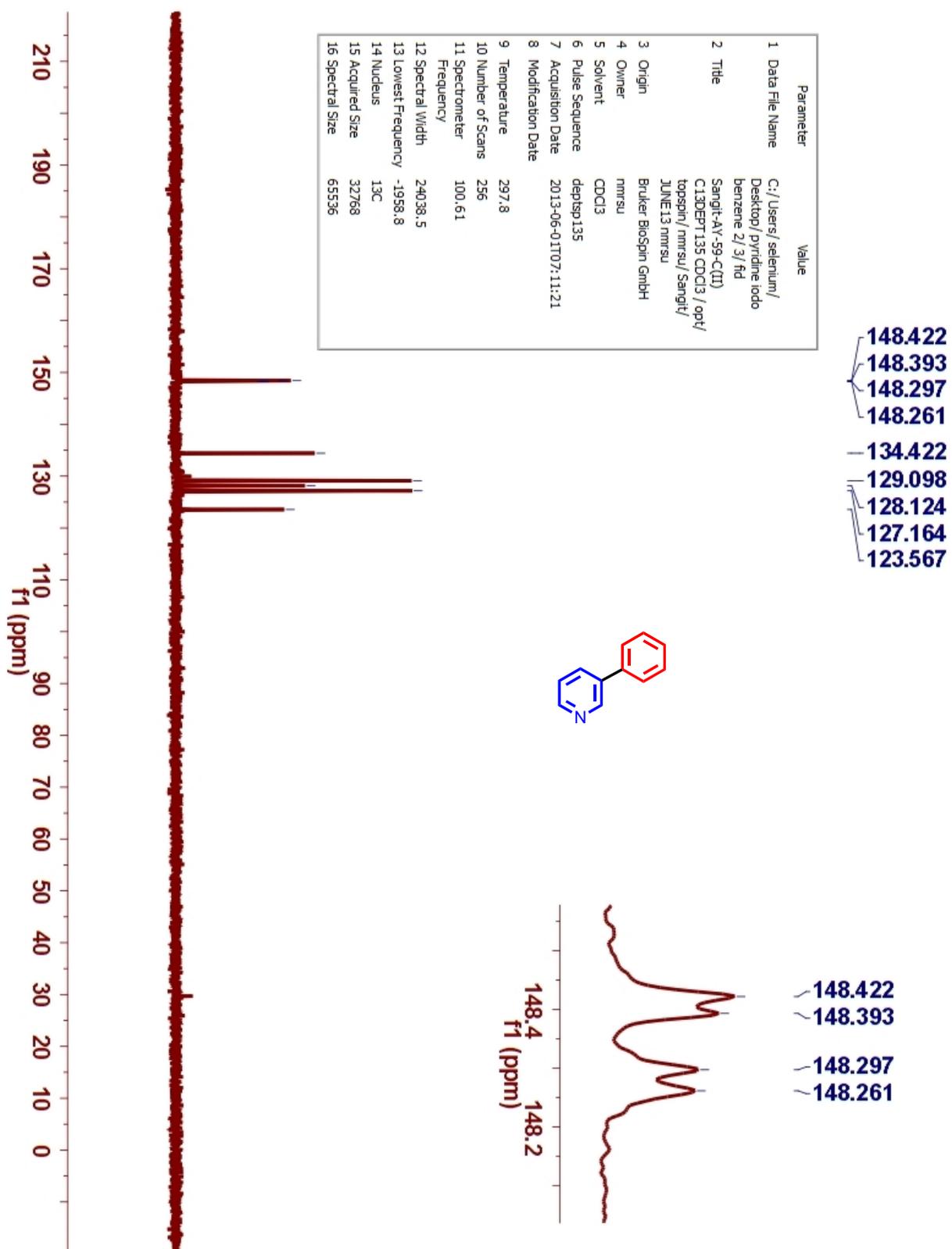


Figure S77 <sup>1</sup>H NMR spectrum of **23**

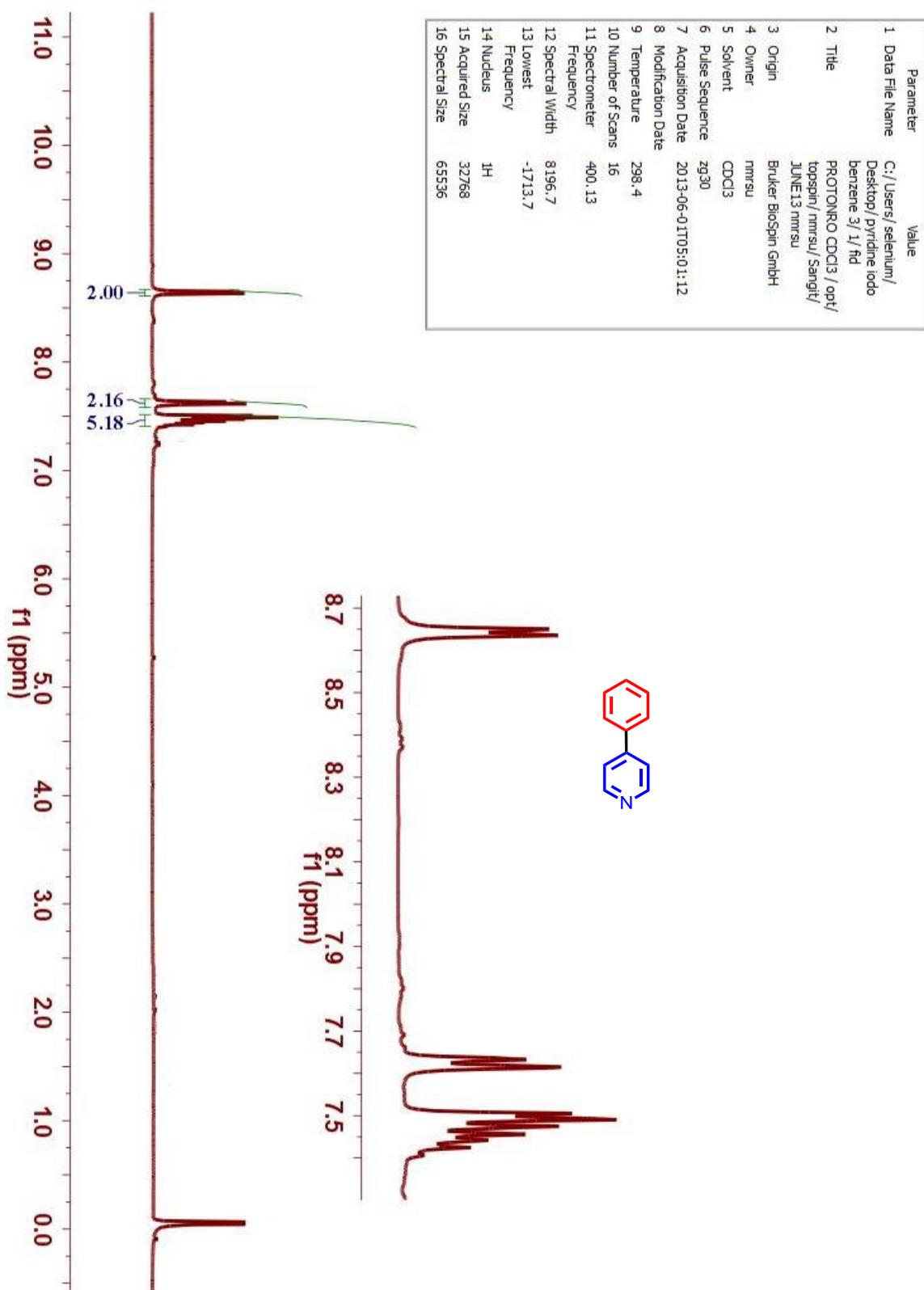


Figure S78  $^{13}\text{C}$  NMR spectrum of **23**

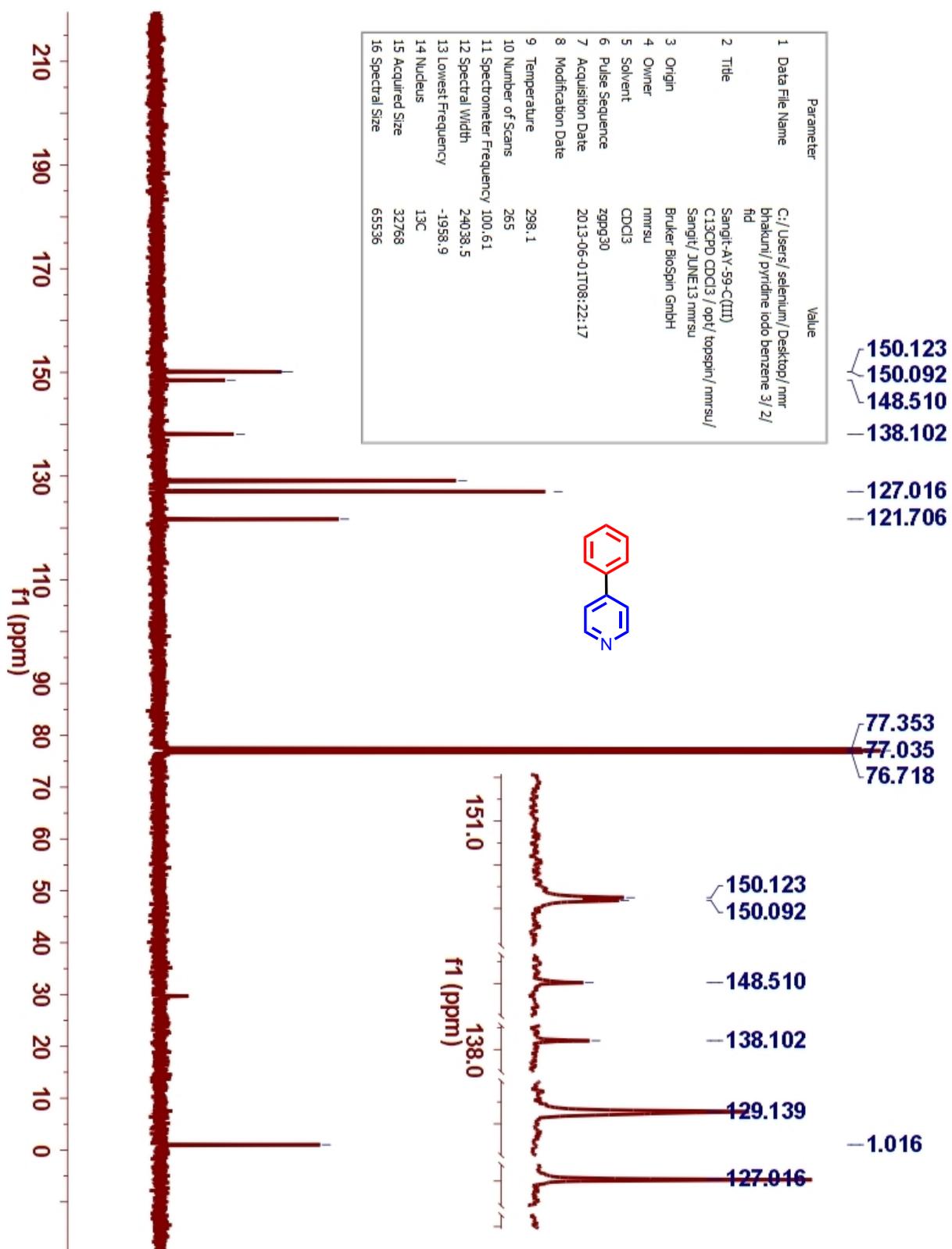


Figure S79  $^{13}\text{C}$  NMR DEPT-135 of **23**

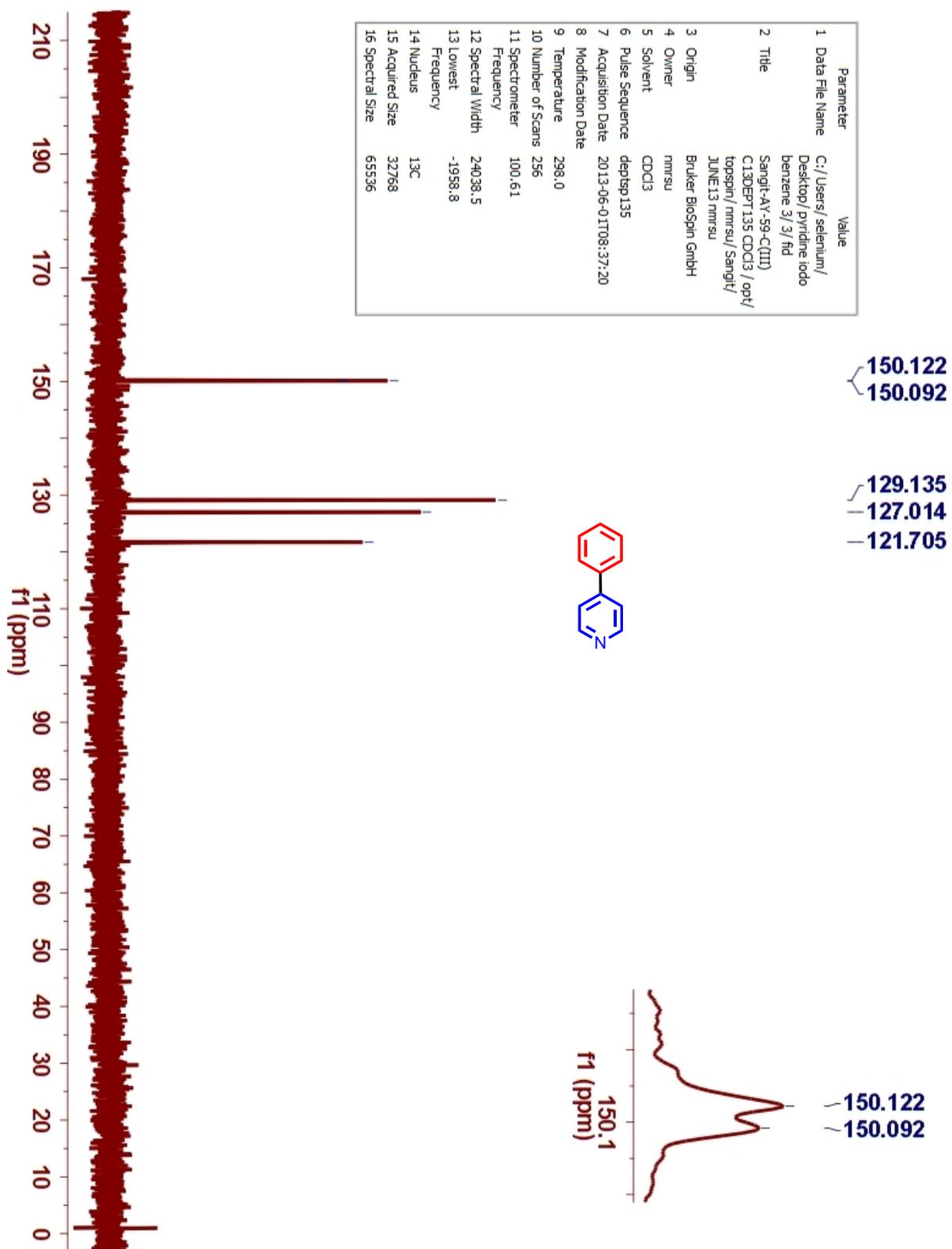


Figure S80  $^1\text{H}$  NMR of **24**

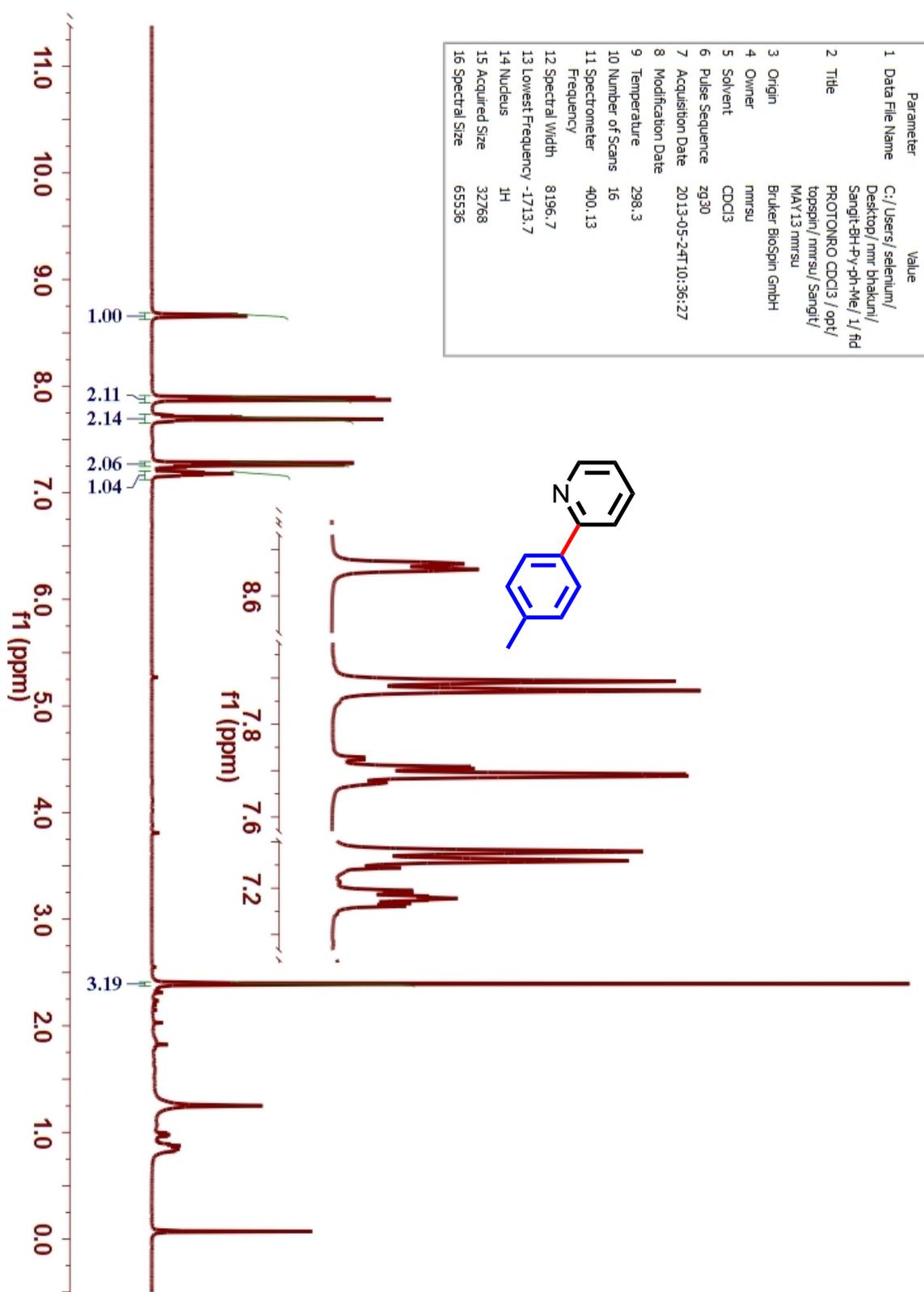


Figure S81  $^{13}\text{C}$  NMR spectrum of **24**

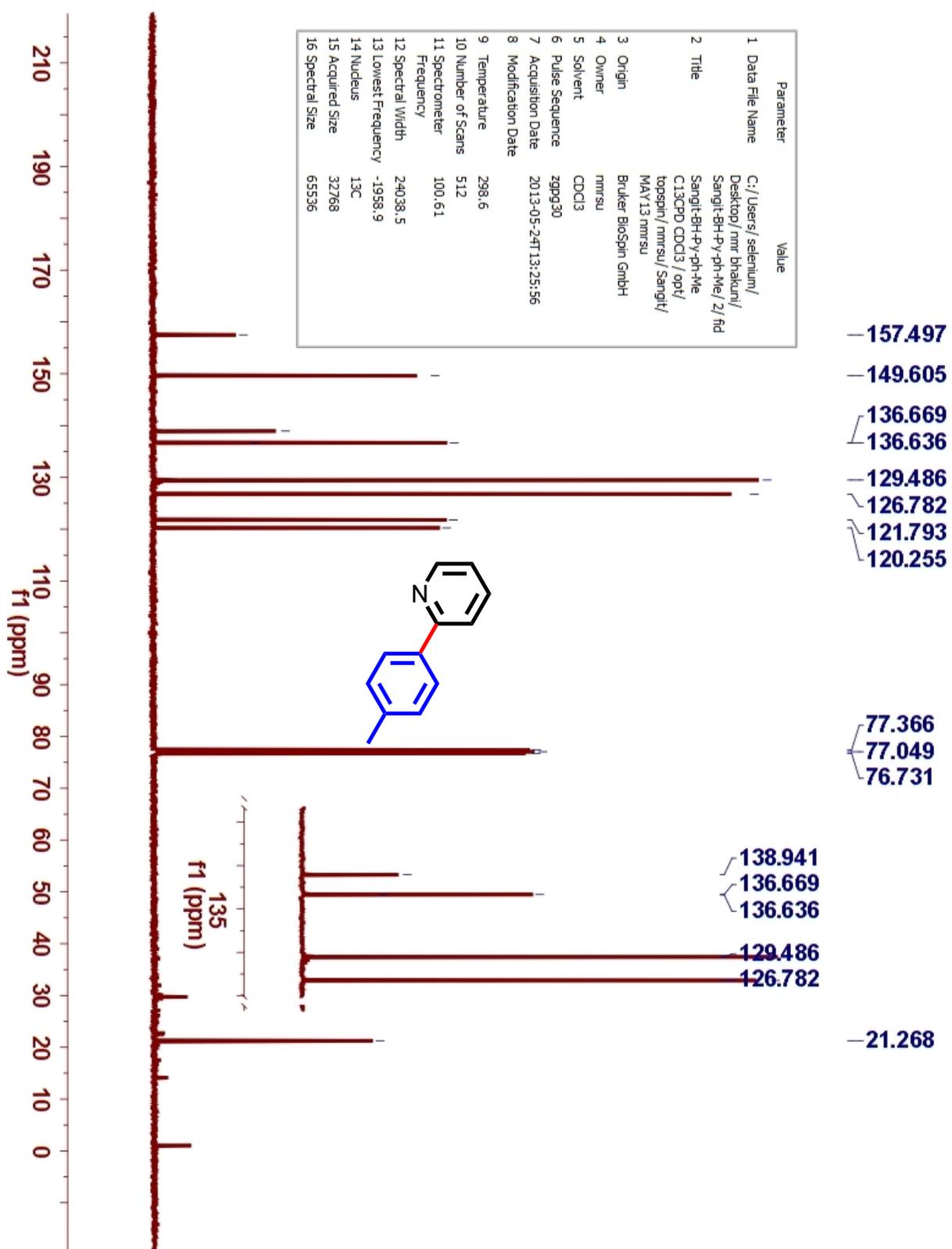


Figure S82  $^{13}\text{C}$  NMR DEPT-135 of **24**

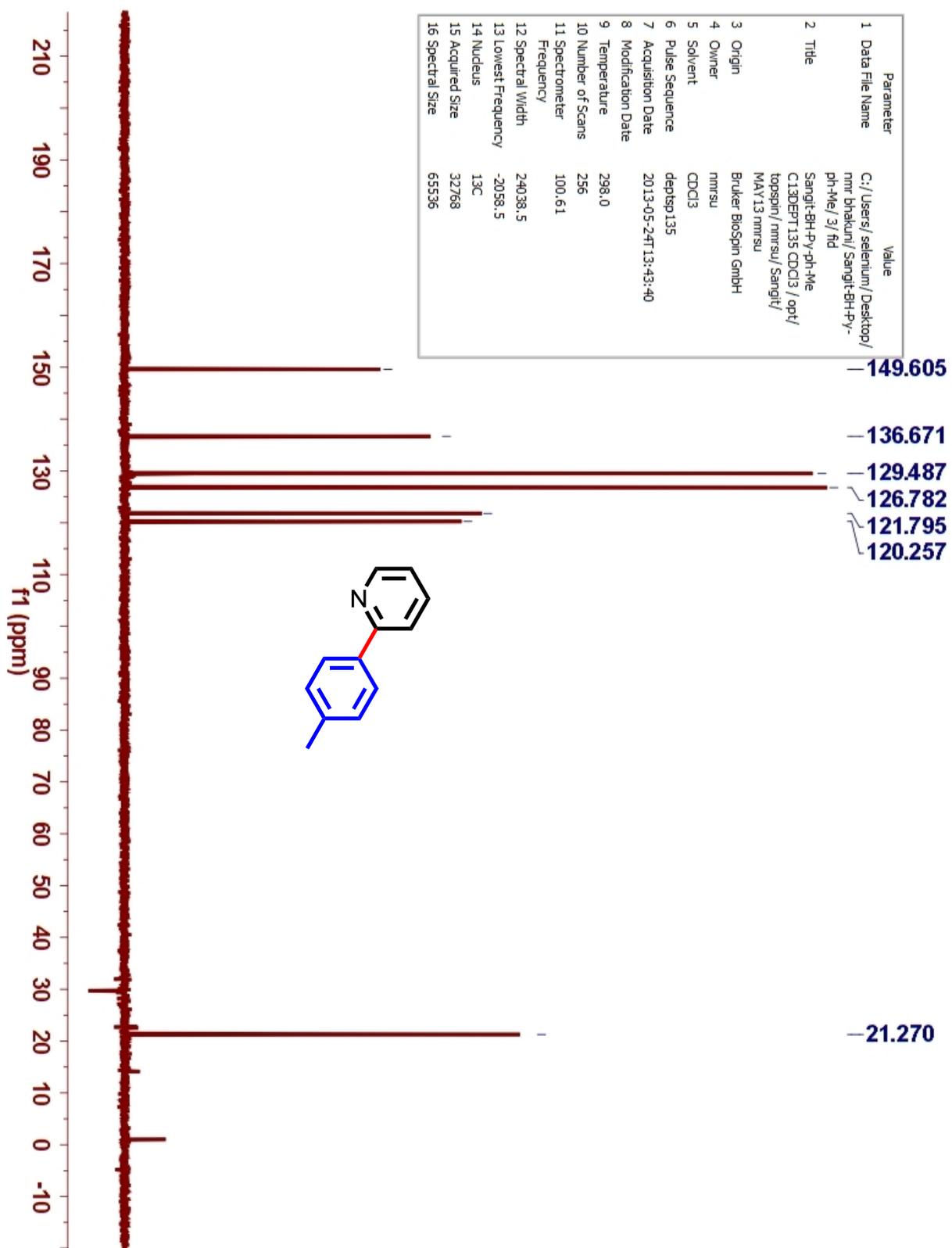


Figure S83  $^1\text{H}$  NMR of **25**

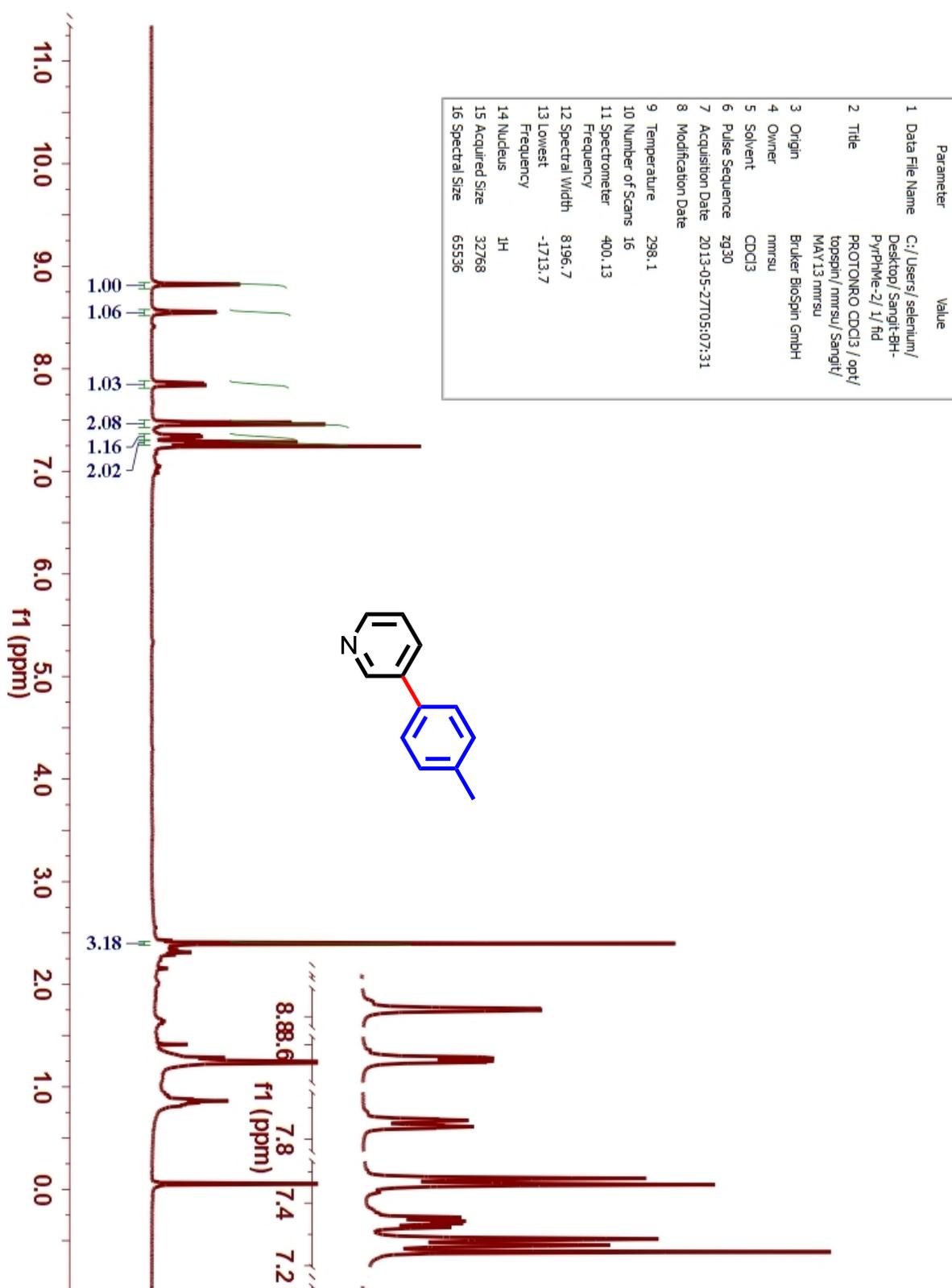


Figure S84  $^{13}\text{C}$  NMR spectrum of **25**

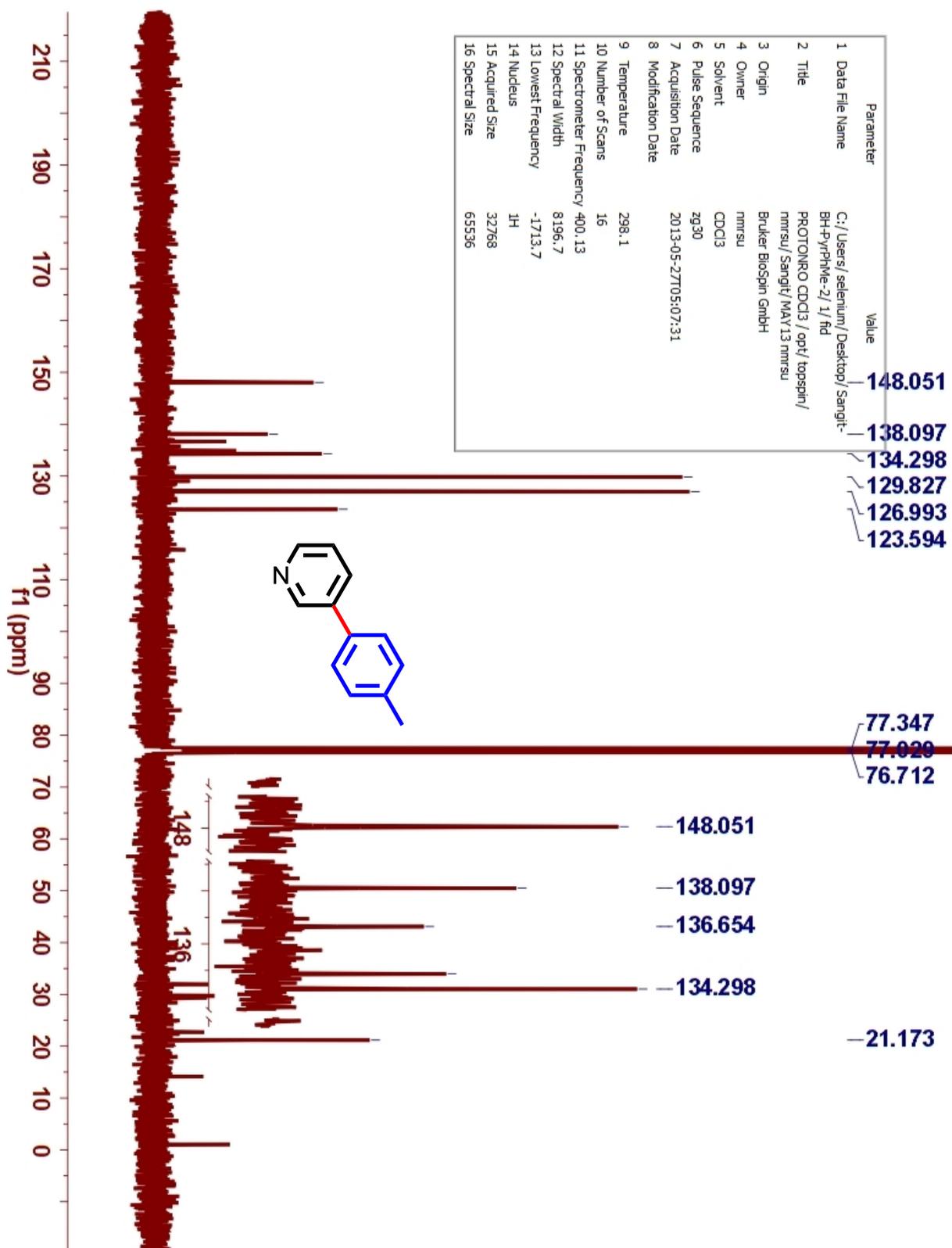


Figure S85  $^{13}\text{C}$  NMR DEPT-135 of **25**

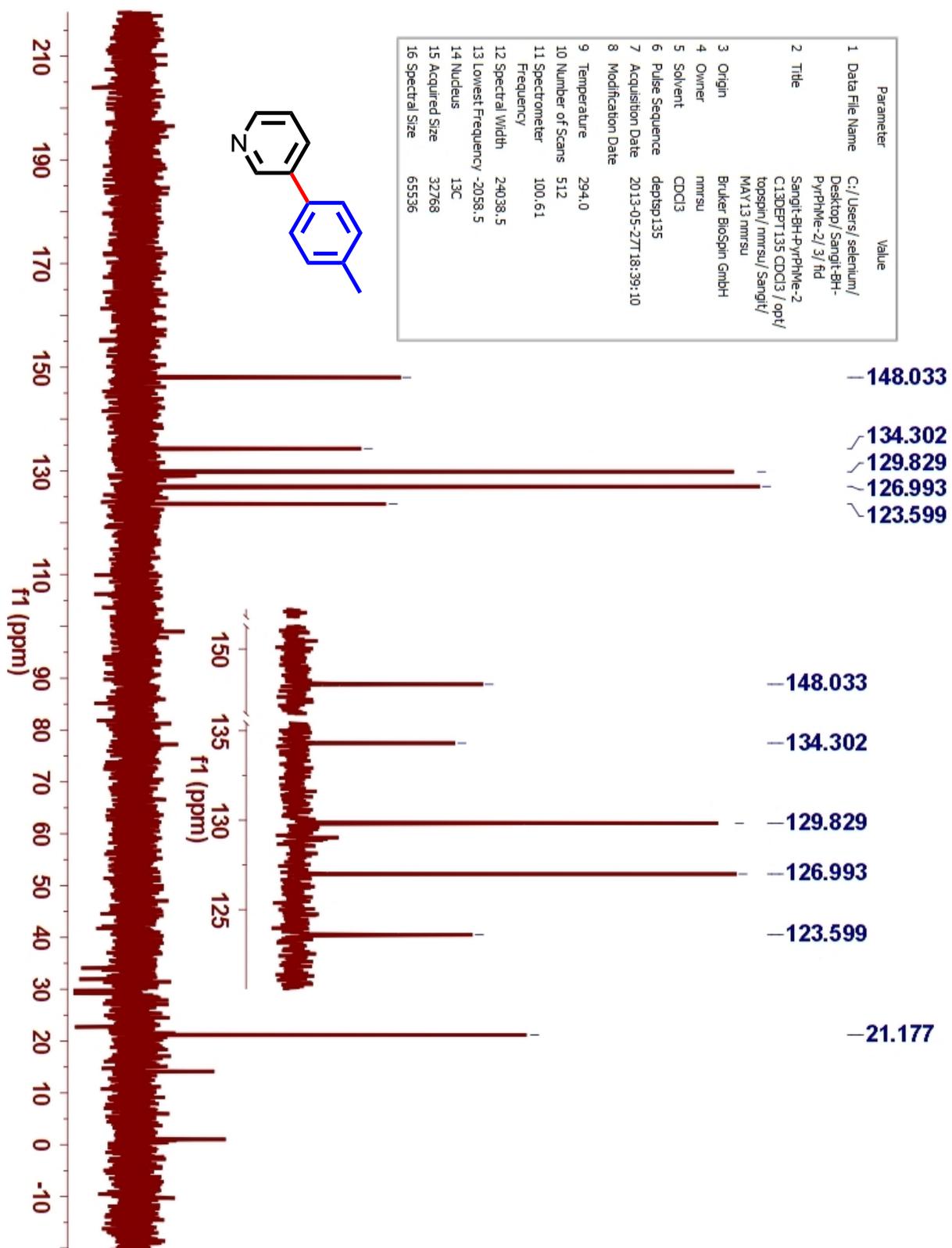




Figure S87  $^{13}\text{C}$  NMR spectrum of **26**

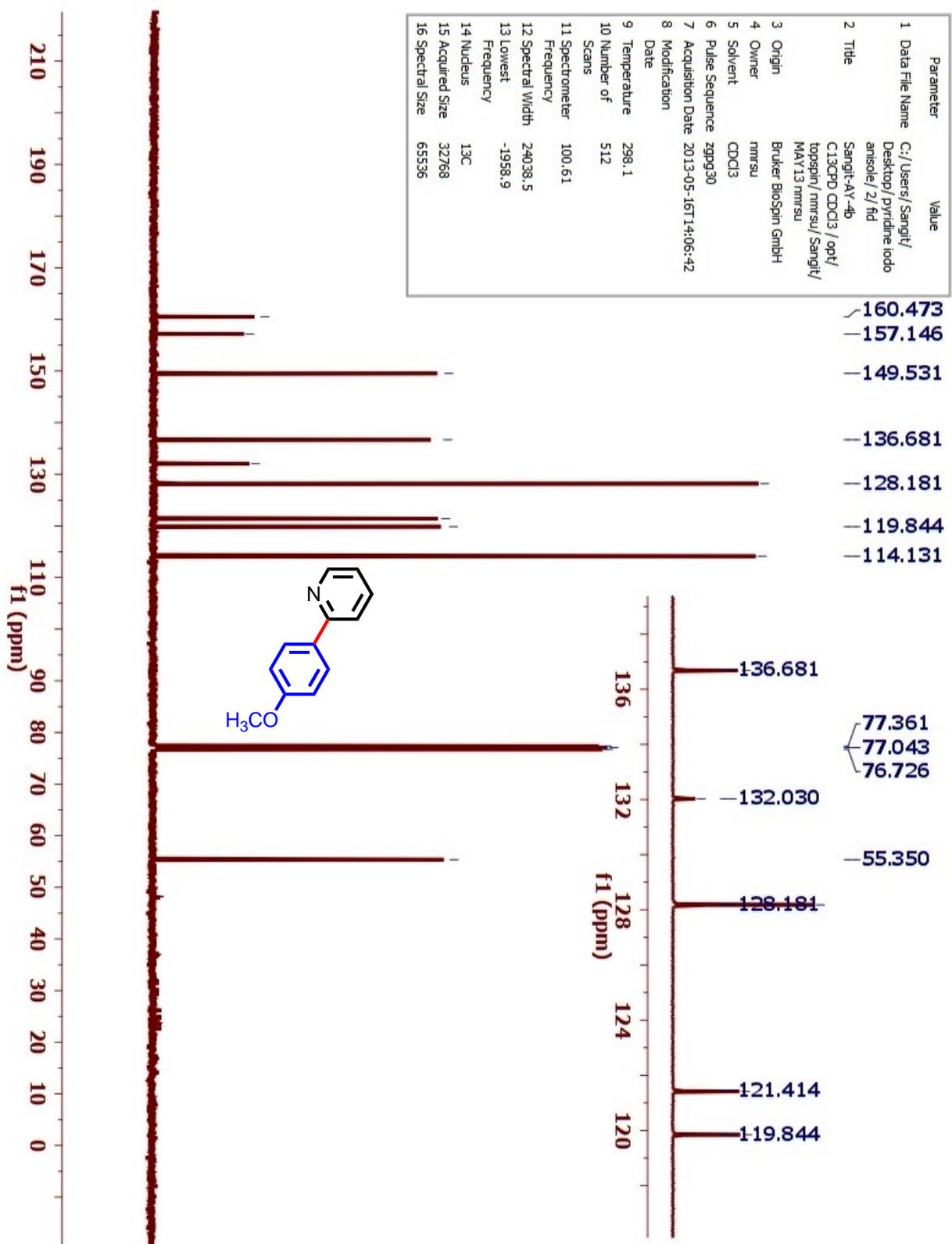


Figure S88  $^{13}\text{C}$  NMR DEPT-135 of **26**

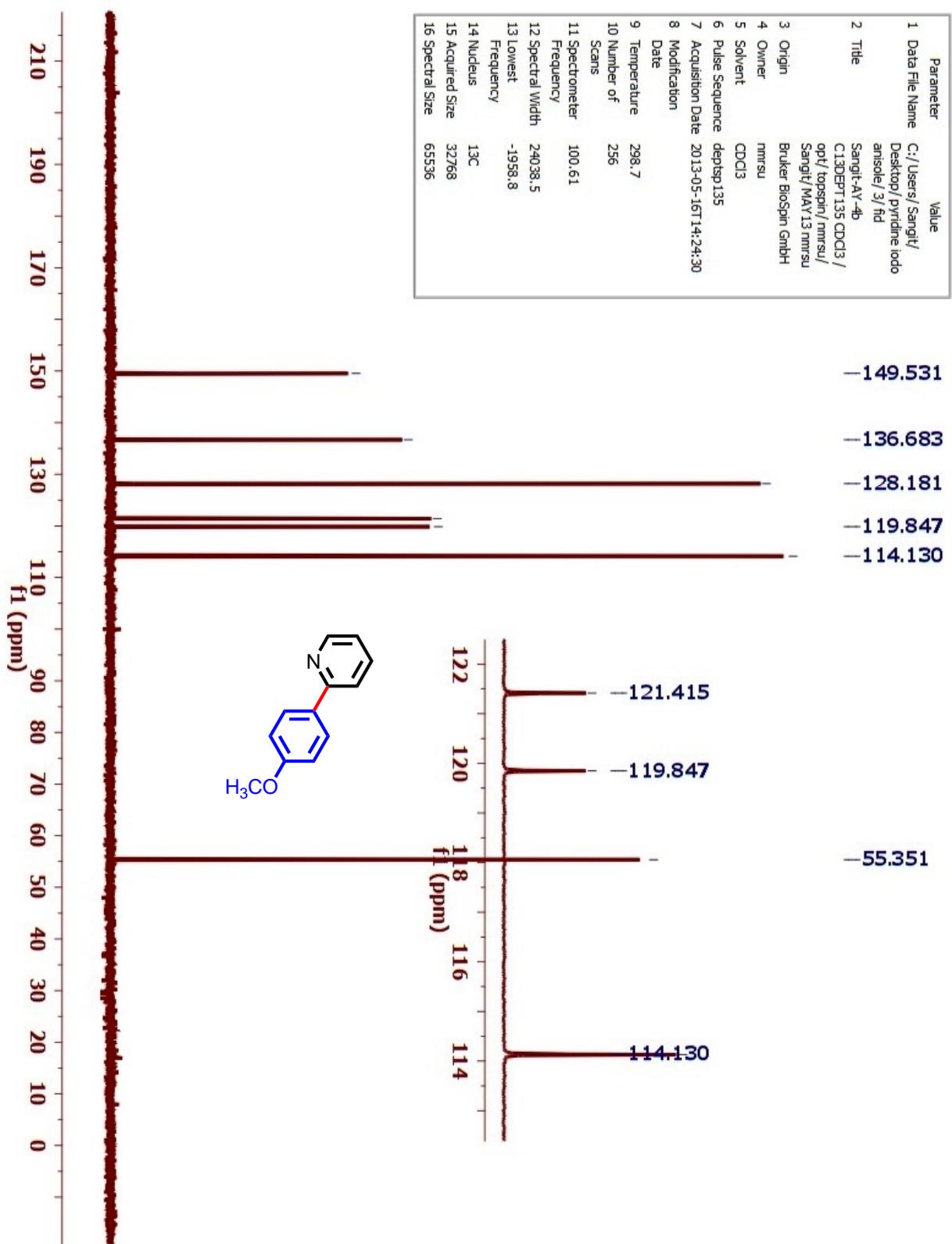


Figure S89 <sup>1</sup>H NMR of 27

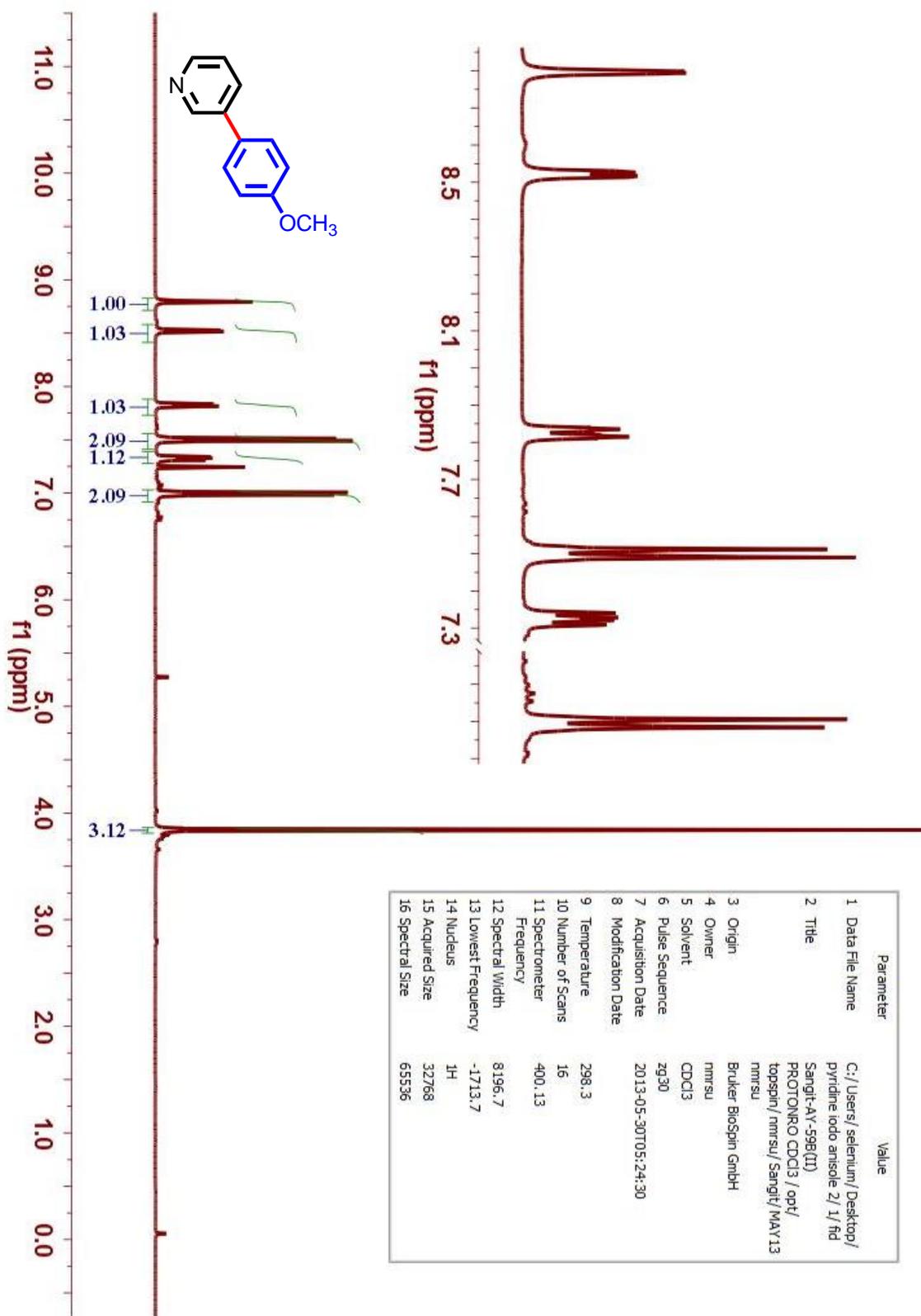


Figure S90  $^{13}\text{C}$  NMR spectrum of **27**

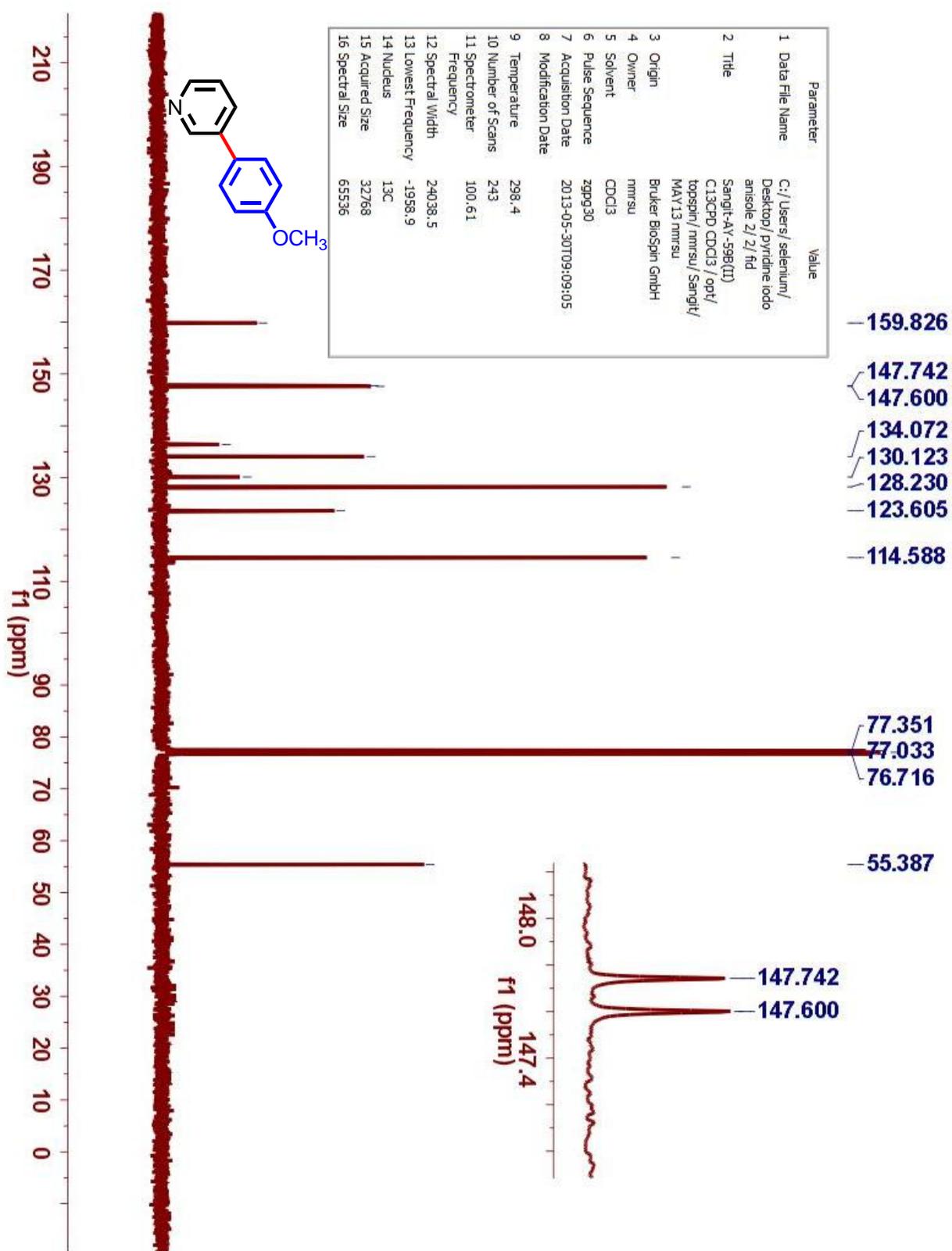


Figure S91  $^{13}\text{C}$  NMR spectrum of **27**

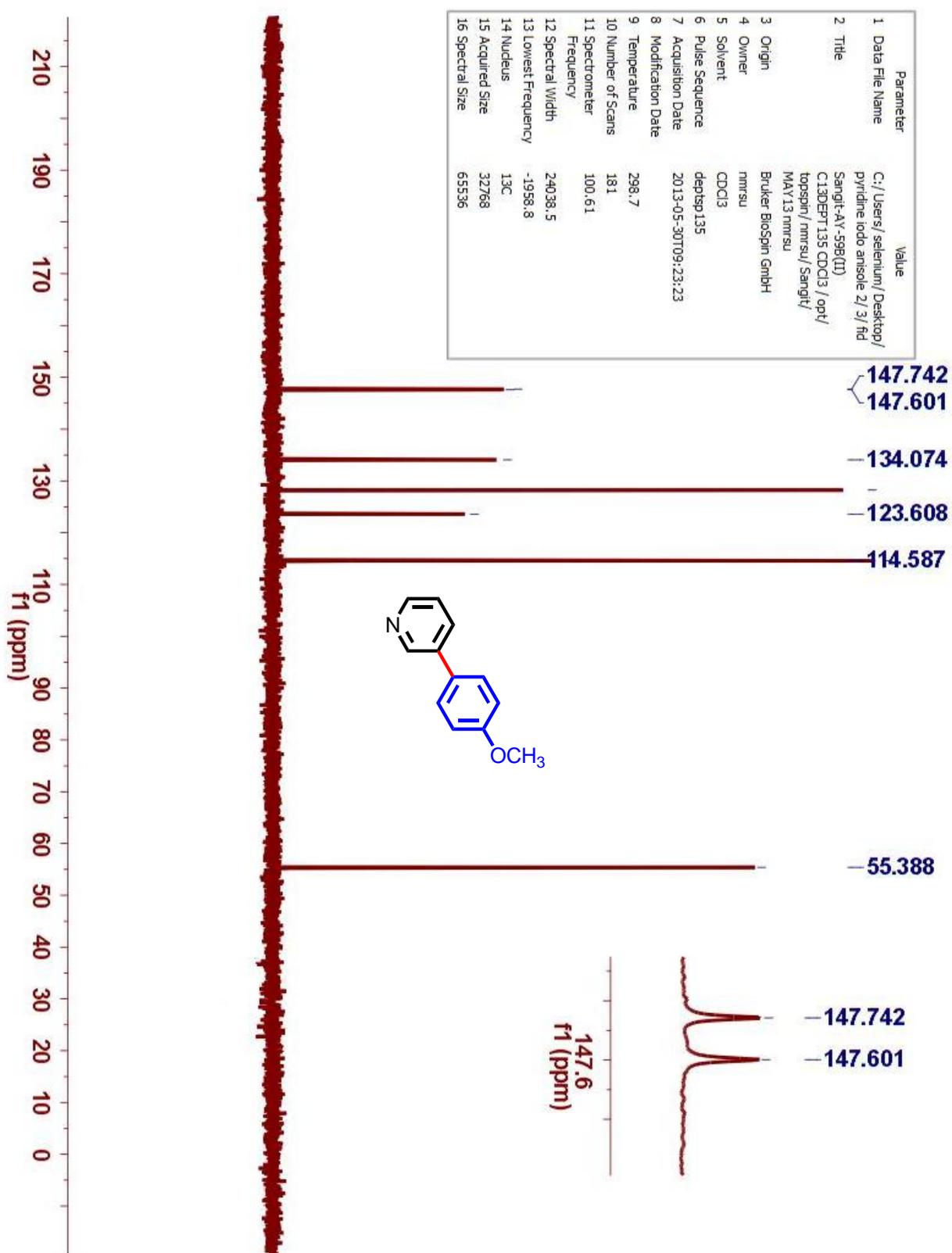


Figure S92  $^1\text{H}$  NMR of **28**

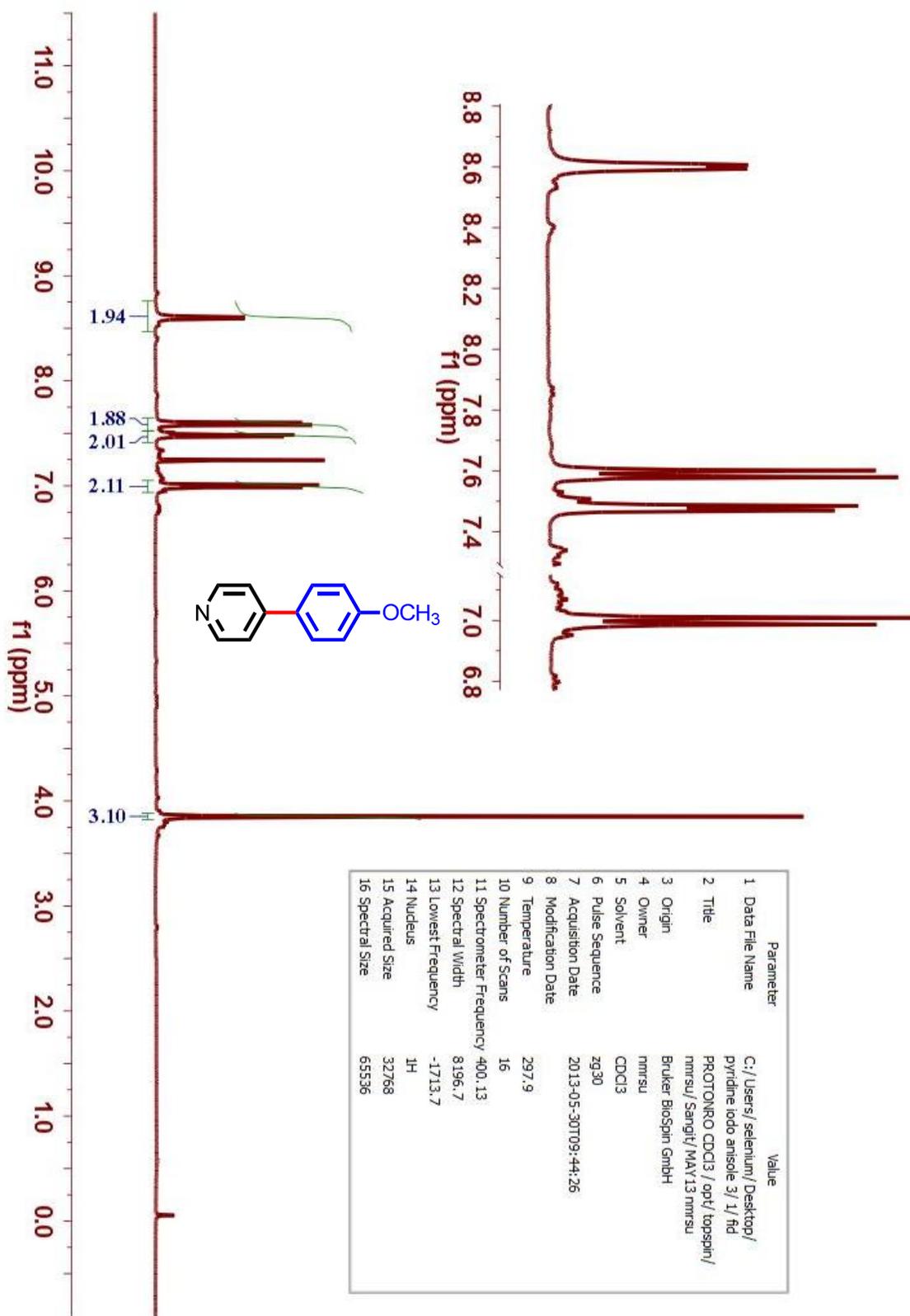


Figure S93 <sup>13</sup>C NMR spectrum of **28**

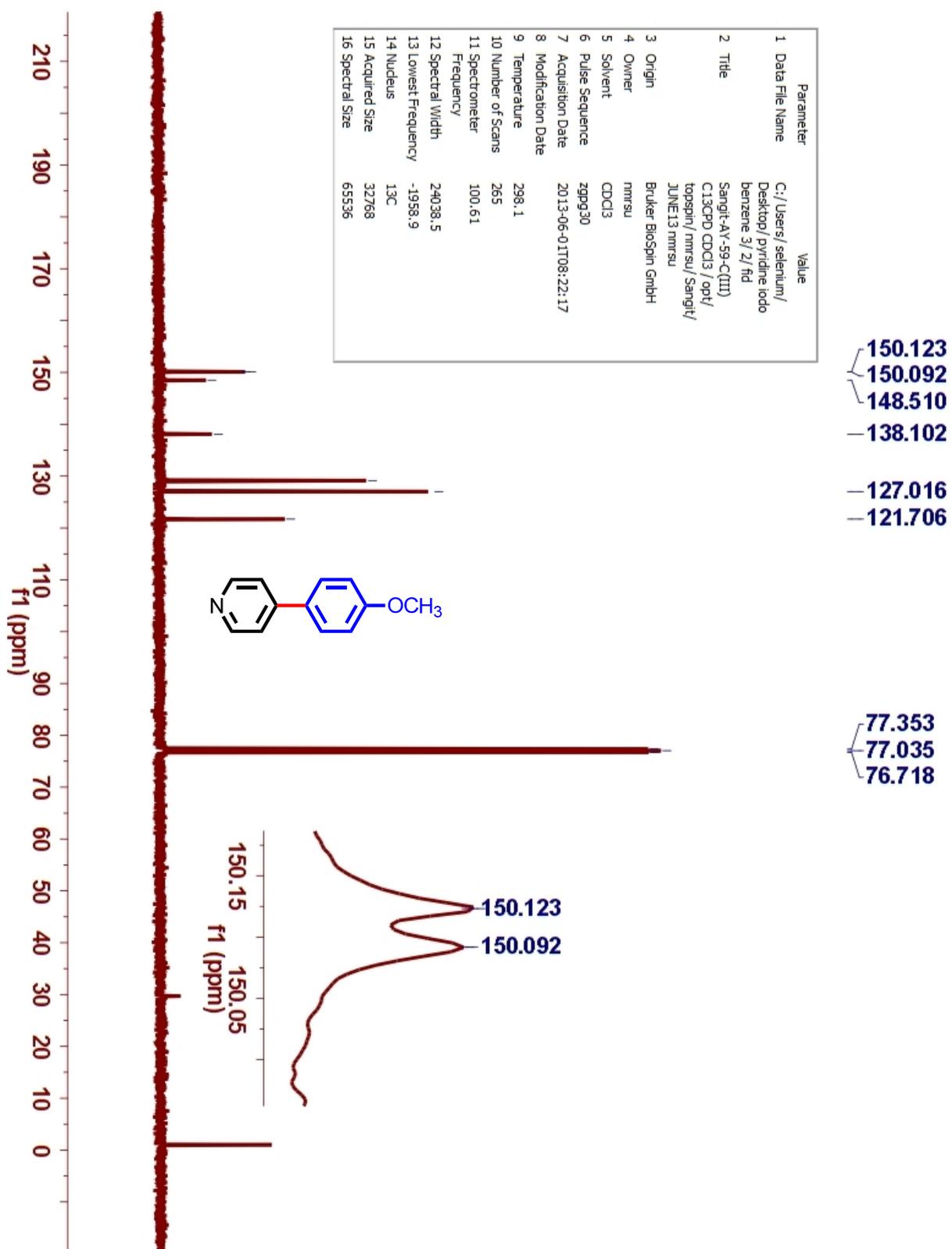


Figure S94  $^{13}\text{C}$  NMR spectrum of **28**

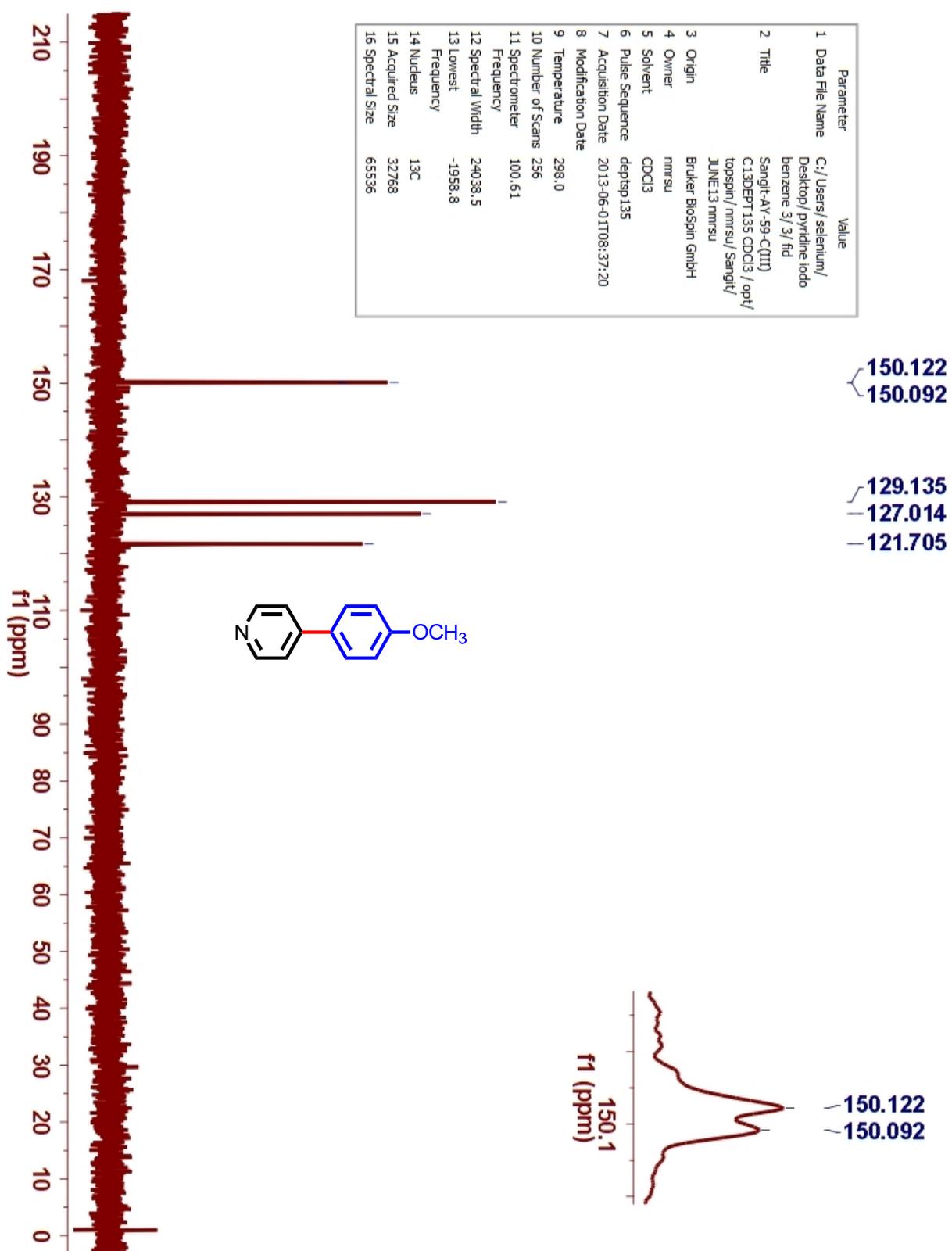


Figure S95  $^1\text{H}$  NMR of **29**

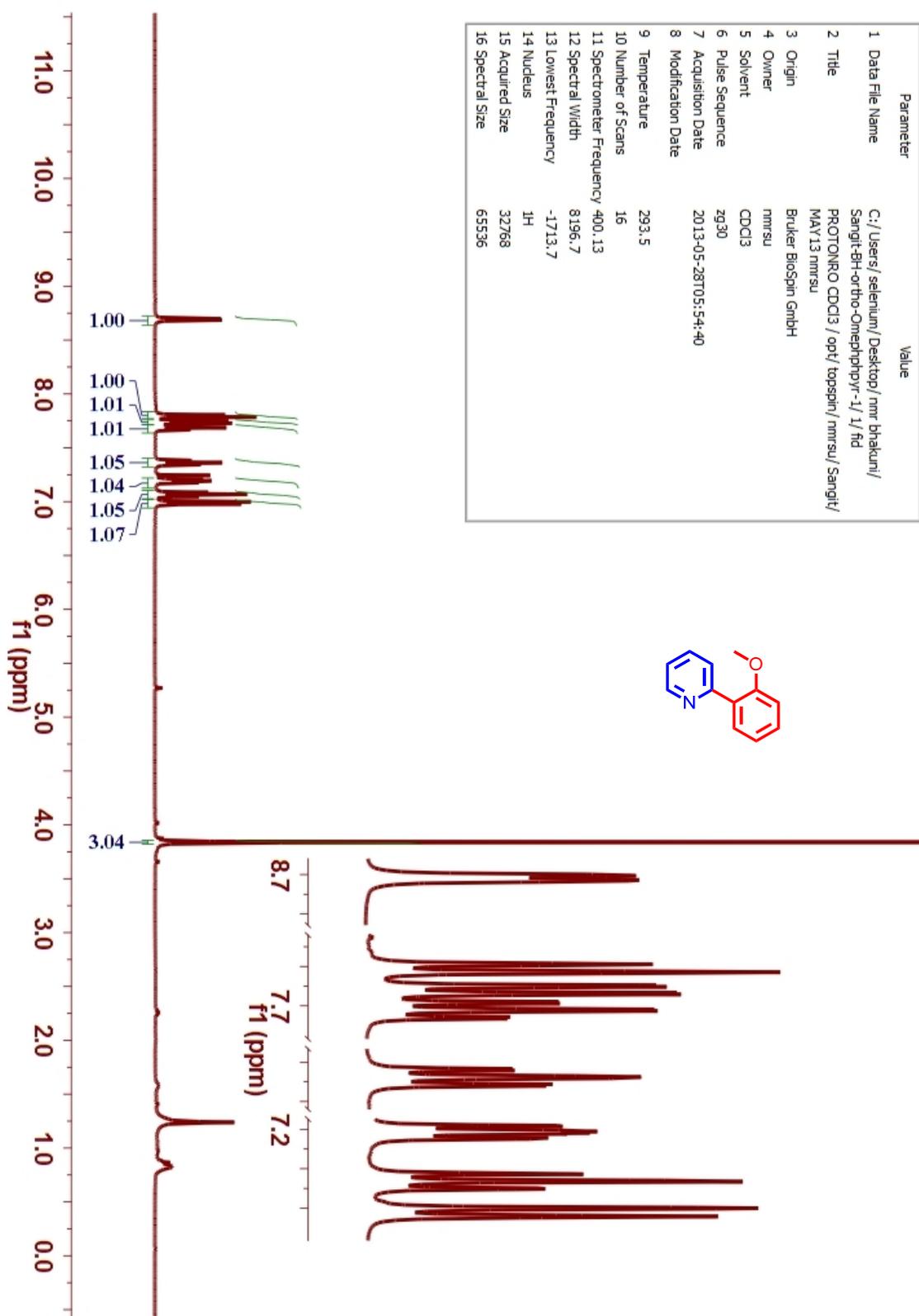


Figure S96 <sup>13</sup>C NMR spectrum of **29**

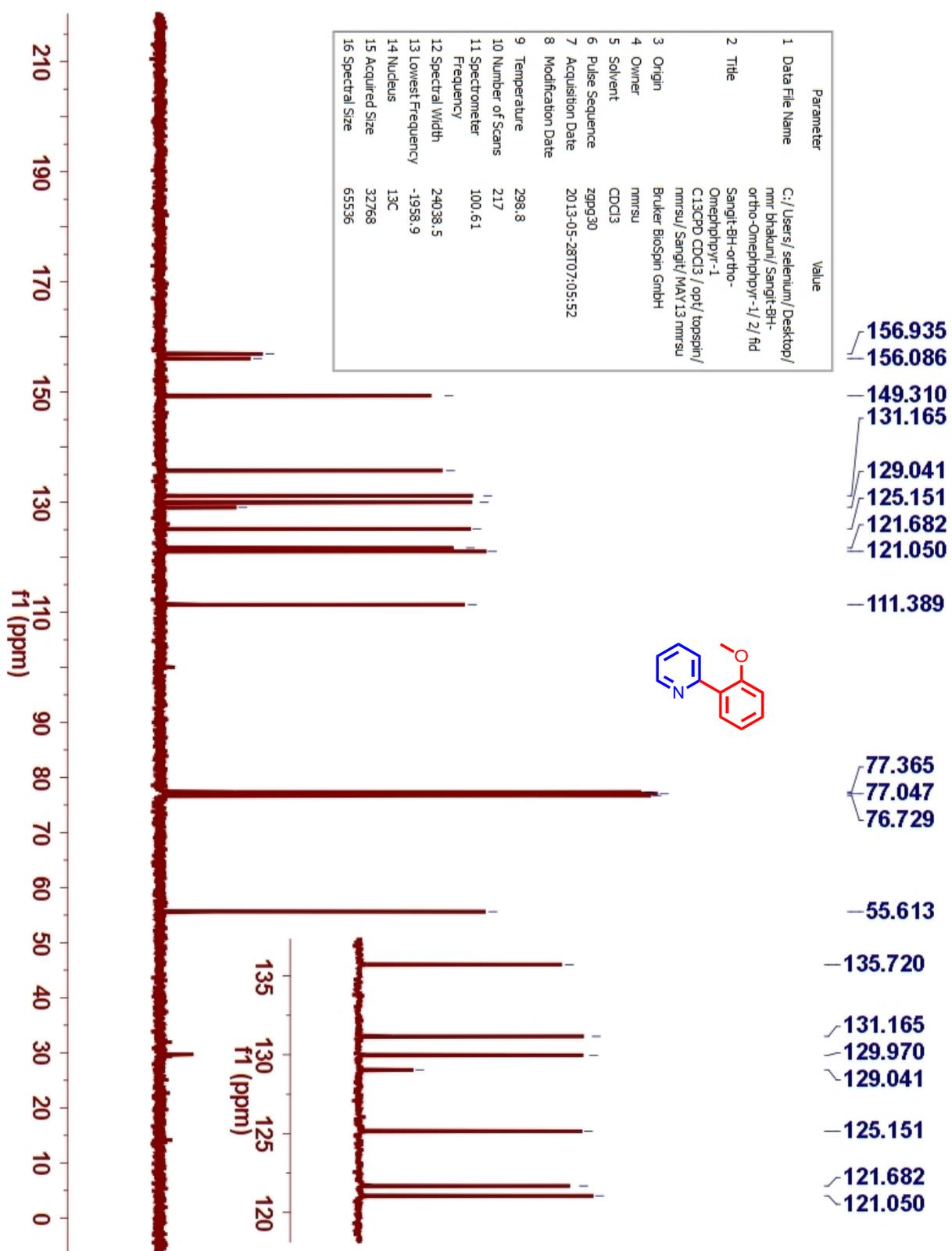


Figure S97  $^{13}\text{C}$  NMR DEPT-135 of **29**

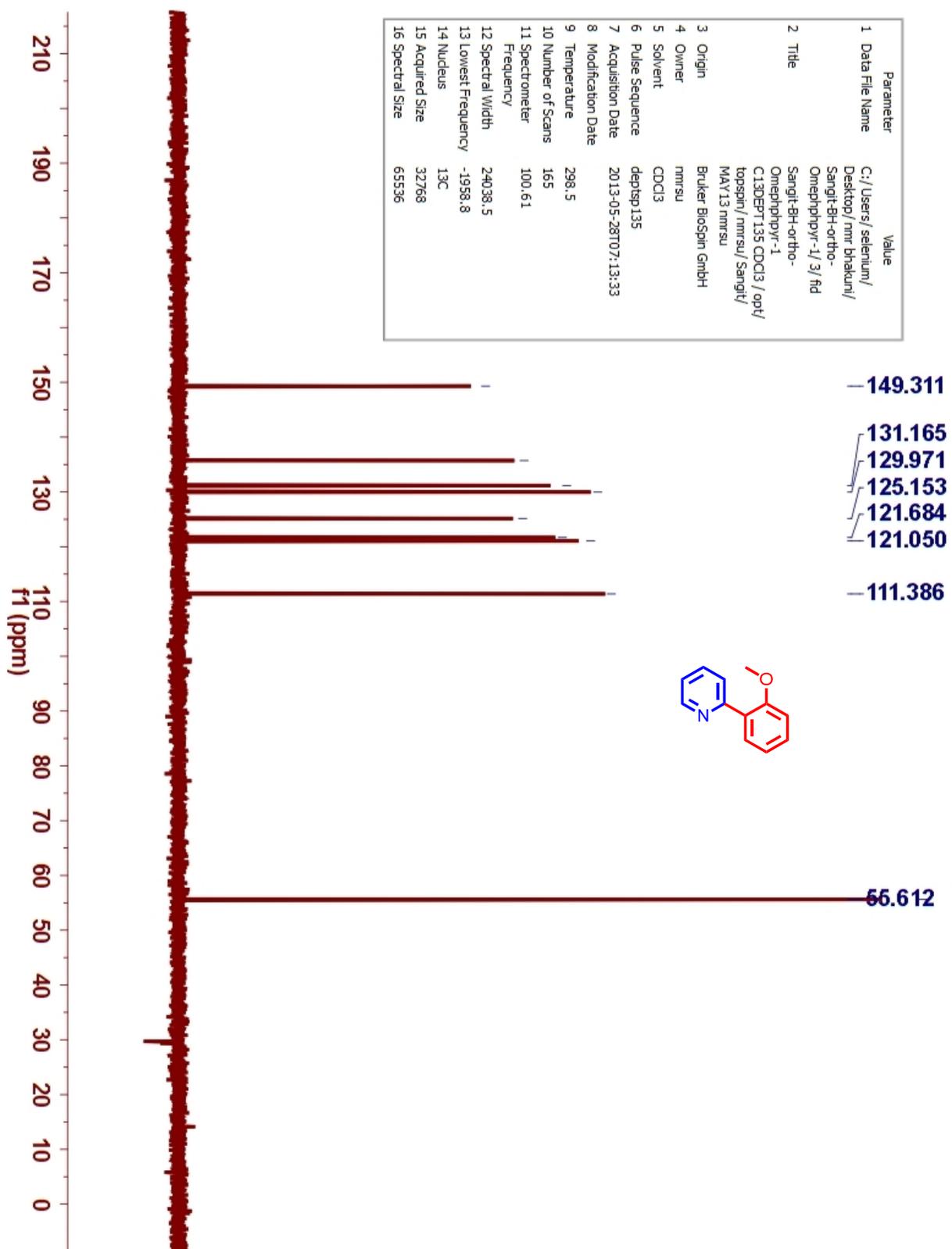


Figure S98 <sup>1</sup>H NMR of **30**

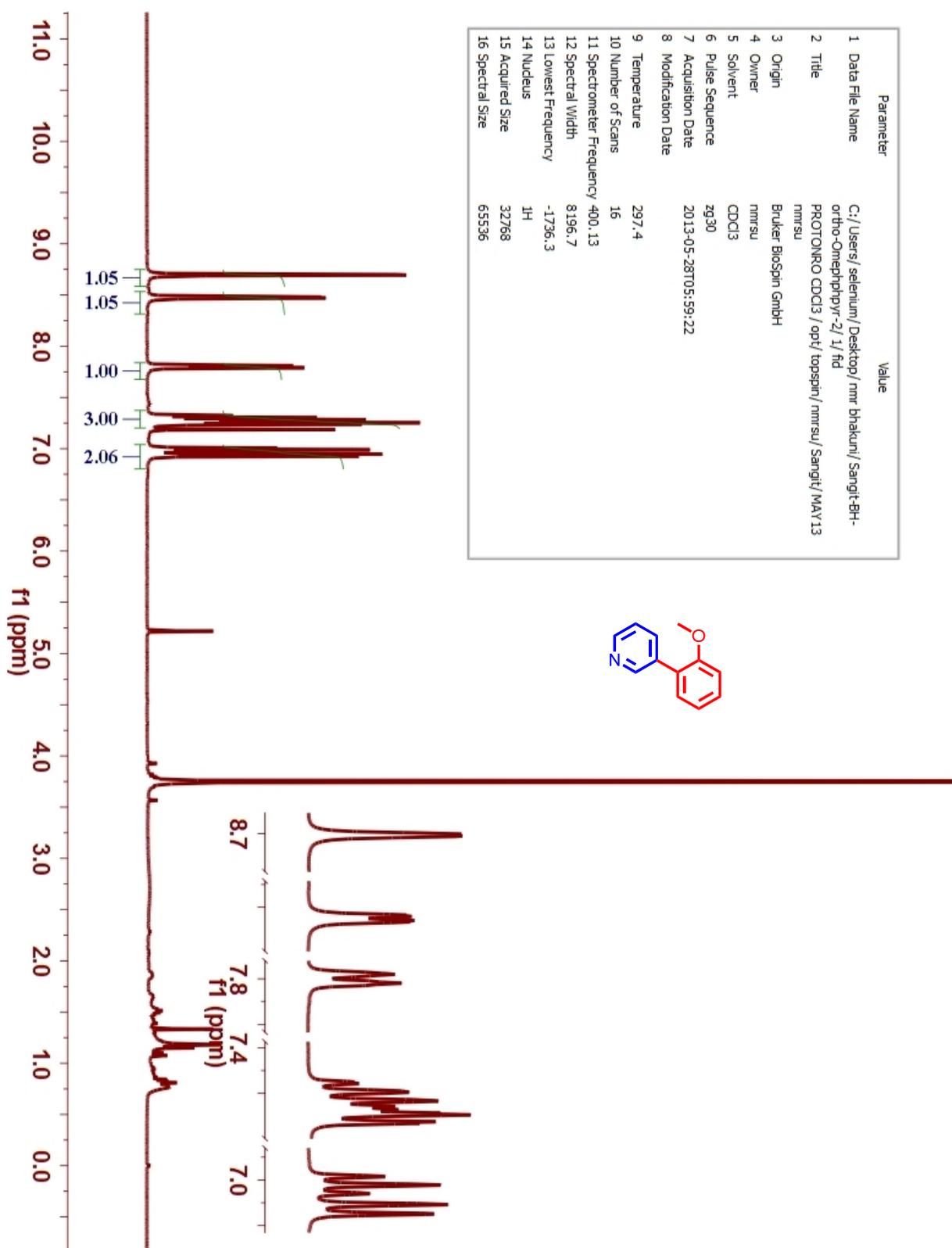


Figure S99  $^{13}\text{C}$  NMR spectrum of **30**

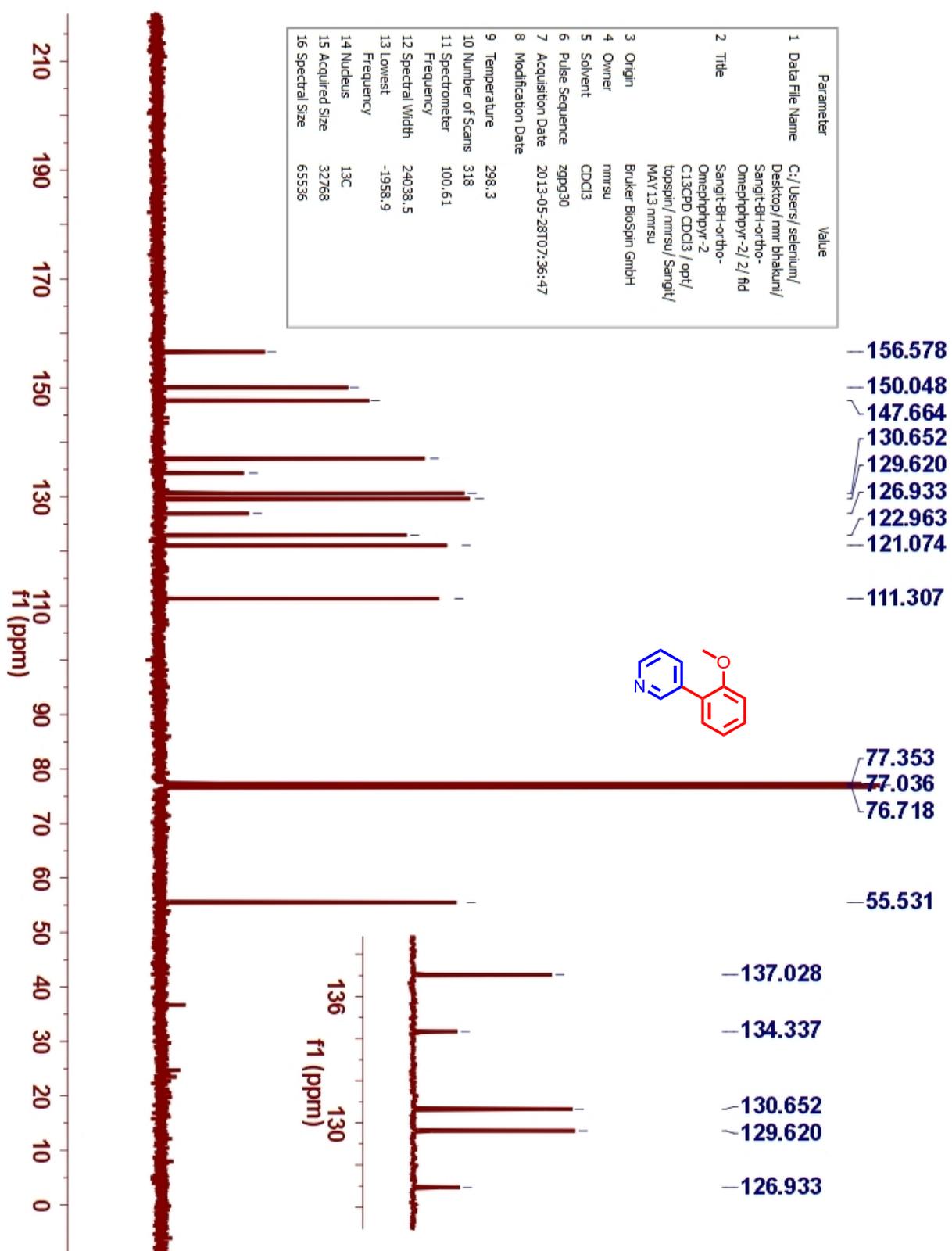


Figure S100  $^{13}\text{C}$  NMR DEPT-135 of **30**

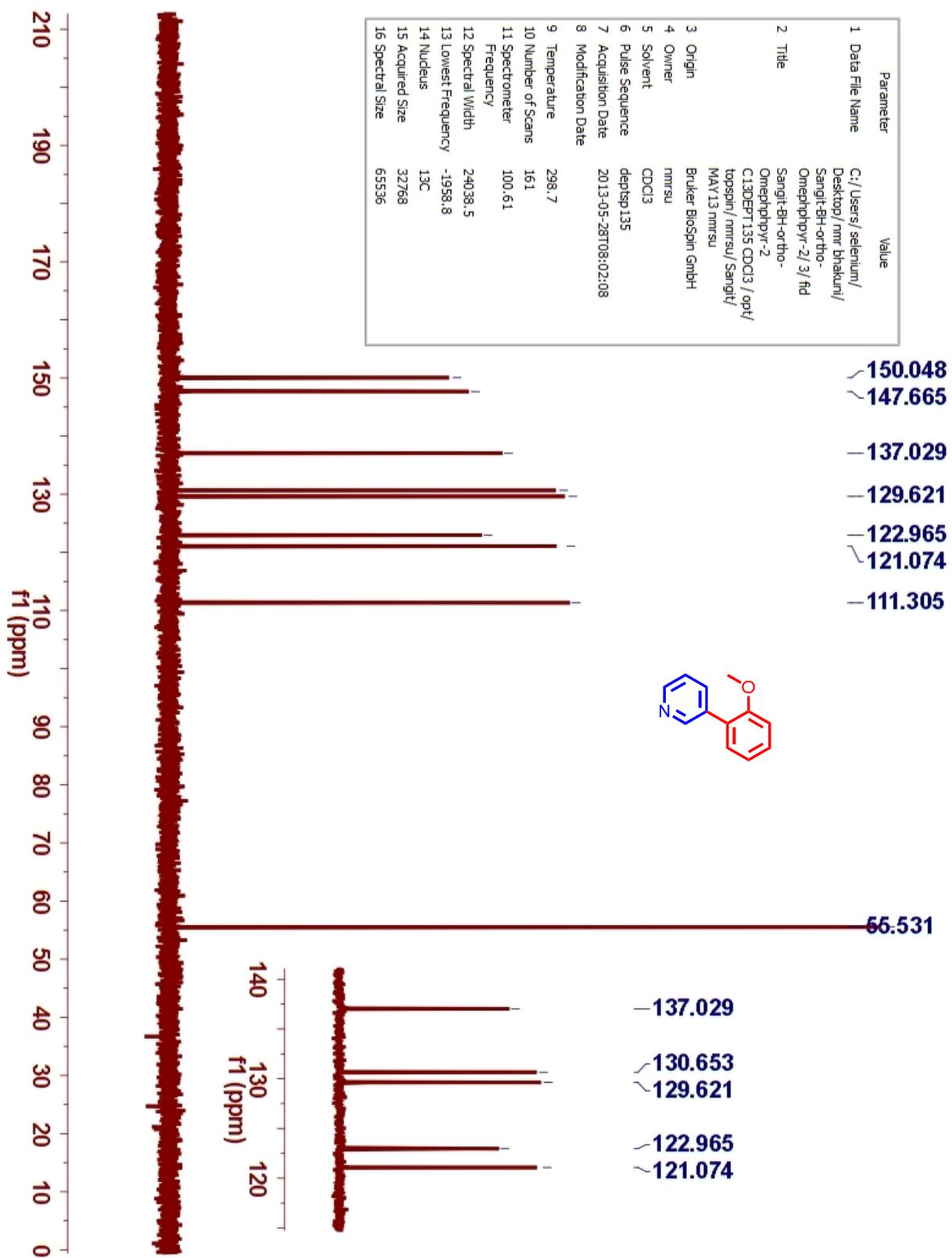


Figure S101 <sup>1</sup>H NMR of **31**

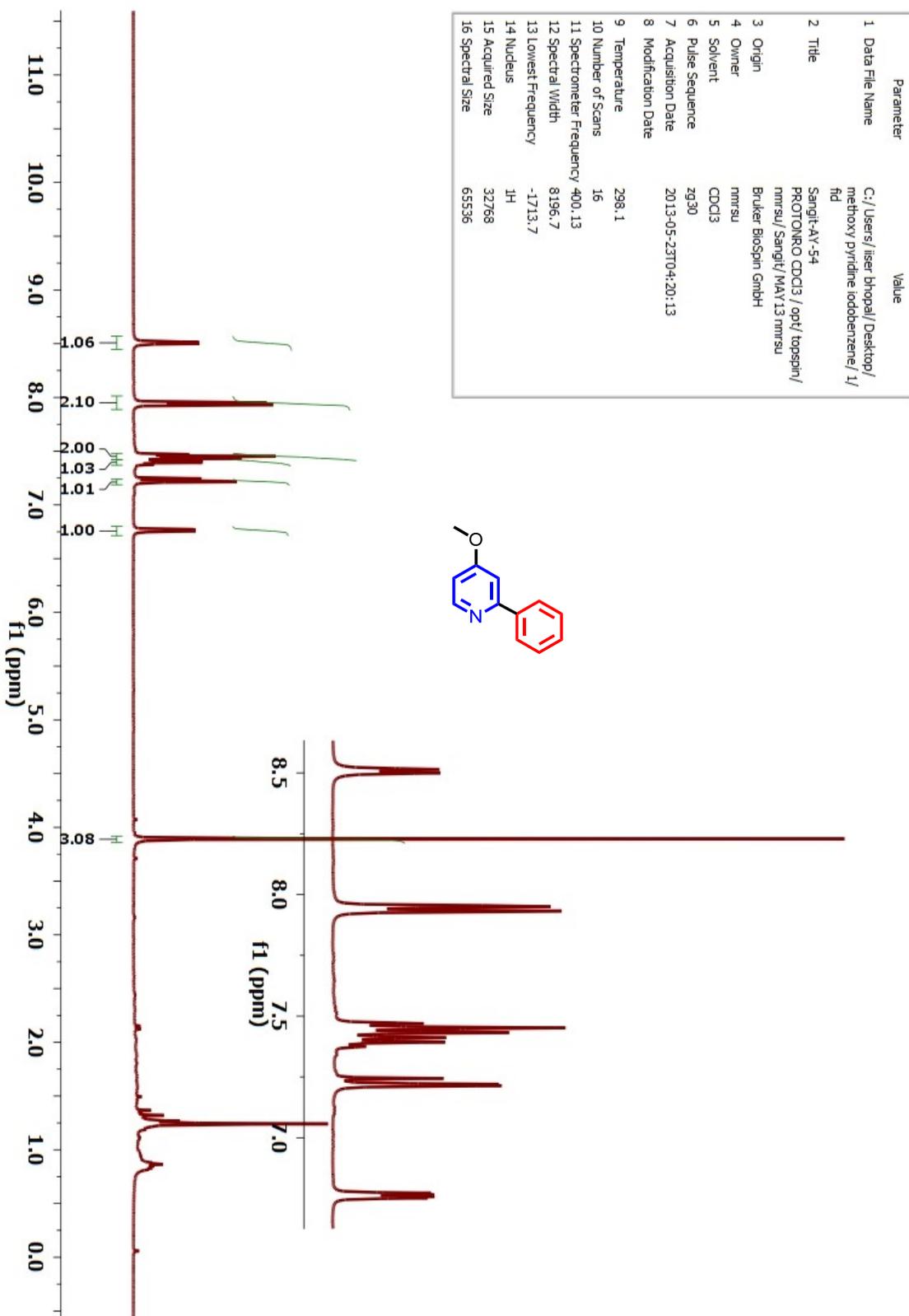


Figure S102  $^{13}\text{C}$  NMR spectrum of **31**

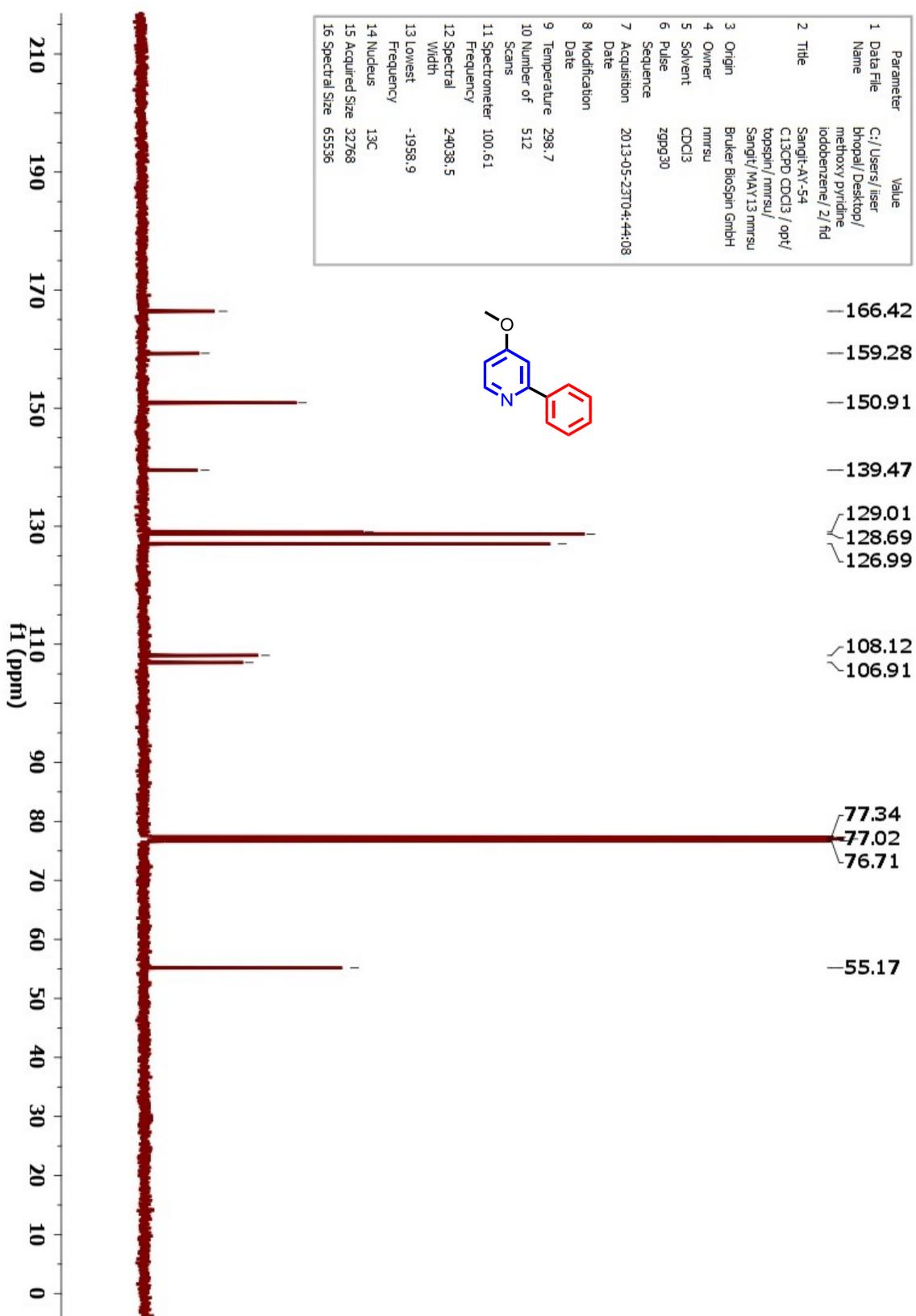


Figure S103  $^{13}\text{C}$  NMR DEPT-135 of **31**

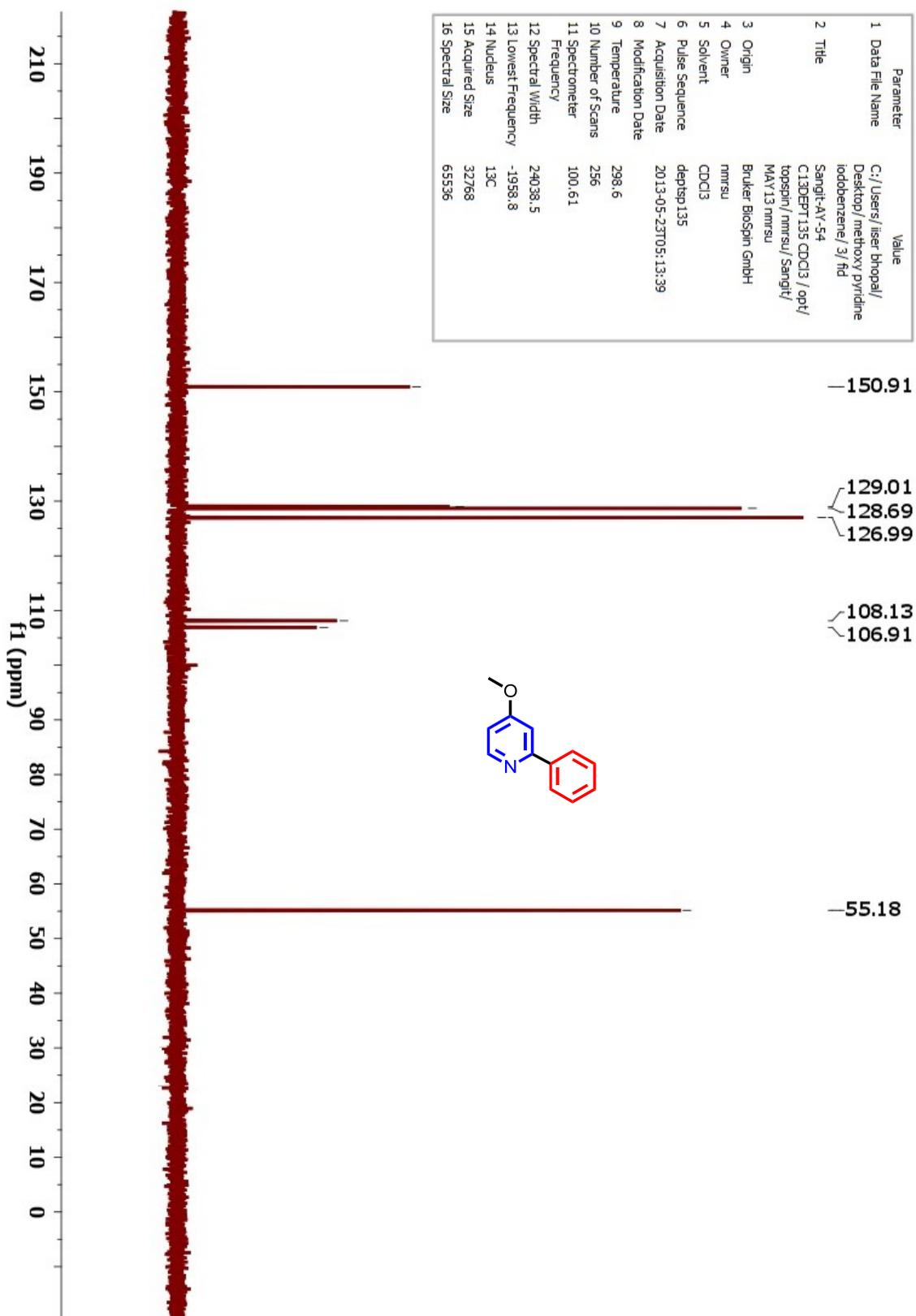


Figure S104  $^1\text{H}$  NMR of **32**

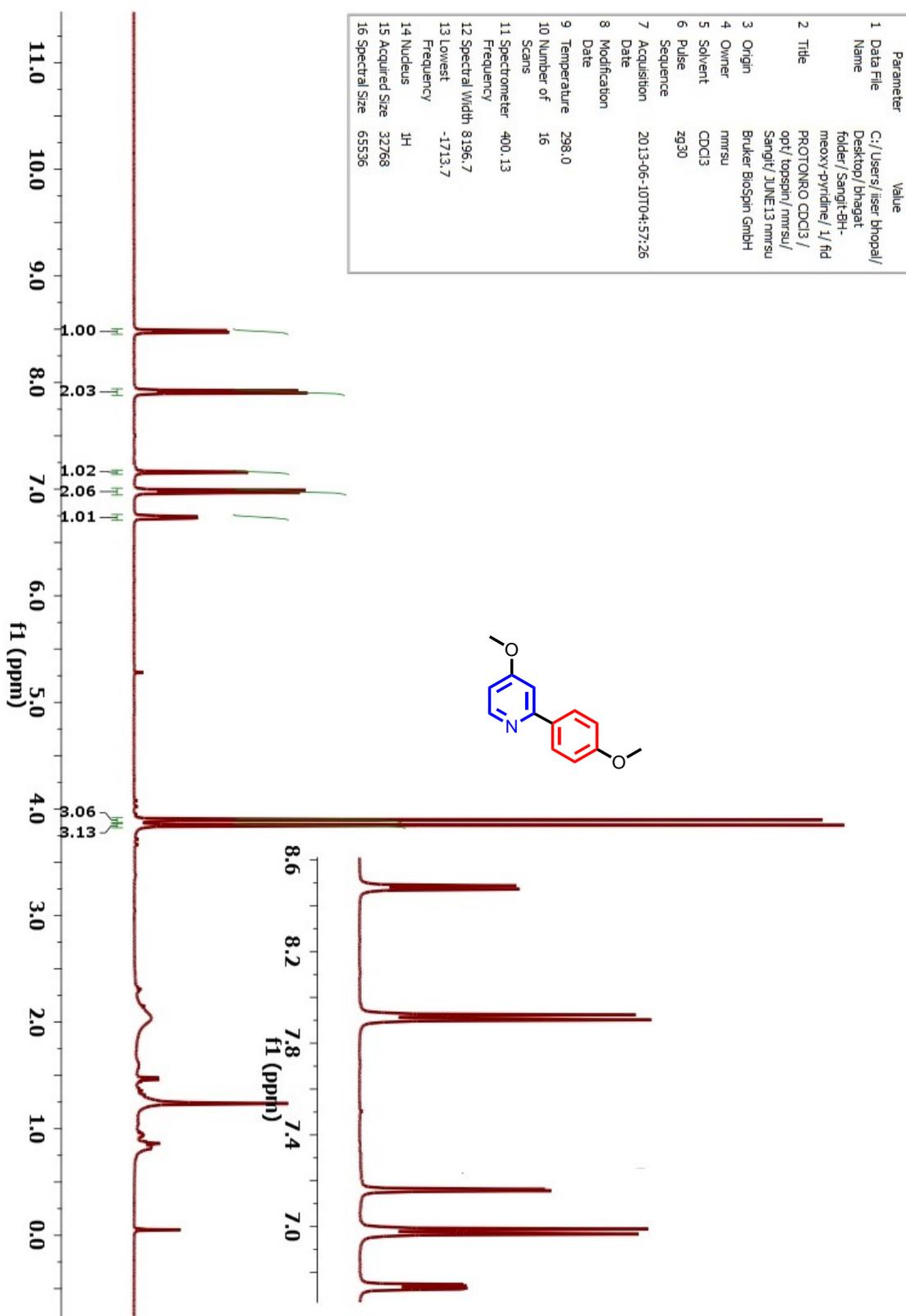


Figure S105 <sup>13</sup>C NMR spectrum of **32**

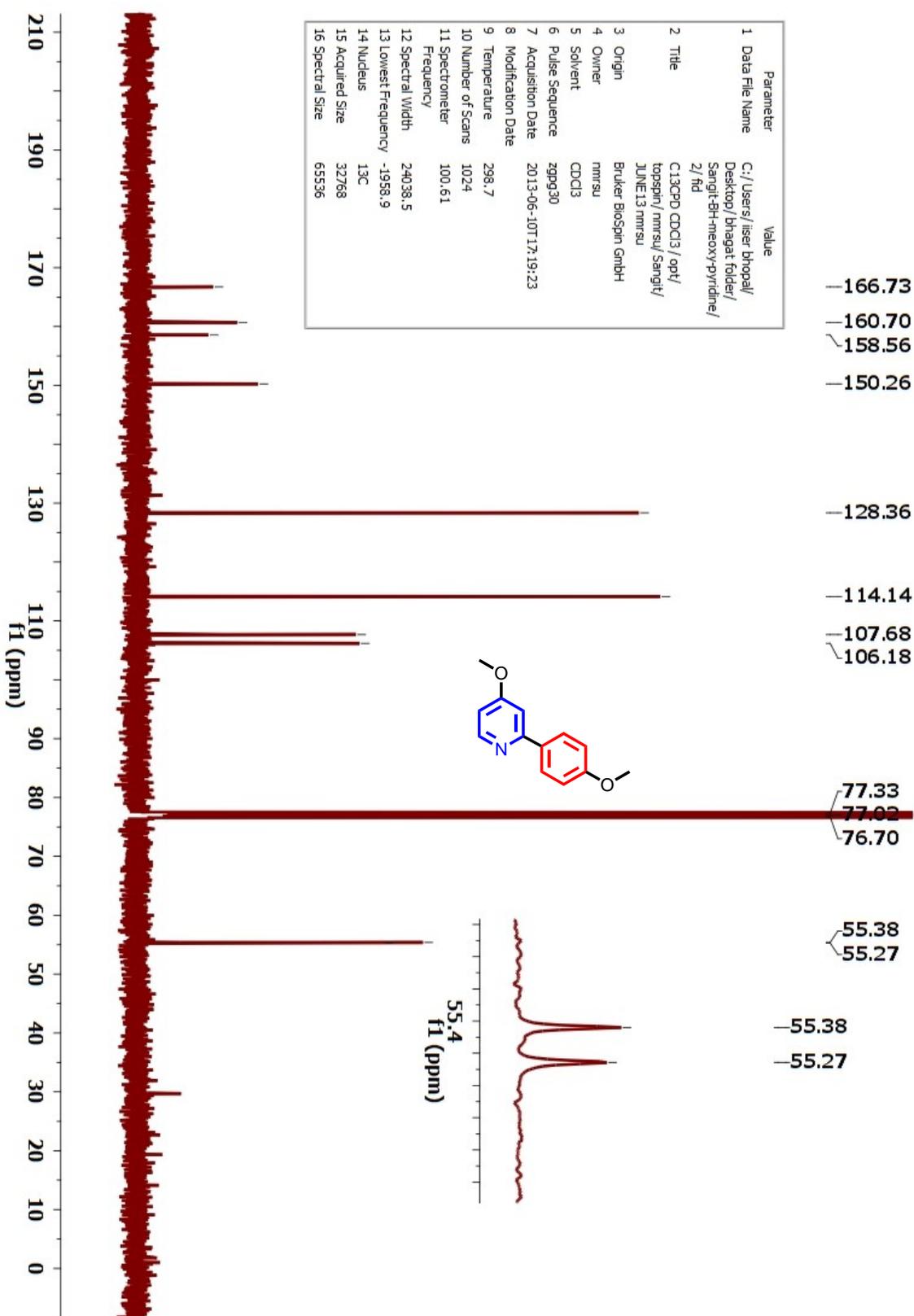


Figure S106  $^{13}\text{C}$  NMR spectrum of **32**

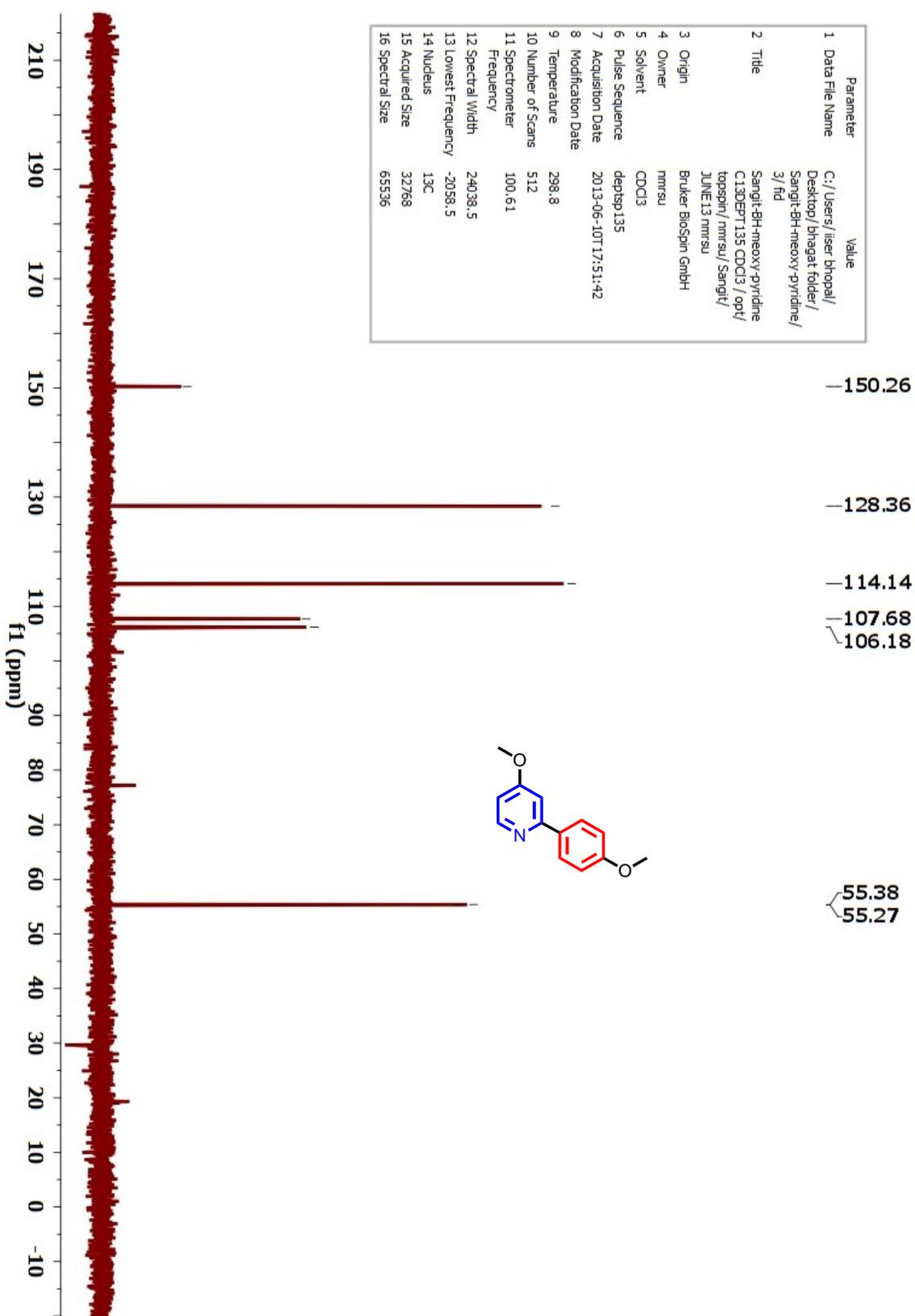


Figure S107  $^1\text{H}$  NMR of **33**

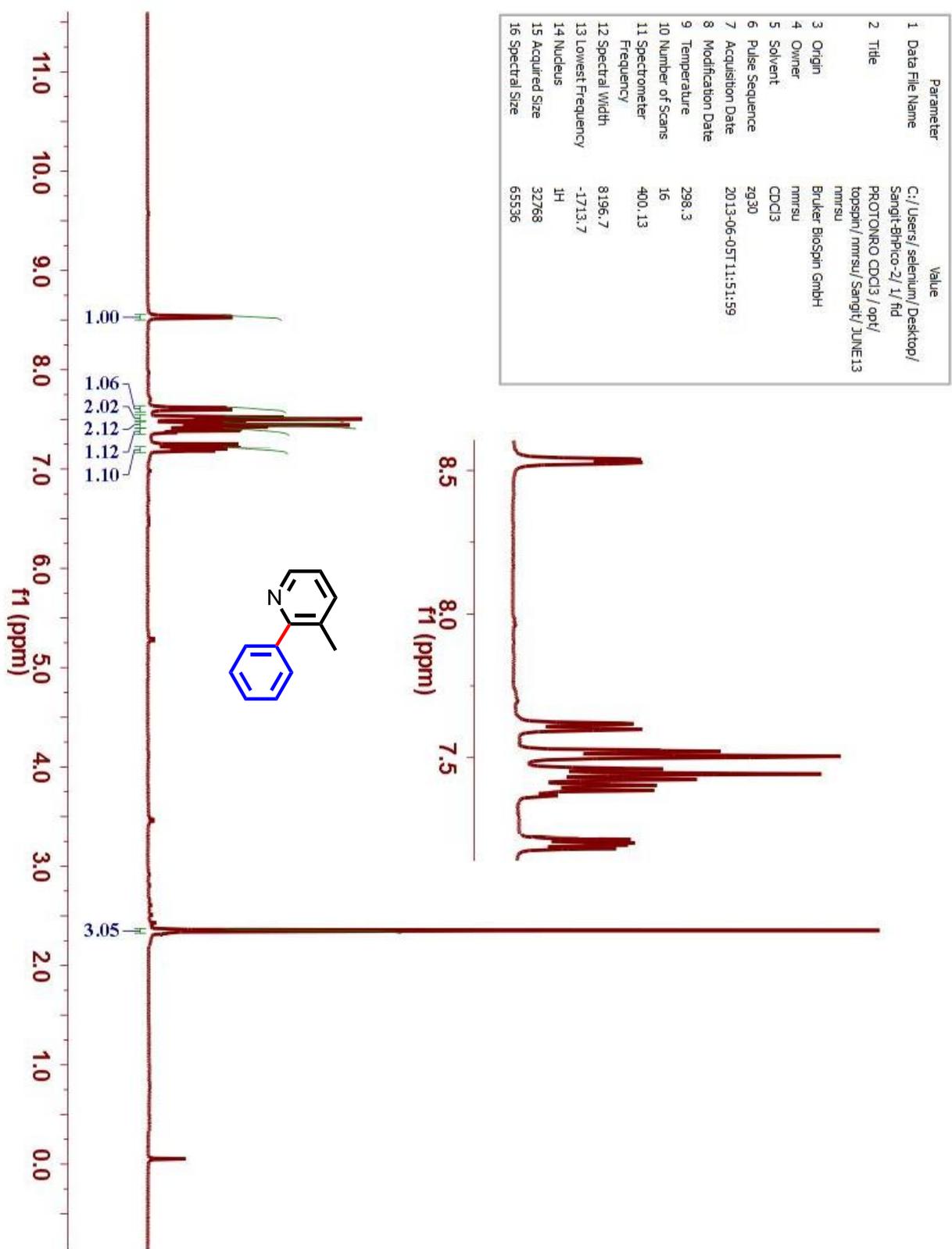


Figure S108 <sup>1</sup>H NMR of **34**

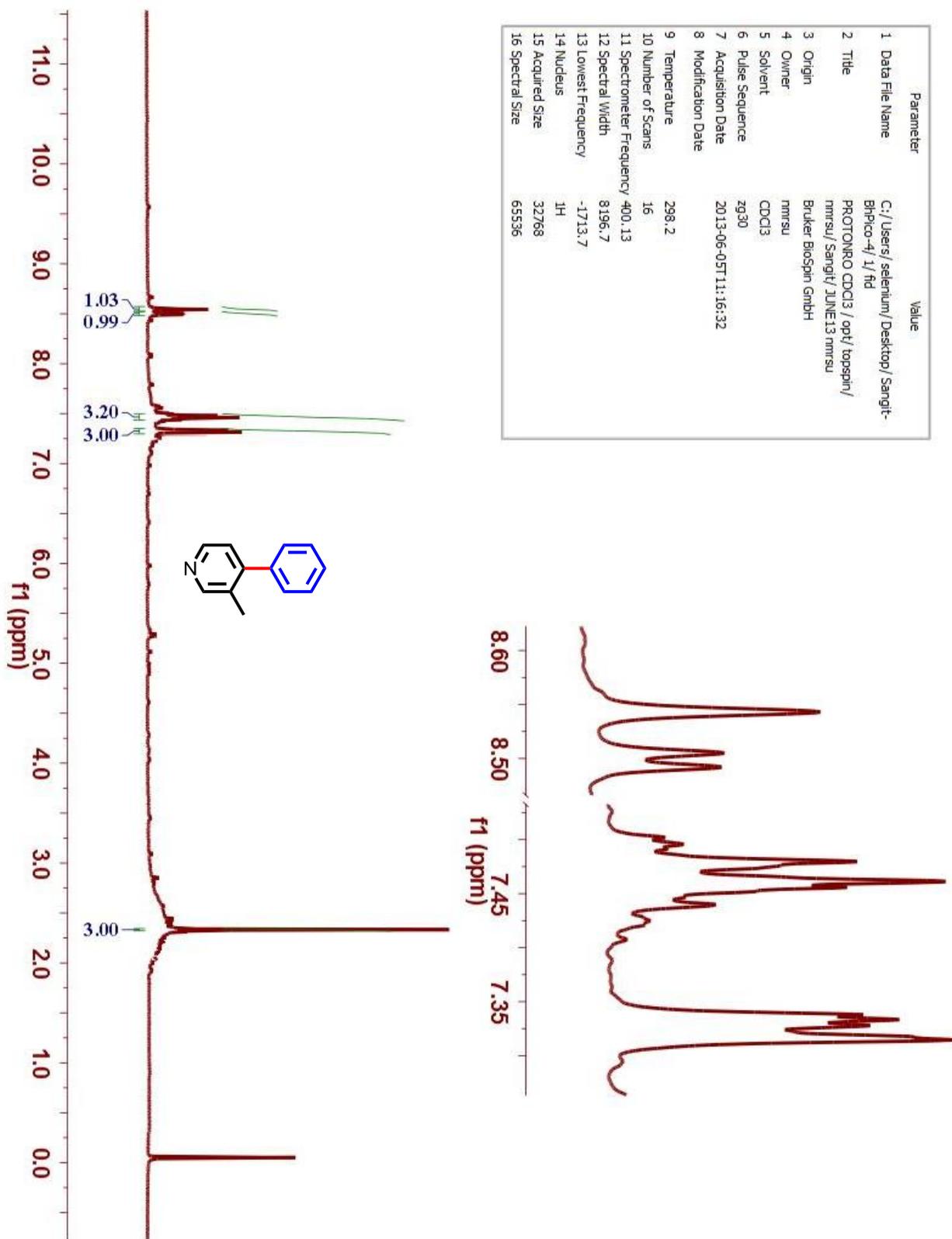




Figure S110  $^1\text{H}$  NMR of **36**

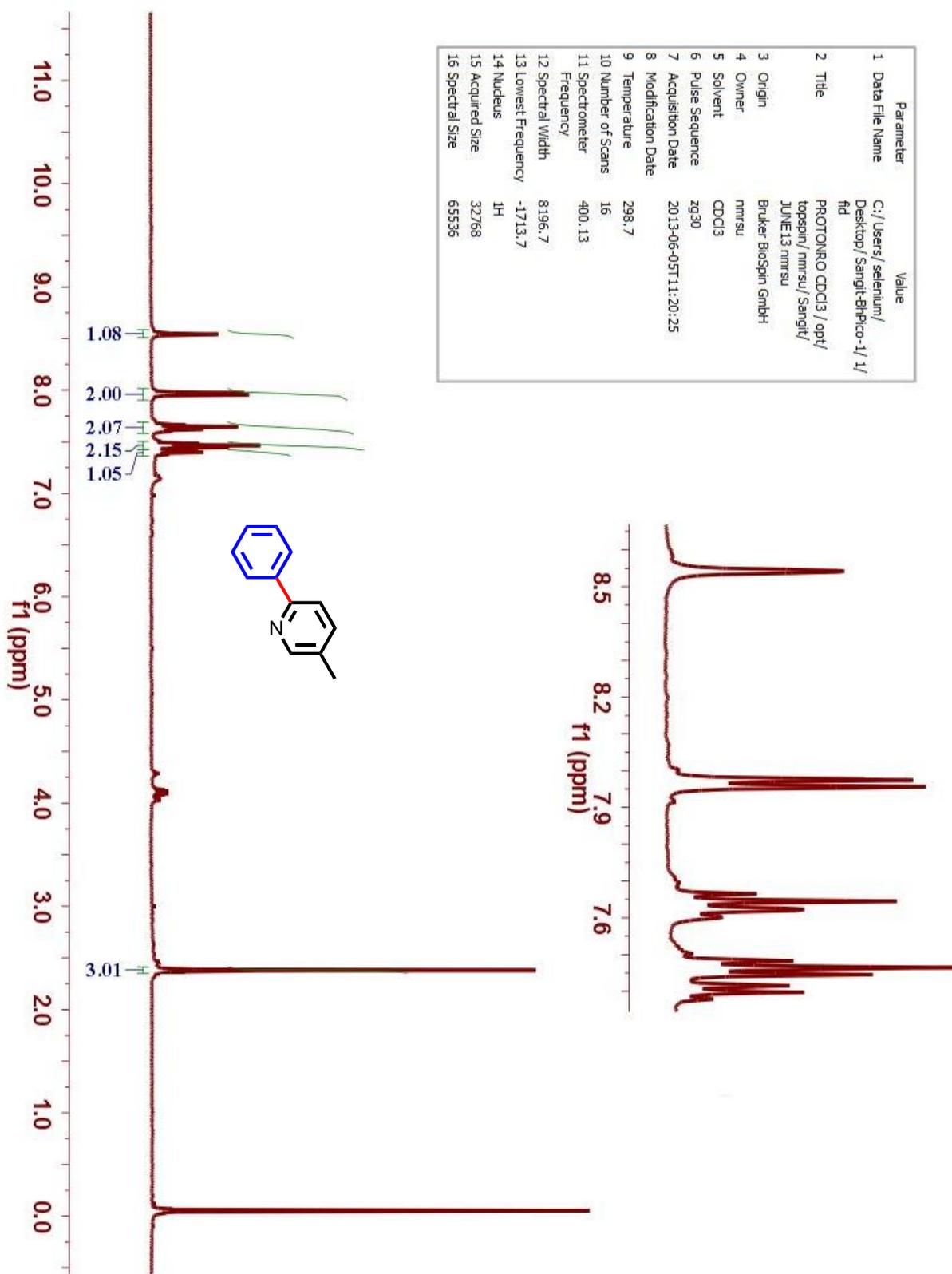


Figure S111  $^1\text{H}$  NMR of **37**

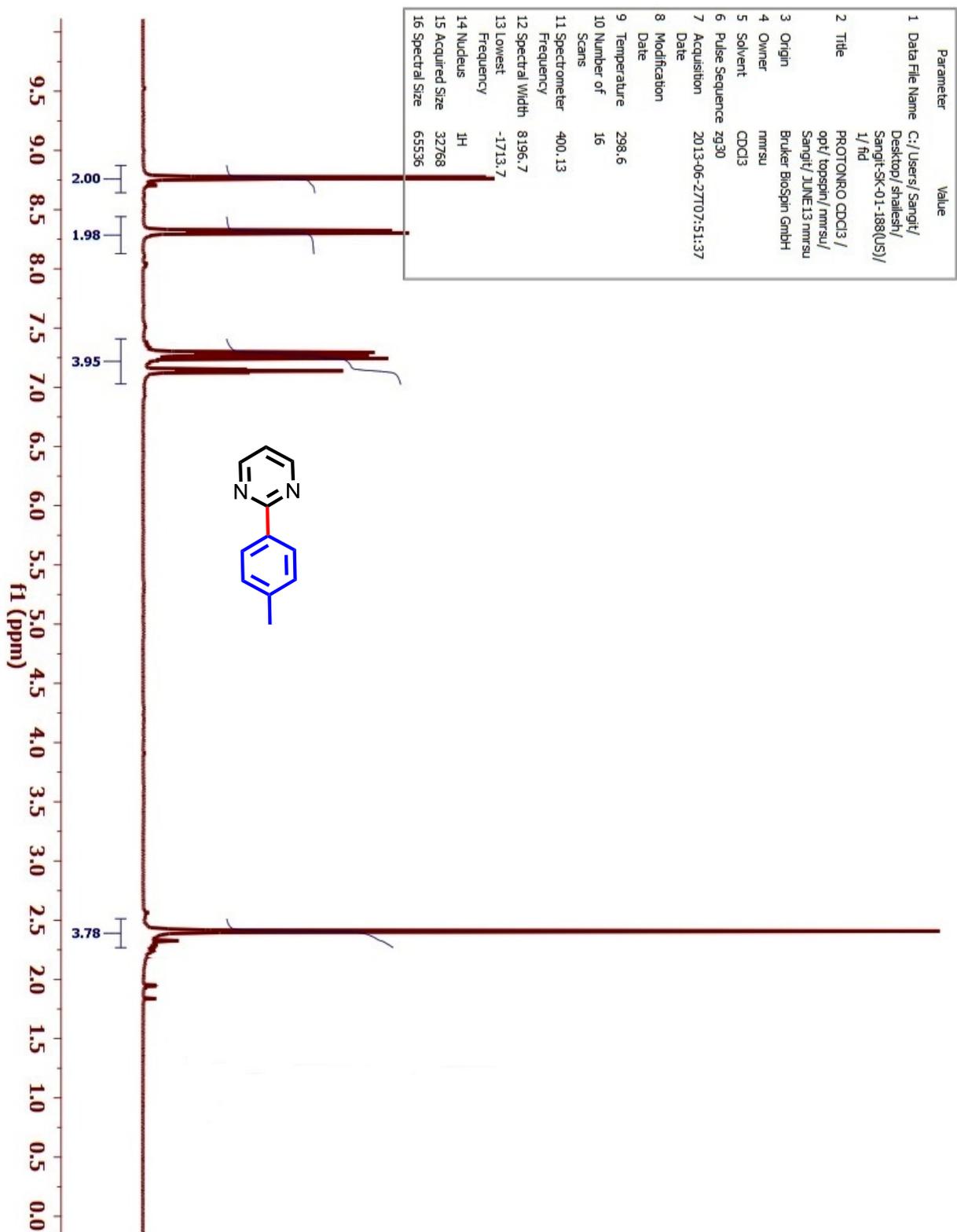


Figure S112  $^{13}\text{C}$  NMR of **37**

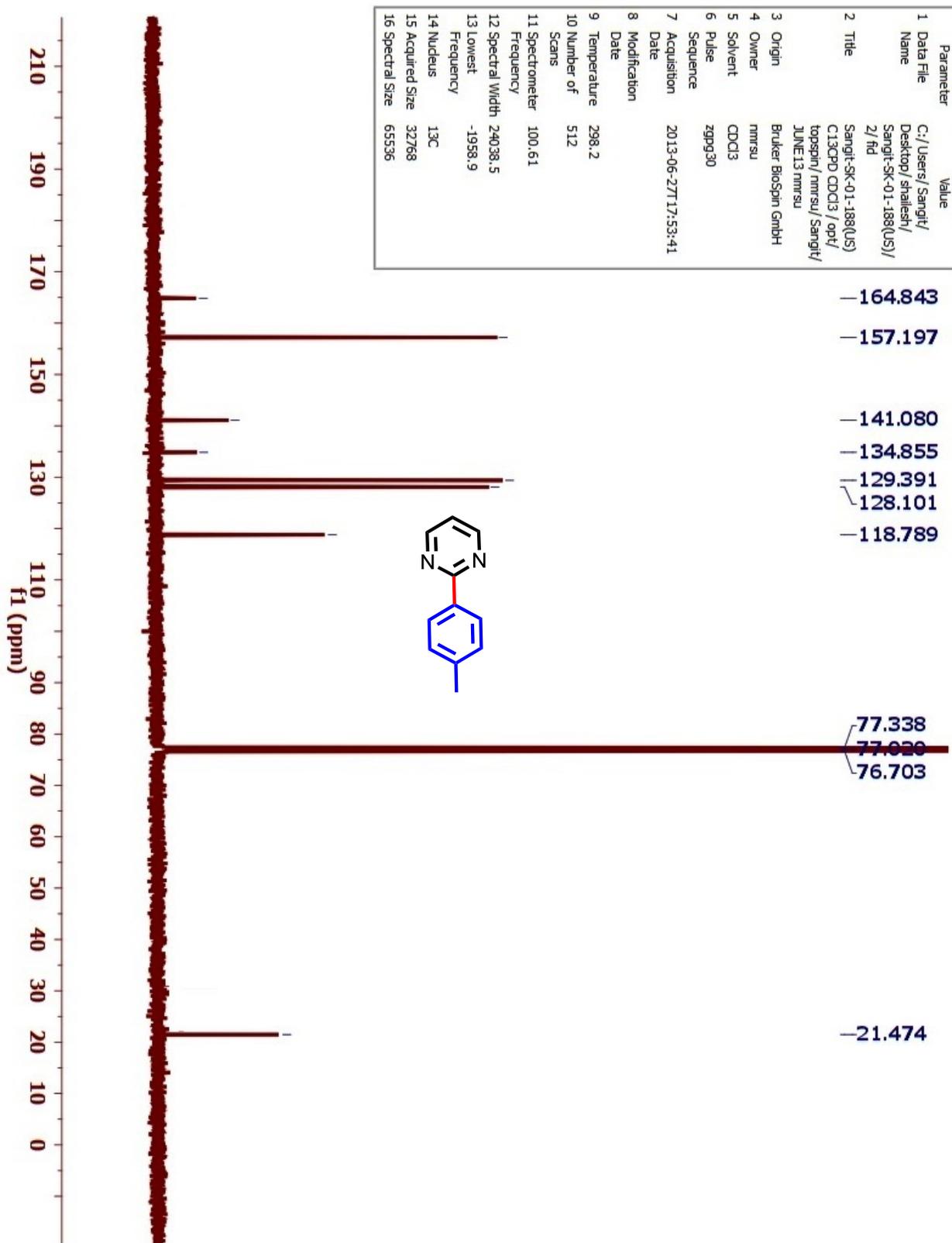


Figure S113  $^1\text{H}$  NMR of **38** and **39**

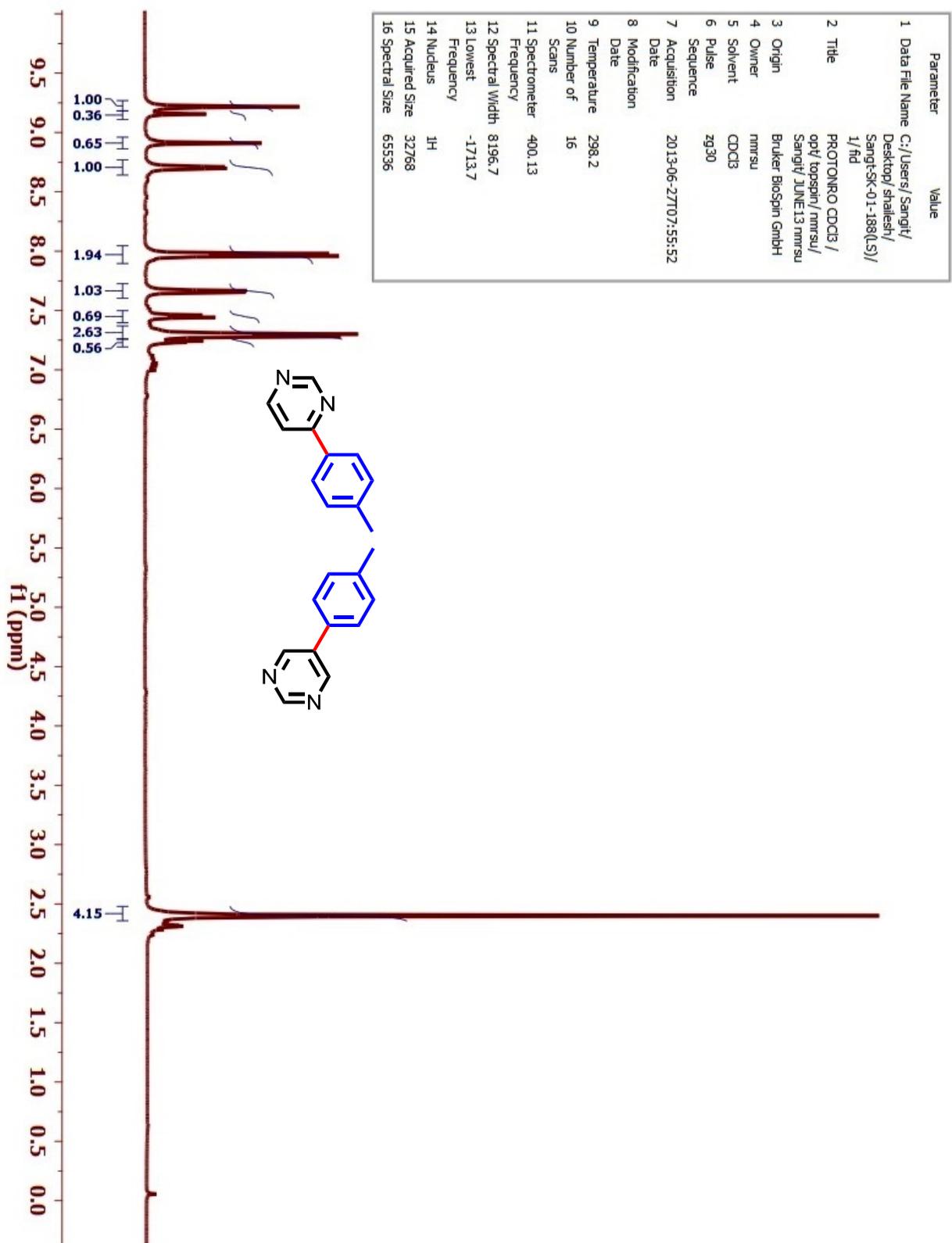


Figure S114  $^{13}\text{C}$  NMR of **38** and **39**

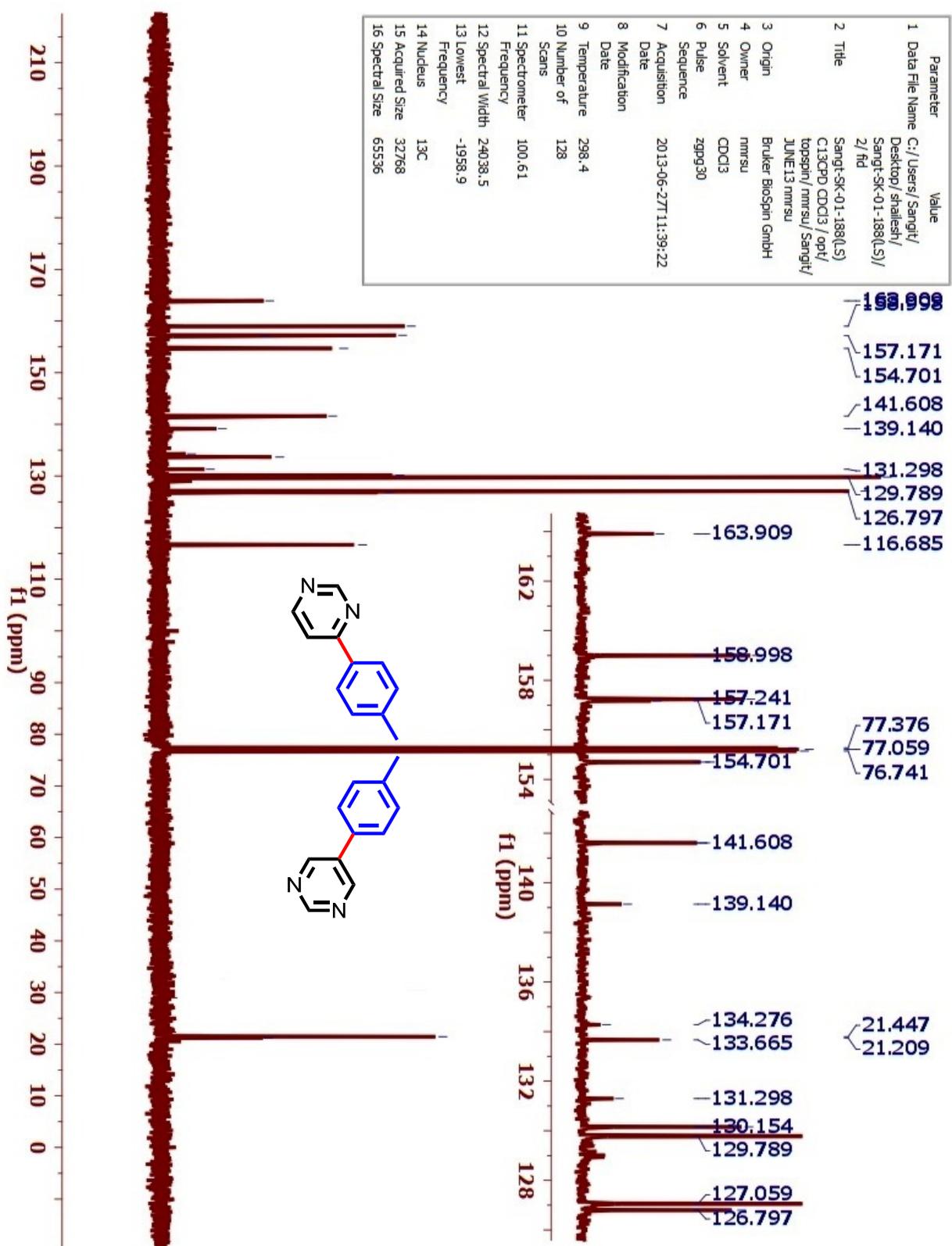


Figure S115  $^1\text{H}$  NMR of **40**

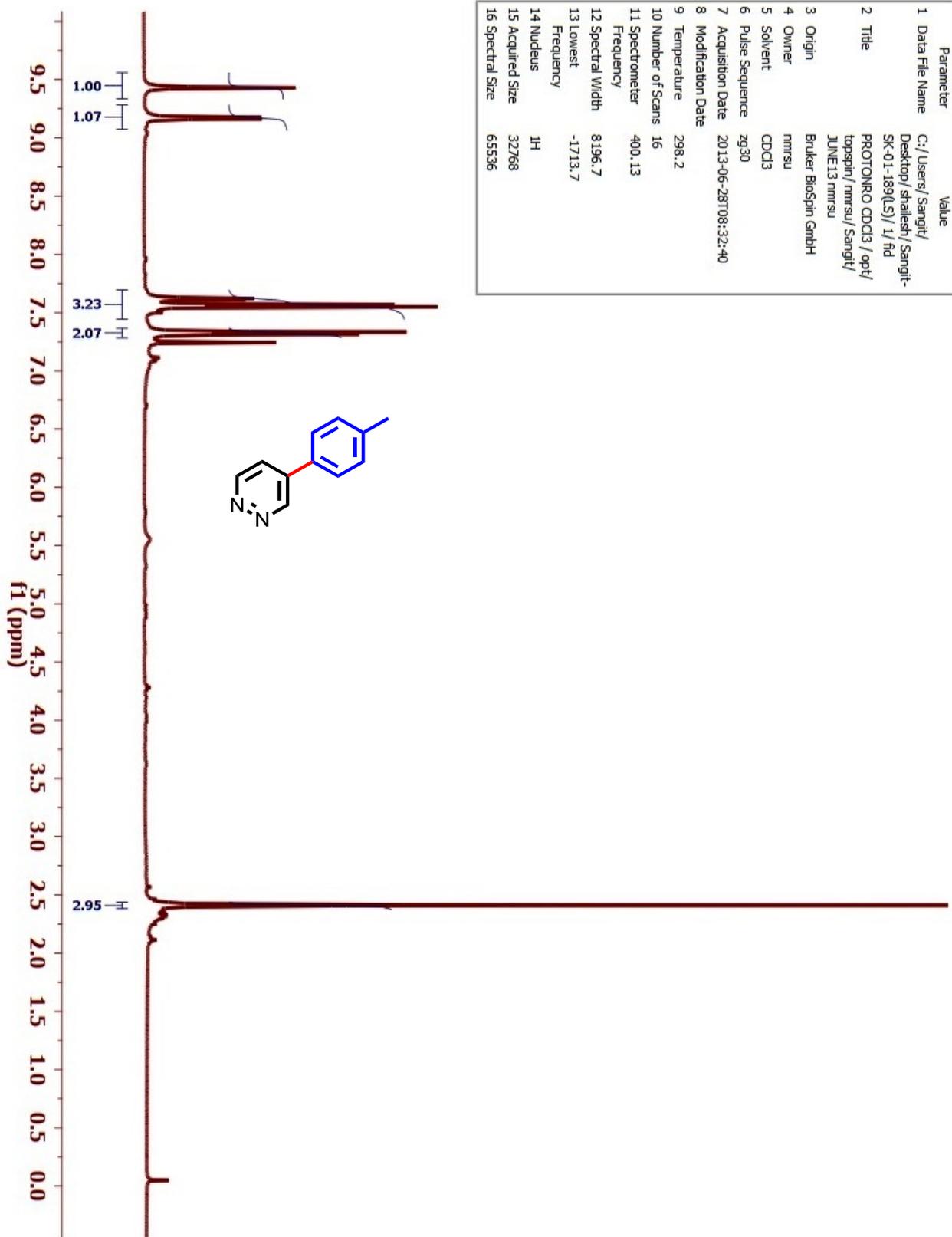


Figure S116  $^{13}\text{C}$  NMR of **40**

