

SUPPLEMENTARY MATERIALS

Synthesis of novel saccharin derivatives

Gregory M. Rankin and Sally-Ann Poulsen*

Griffith Institute for Drug Discovery, Griffith University, Don Young Road, Nathan, Queensland 4111, Australia

E-mail: s.poulsen@griffith.edu.au

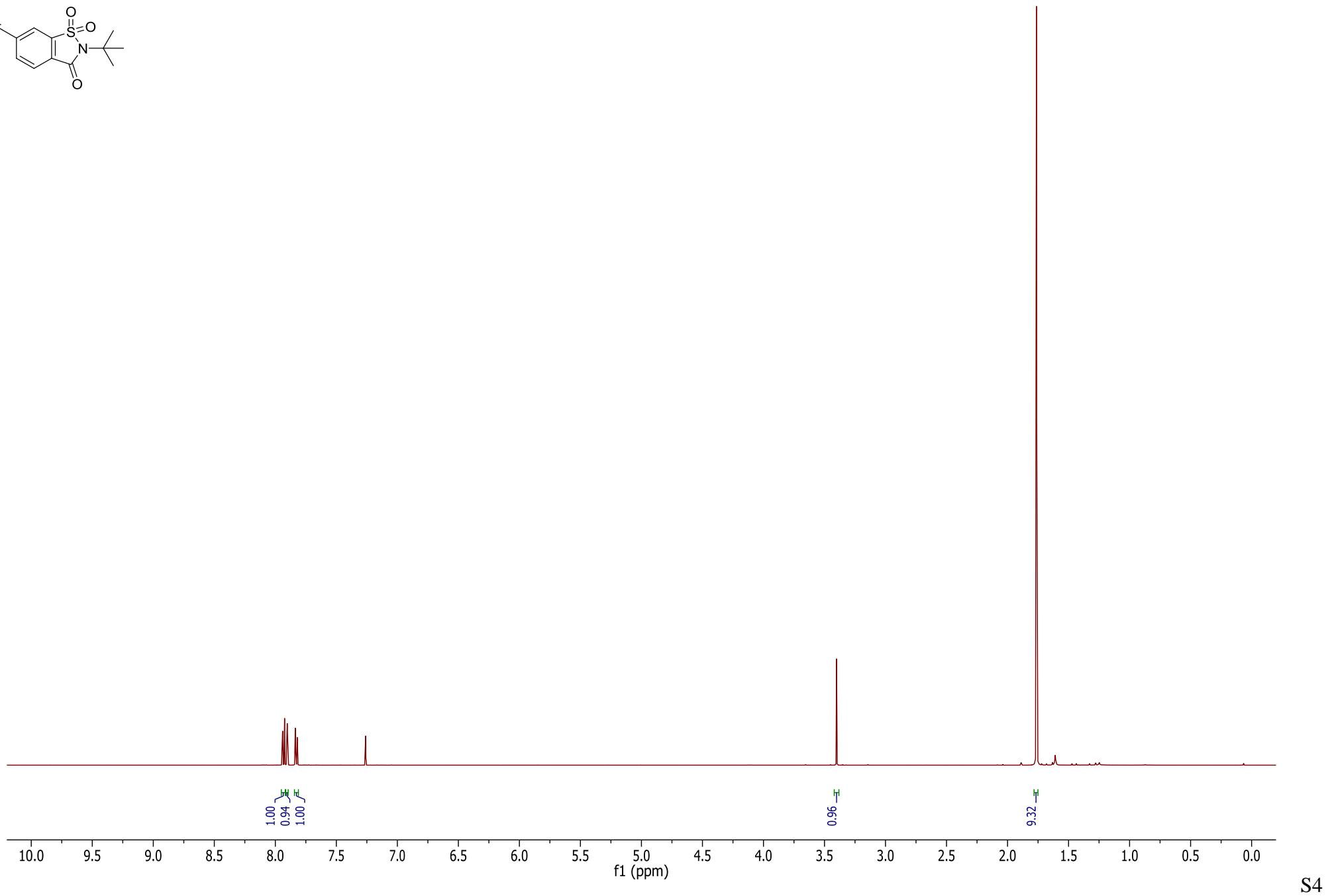
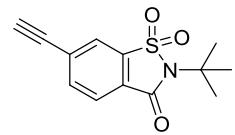
¹H, ¹³C and ¹⁹F NMR spectra

Compound 5 500 MHz ¹ H NMR CDCl ₃	S4
Compound 5 125 MHz ¹³ C NMR CDCl ₃	S5
Compound 6 500 MHz ¹ H NMR (CD ₃) ₂ SO	S6
Compound 6 125 MHz ¹³ C NMR (CD ₃) ₂ SO	S7
Compound 8 500 MHz ¹ H NMR CDCl ₃	S8
Compound 8 125 MHz ¹³ C NMR CDCl ₃	S9
Compound 9 500 MHz ¹ H NMR CDCl ₃	S10
Compound 9 125 MHz ¹³ C NMR CDCl ₃	S11
Compound 10 500 MHz ¹ H NMR (CD ₃) ₂ SO	S12
Compound 10 125 MHz ¹³ C NMR (CD ₃) ₂ SO	S13
Compound 11 500 MHz ¹ H NMR (CD ₃) ₂ SO	S14
Compound 11 125 MHz ¹³ C NMR (CD ₃) ₂ SO	S15
Compound 12 500 MHz ¹ H NMR (CD ₃) ₂ SO	S16
Compound 12 125 MHz ¹³ C NMR (CD ₃) ₂ SO	S17
Compound 13 500 MHz ¹ H NMR (CD ₃) ₂ SO	S18
Compound 13 125 MHz ¹³ C NMR (CD ₃) ₂ SO	S19
Compound 14 376 MHz ¹⁹ F NMR (CD ₃) ₂ SO.....	S20
Compound 14 500 MHz ¹ H NMR (CD ₃) ₂ SO	S21

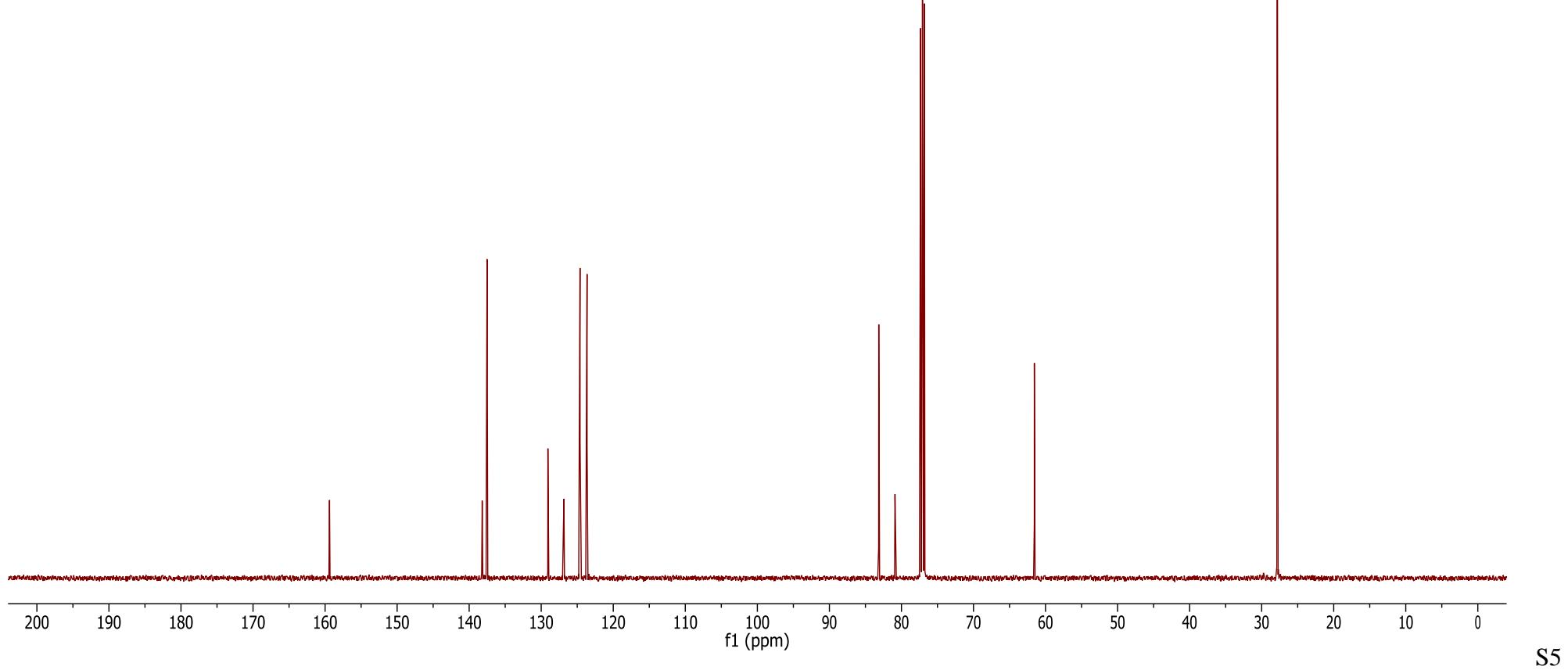
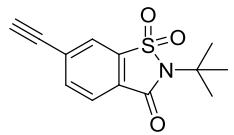
Compound 14 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S22
Compound 15 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S23
Compound 15 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S24
Compound 17 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S25
Compound 17 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S26
Compound 19 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S27
Compound 19 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S28
Compound 20 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S29
Compound 20 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S30
Compound 21 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S31
Compound 21 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S32
Compound 22 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S33
Compound 22 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S34
Compound 24 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S35
Compound 24 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S36
Compound 25 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S37
Compound 25 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S38
Compound 26 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S39
Compound 26 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S40
Compound 27 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S41
Compound 27 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S42
Compound 28 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S43
Compound 28 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S44
Compound 29 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S45
Compound 29 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S46
Compound 29 376 MHz ^{19}F NMR ($\text{CD}_3)_2\text{SO}$	S47
Compound 30 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S48
Compound 30 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S49
Compound 31 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S50
Compound 31 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S51
Compound 31 HSQC NMR ($\text{CD}_3)_2\text{SO}$	S52
Compound 32a + 32b 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S53
Compound 32a + 32b 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S54
Compound 33 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S55
Compound 33 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S56
Compound 34 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S57

Compound 34 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S58
Compound 35 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S59
Compound 35 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S60
Compound 36 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S61
Compound 36 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S62
Compound 37 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S63
Compound 37 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S64
Compound 38 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S65
Compound 38 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S66
Compound 39 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S67
Compound 39 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S68
Compound 40 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S69
Compound 40 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S70
Compound 41 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S71
Compound 41 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S72
Compound 42 500 MHz ^1H NMR ($\text{CD}_3)_2\text{SO}$	S73
Compound 42 125 MHz ^{13}C NMR ($\text{CD}_3)_2\text{SO}$	S74

Compound 5 500 MHz ^1H NMR CDCl_3

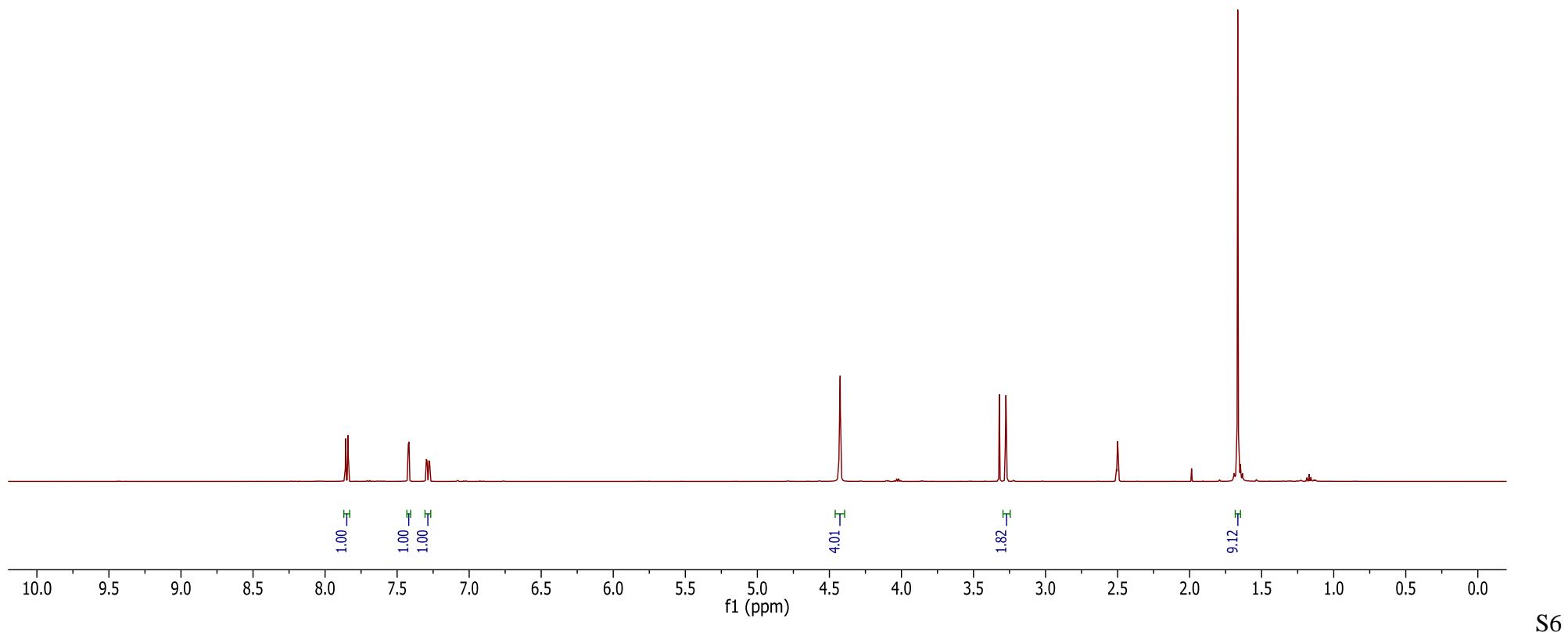
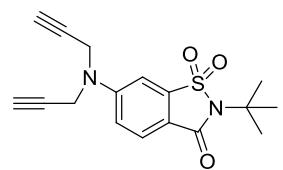


Compound **5** 125 MHz ^{13}C NMR CDCl_3

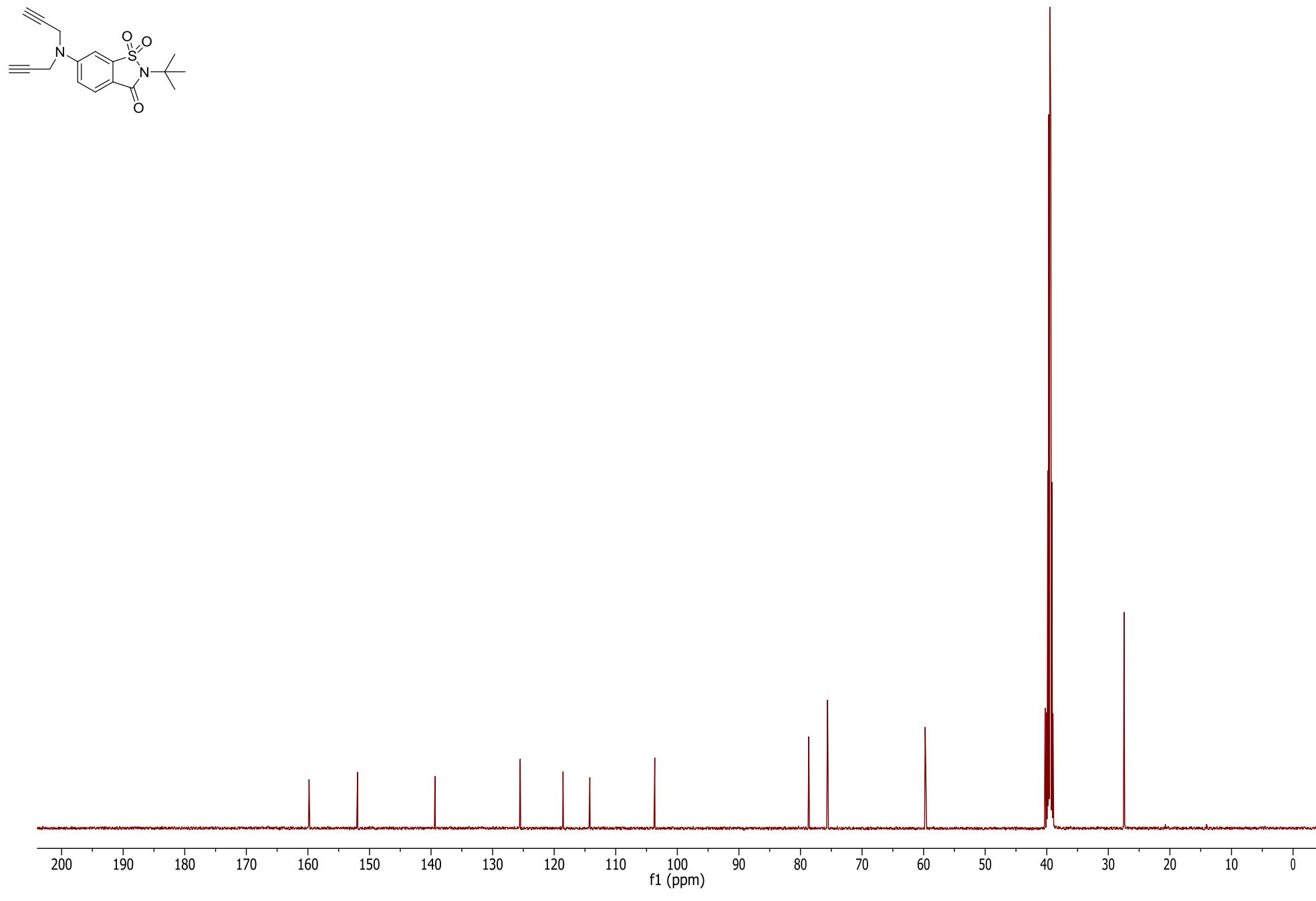


S5

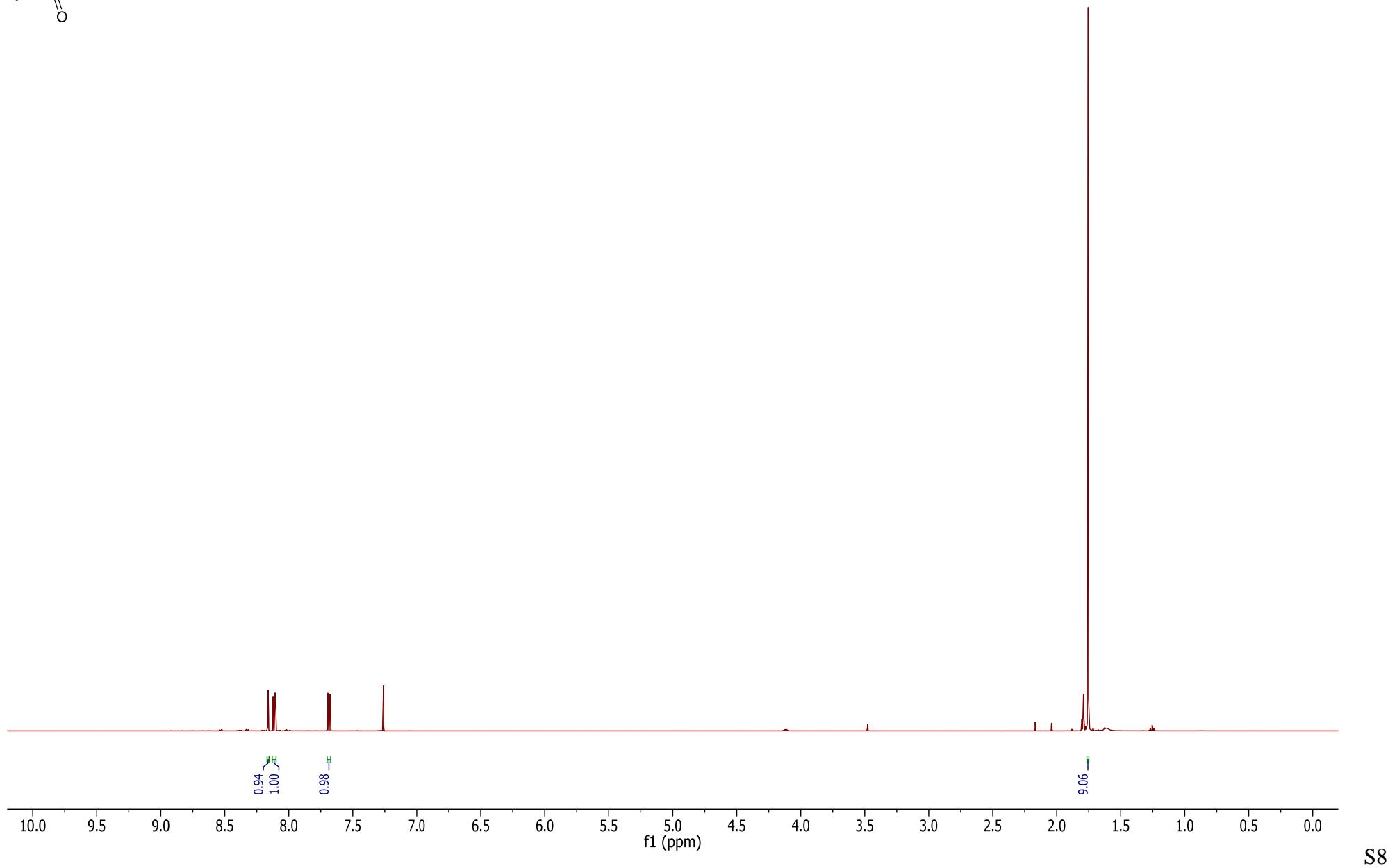
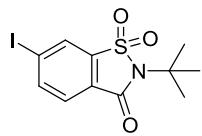
Compound **6** 500 MHz ^1H NMR (CD_3SO_2)



Compound **6** 125 MHz ^{13}C NMR (CD_3SO_2)

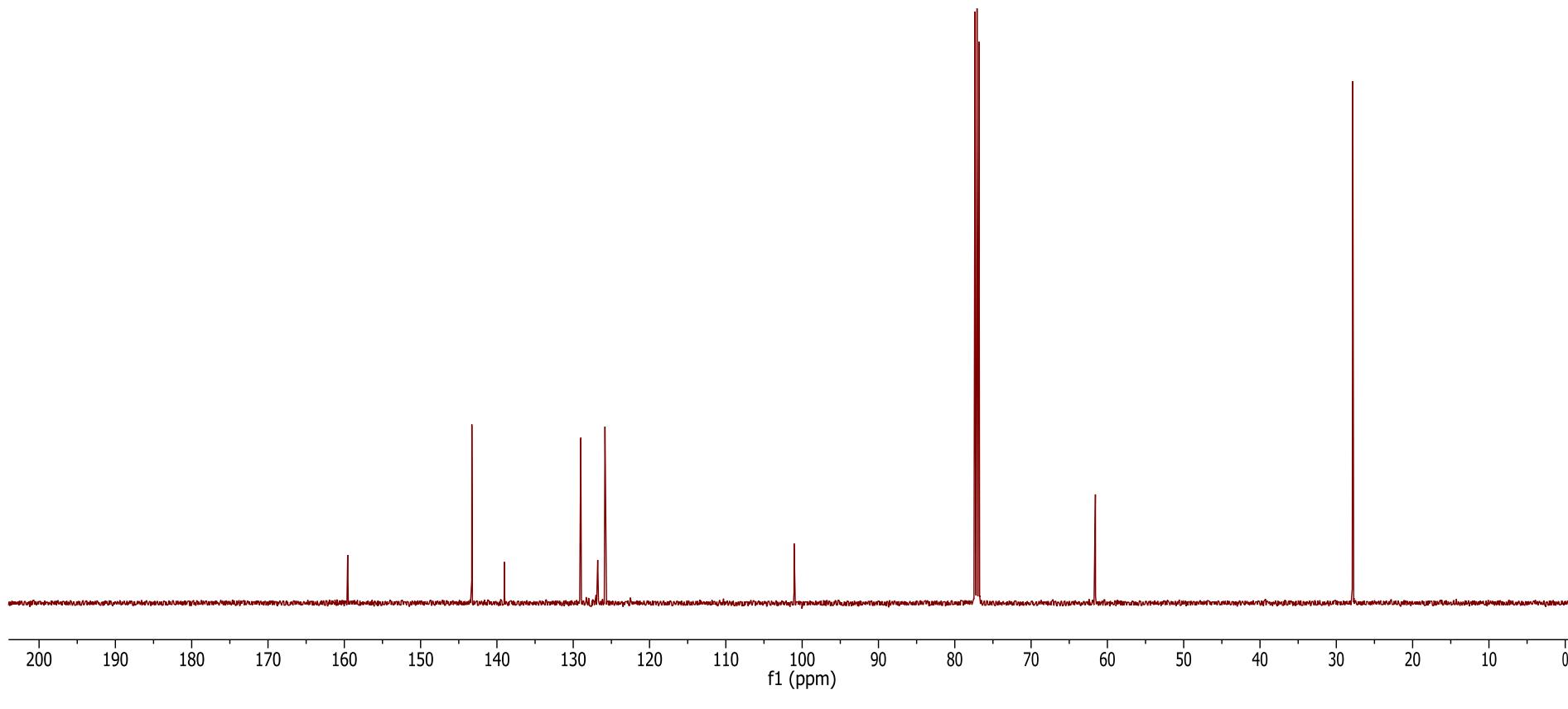
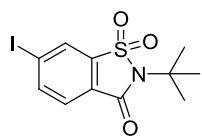


Compound **8** 500 MHz ^1H NMR CDCl_3

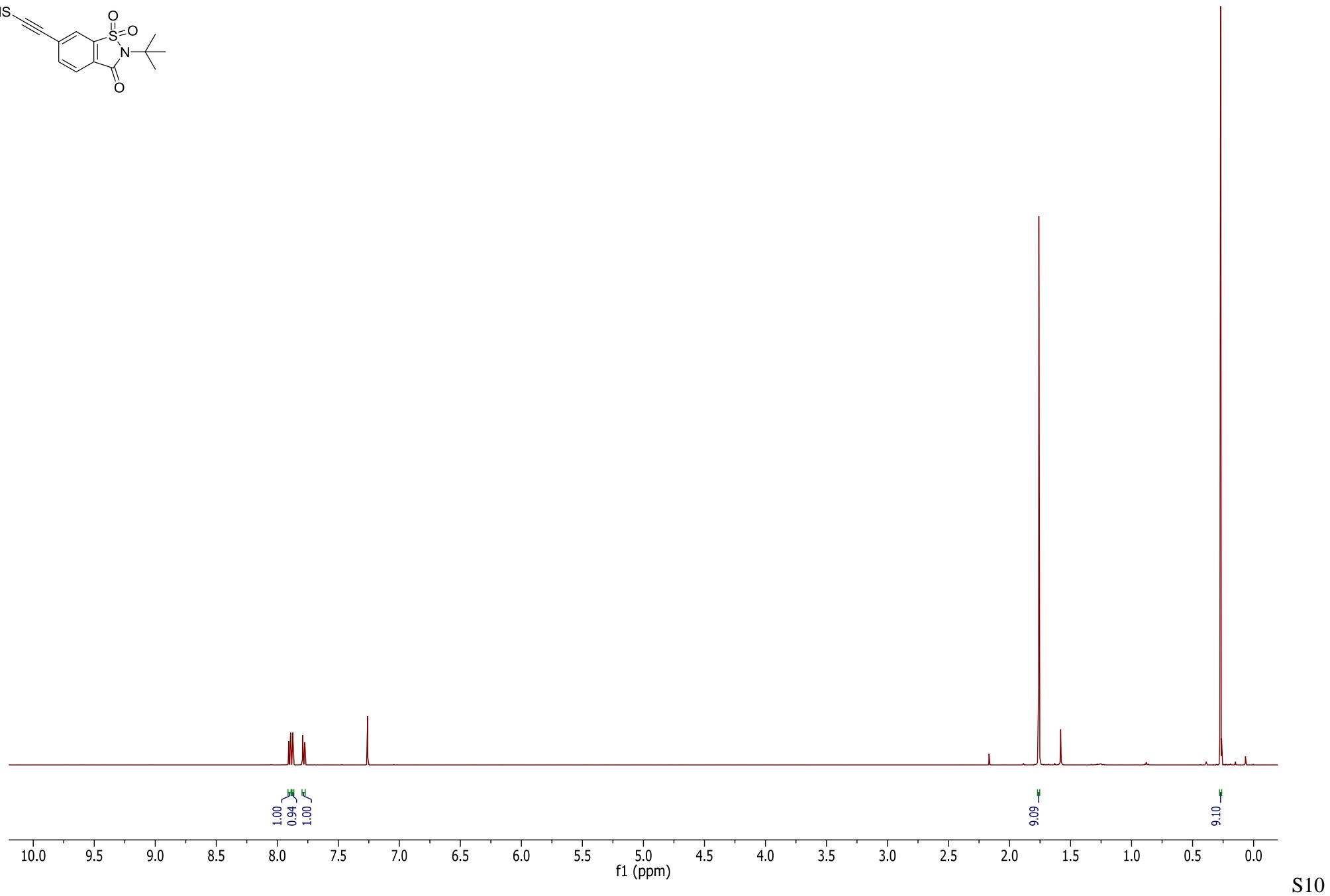
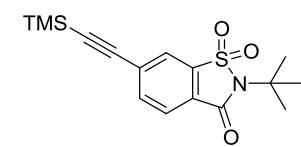


S8

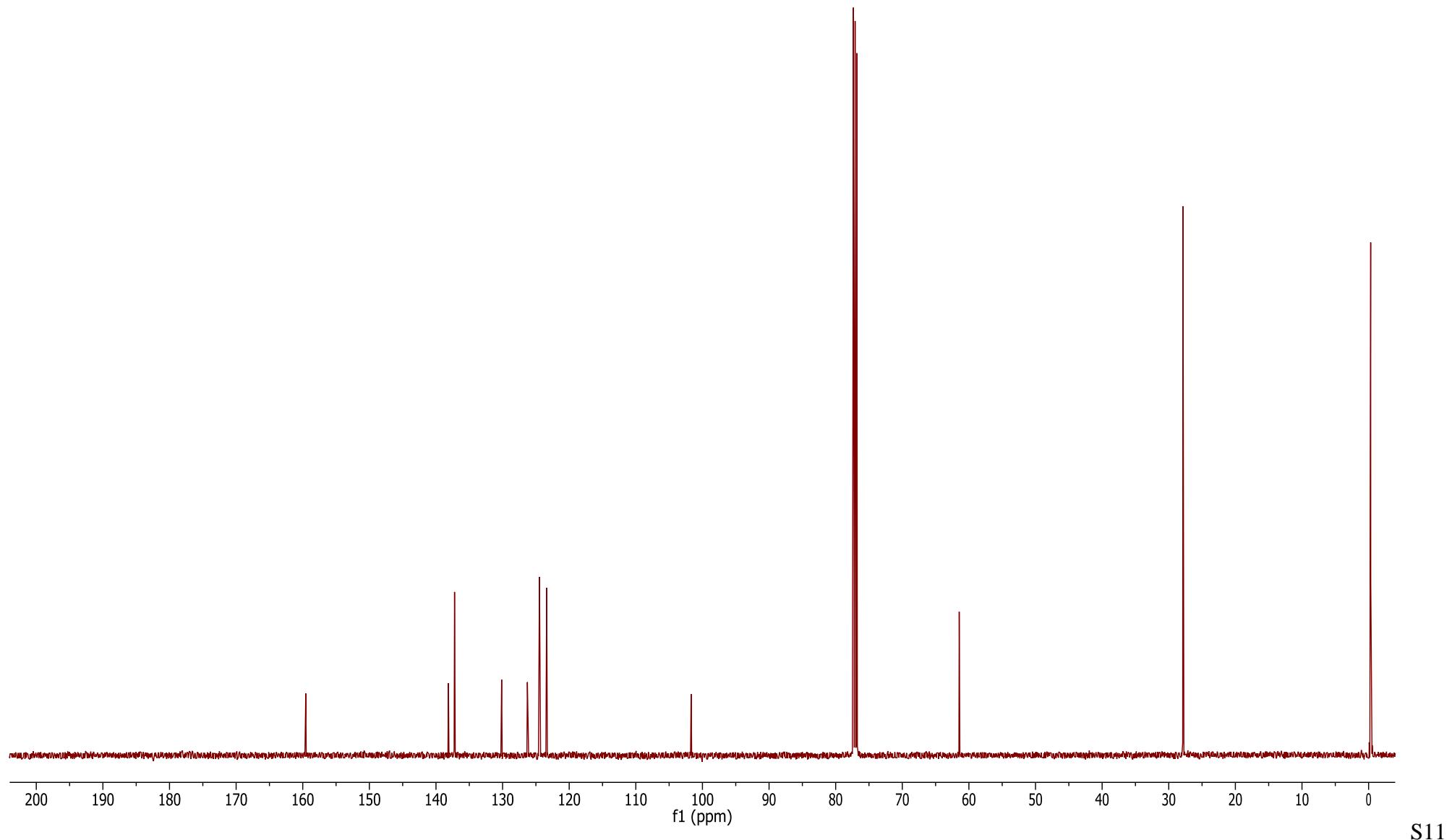
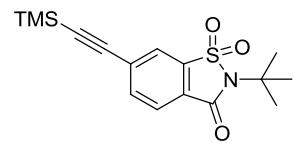
Compound **8** 125 MHz ^{13}C NMR CDCl_3



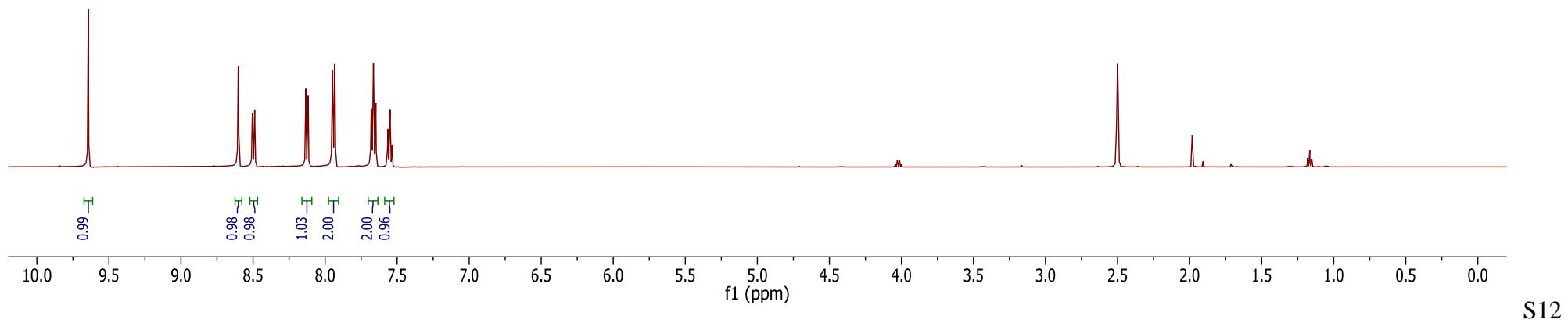
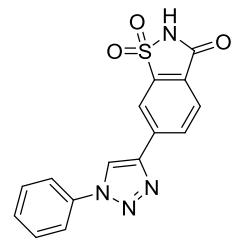
Compound **9** 500 MHz ^1H NMR CDCl_3



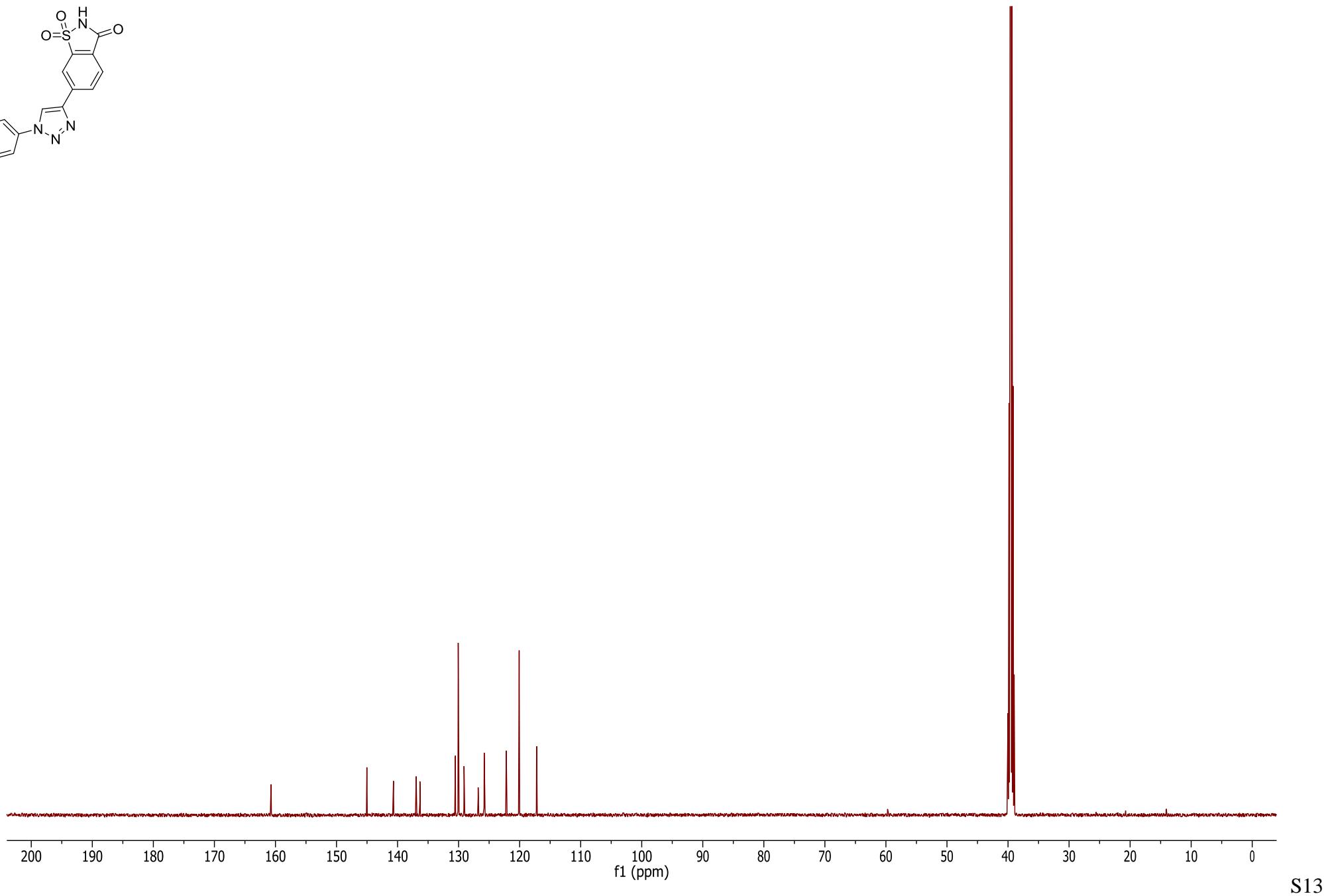
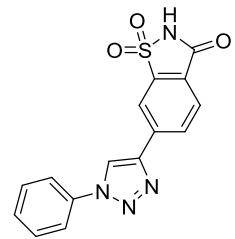
Compound **9** 125 MHz ^{13}C NMR CDCl_3



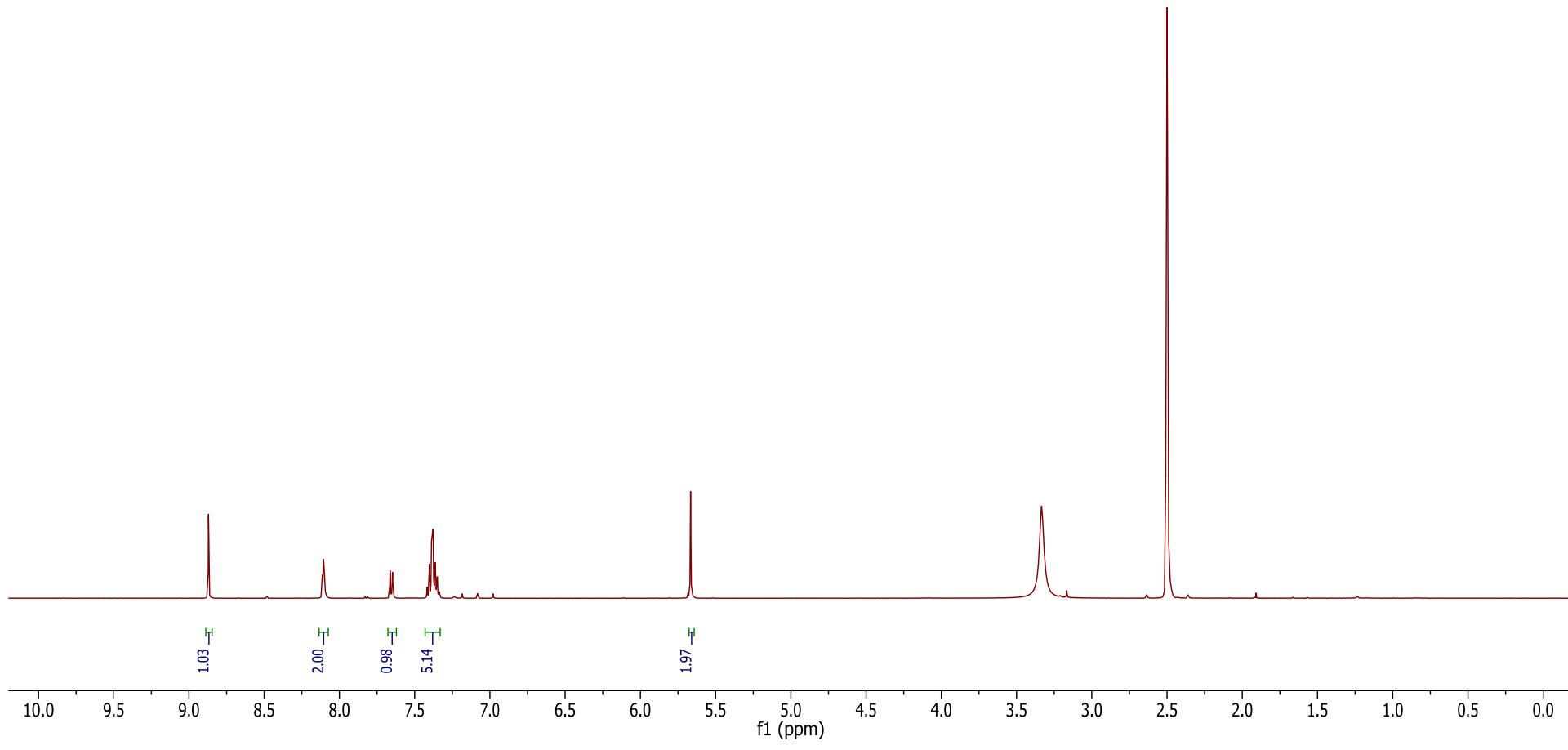
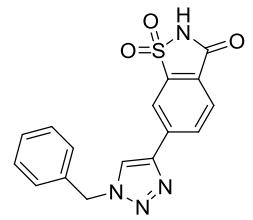
Compound **10** 500 MHz ^1H NMR (CD_3SO)



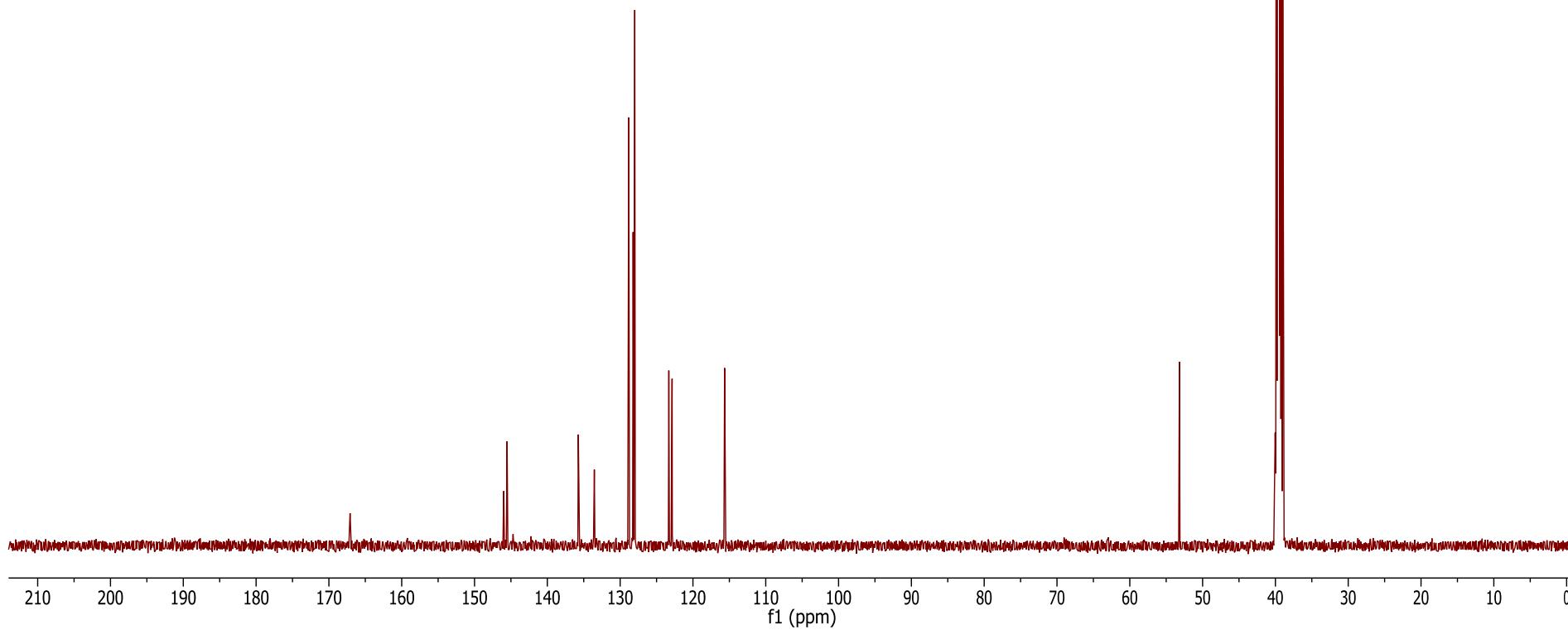
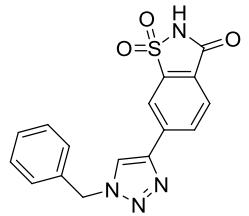
Compound **10** 125 MHz ^{13}C NMR (CD_3SO_2)



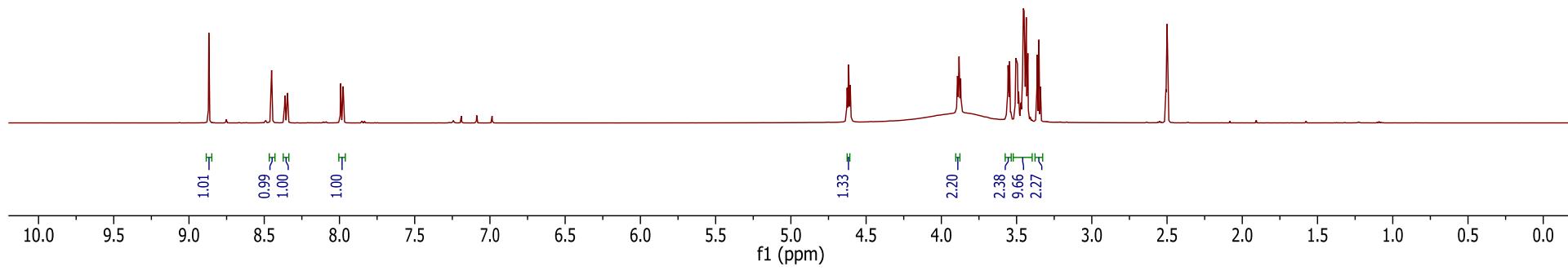
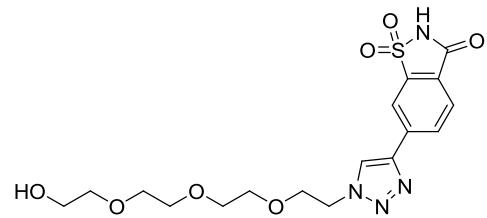
Compound **11** 500 MHz ^1H NMR ($\text{CD}_3\text{}_2\text{SO}$)



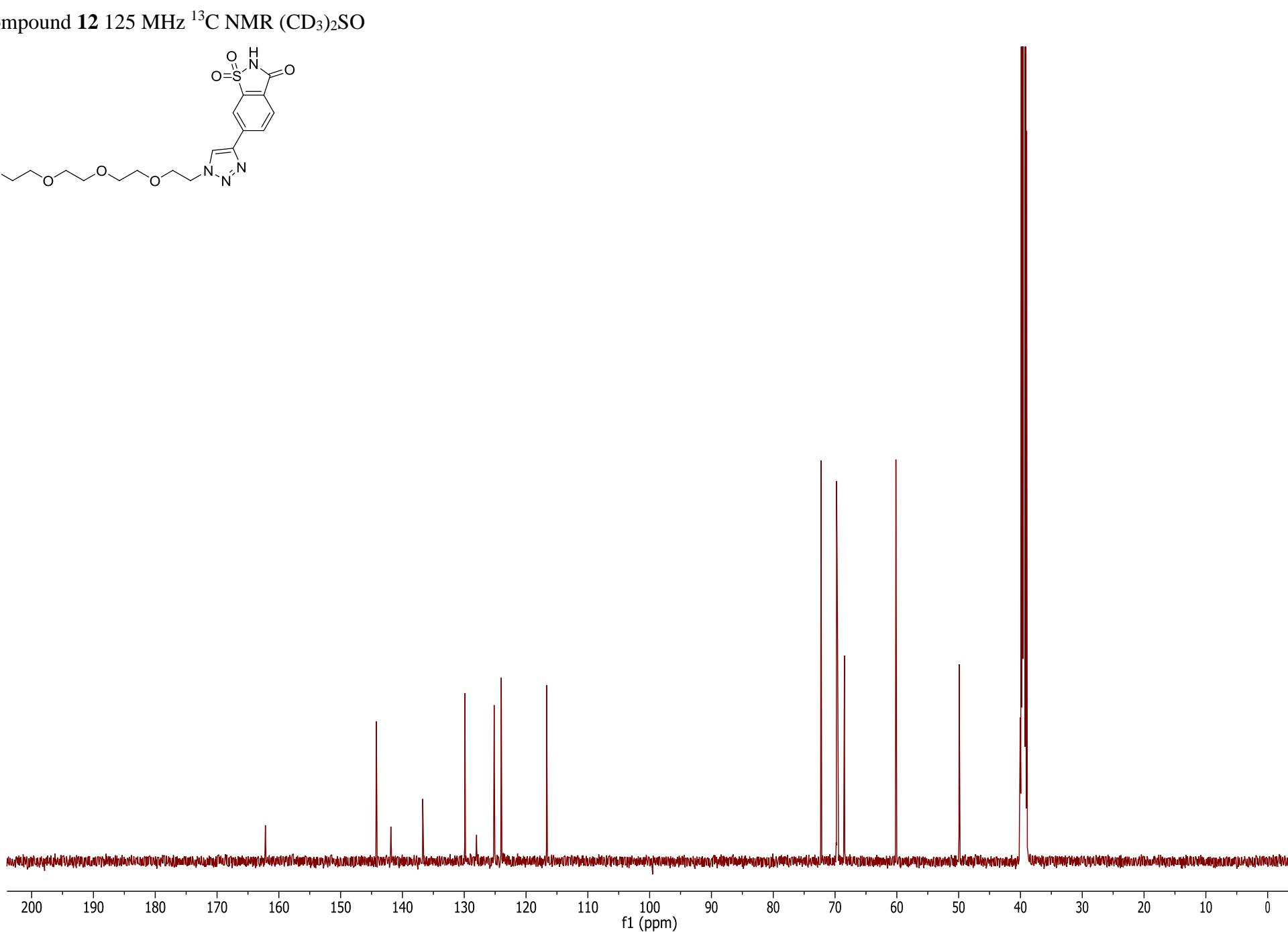
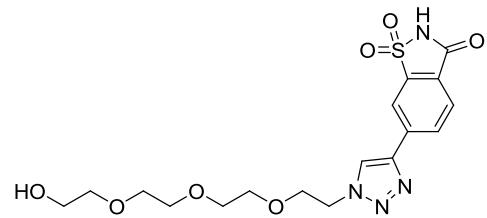
Compound **11** 125 MHz ^{13}C NMR (CD_3SO_2)



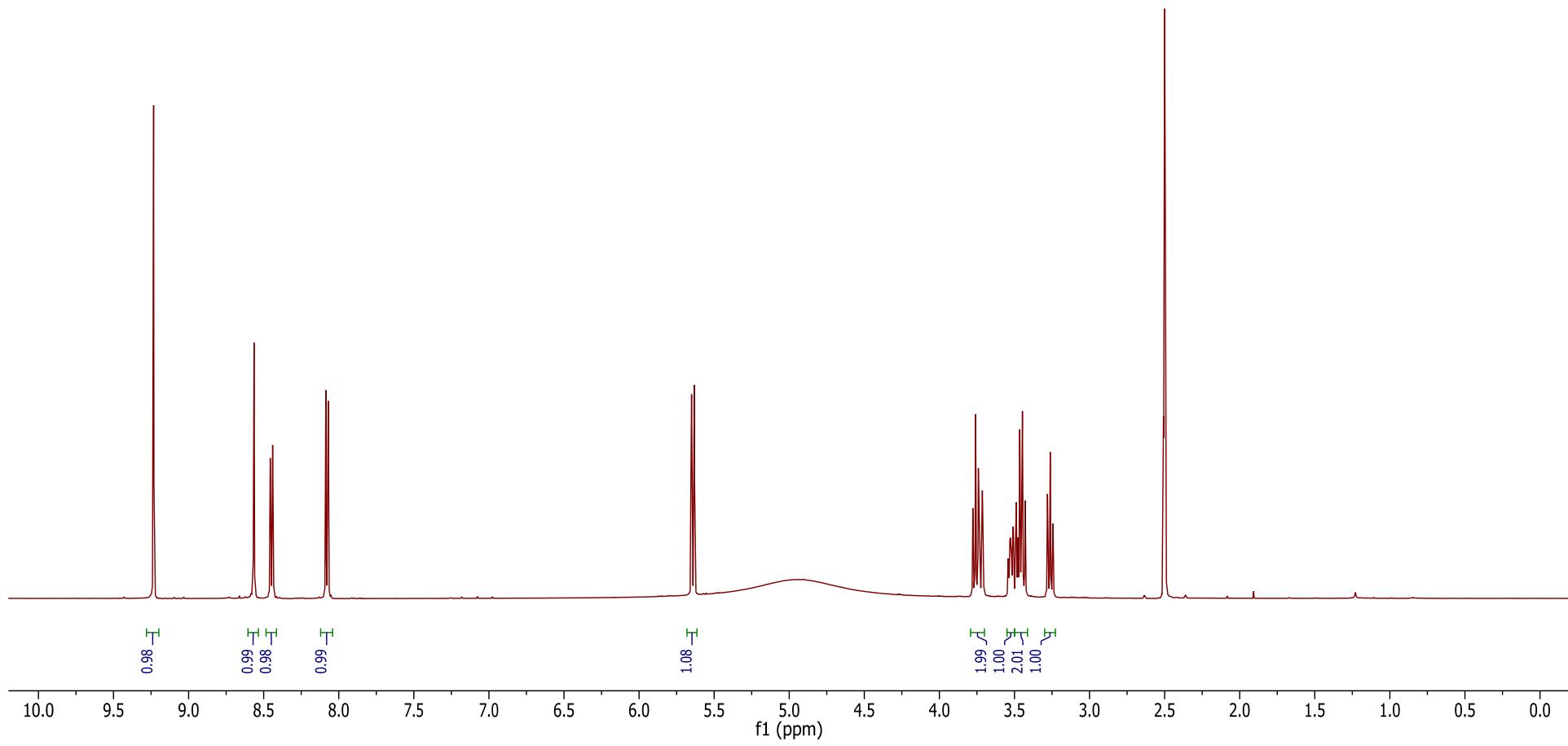
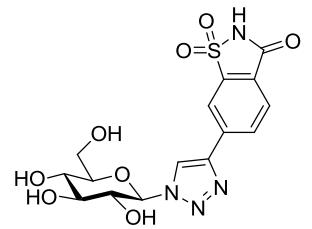
Compound **12** 500 MHz ^1H NMR (CD_3SO)



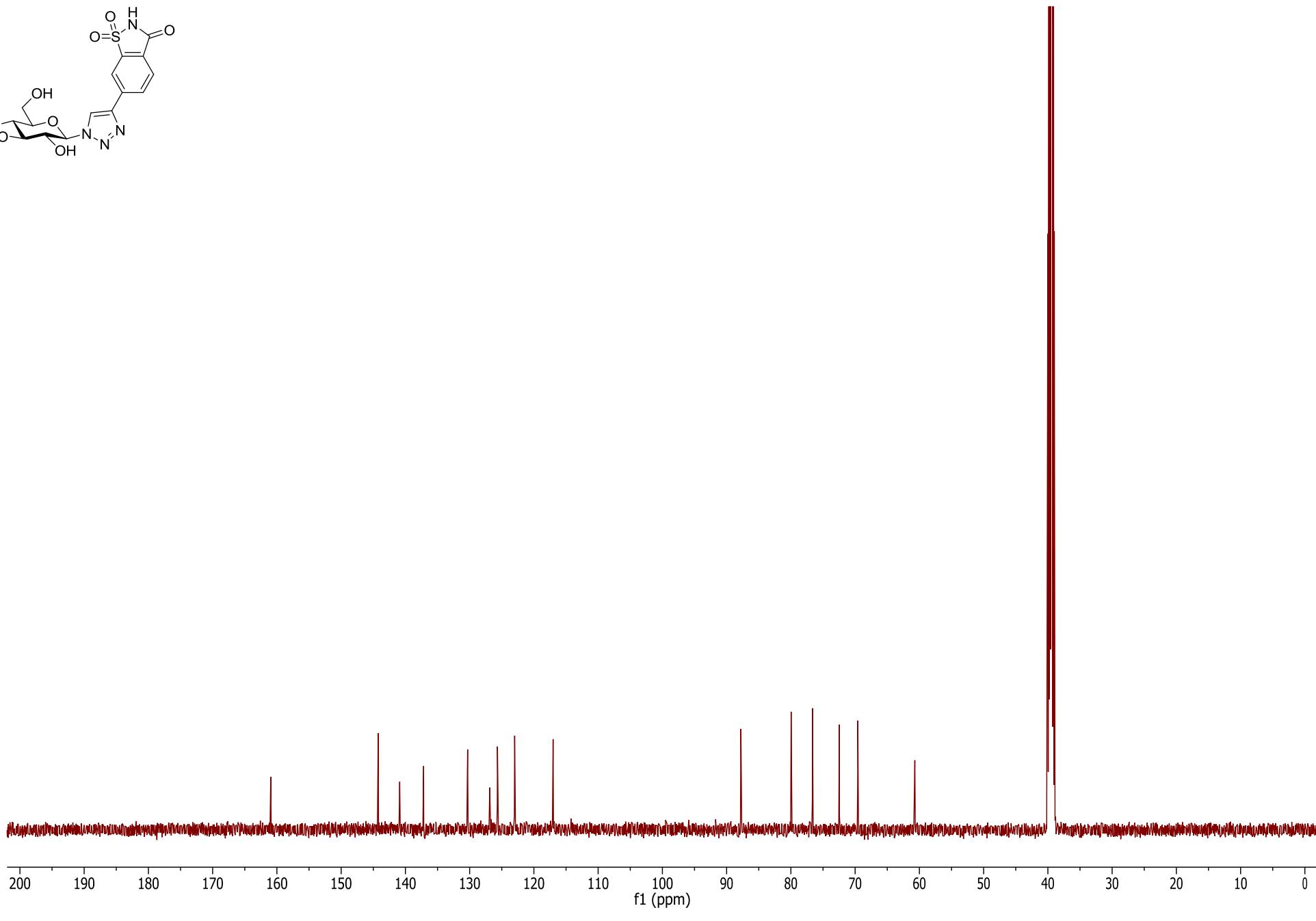
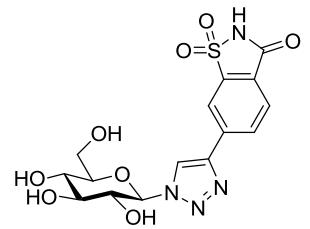
Compound **12** 125 MHz ^{13}C NMR (CD_3SO)



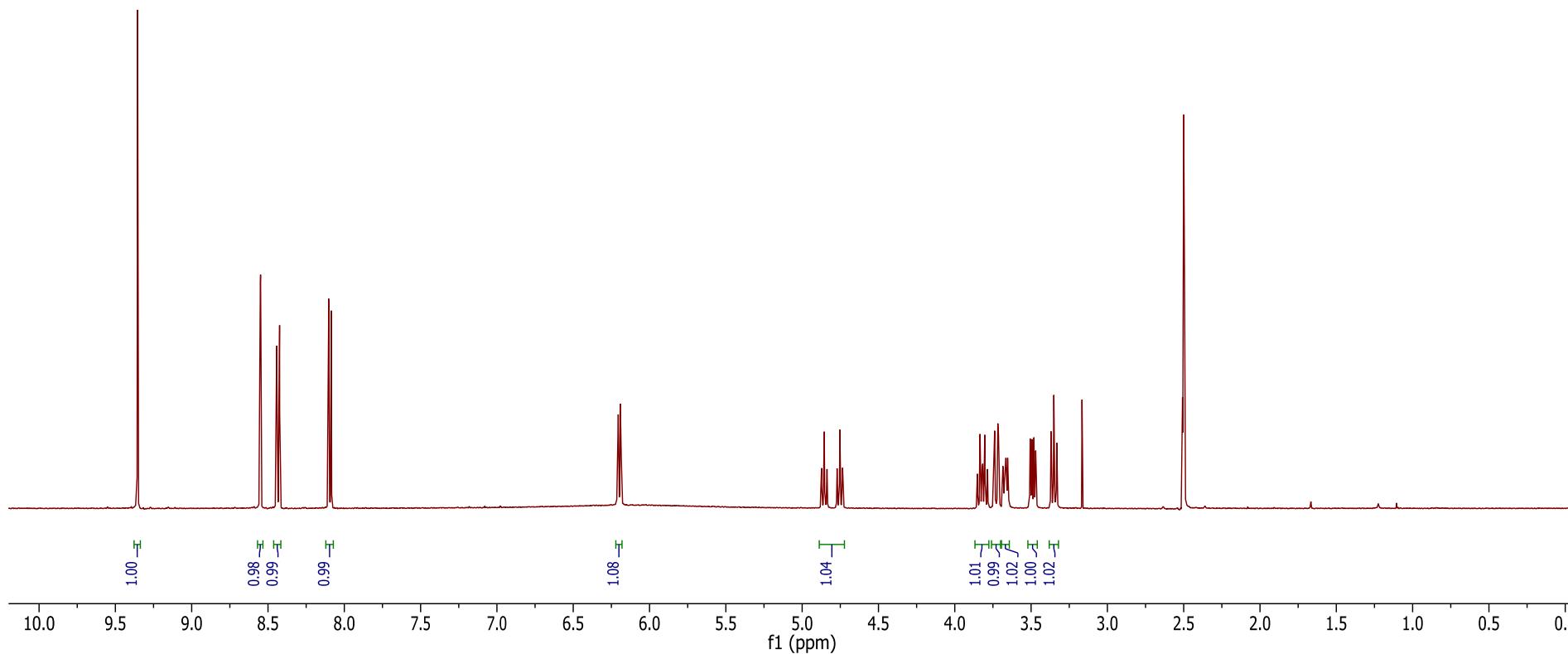
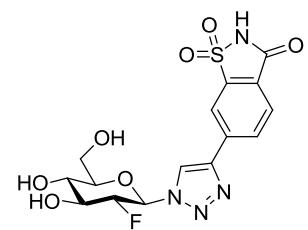
Compound **13** 500 MHz ^1H NMR (CD_3SO)



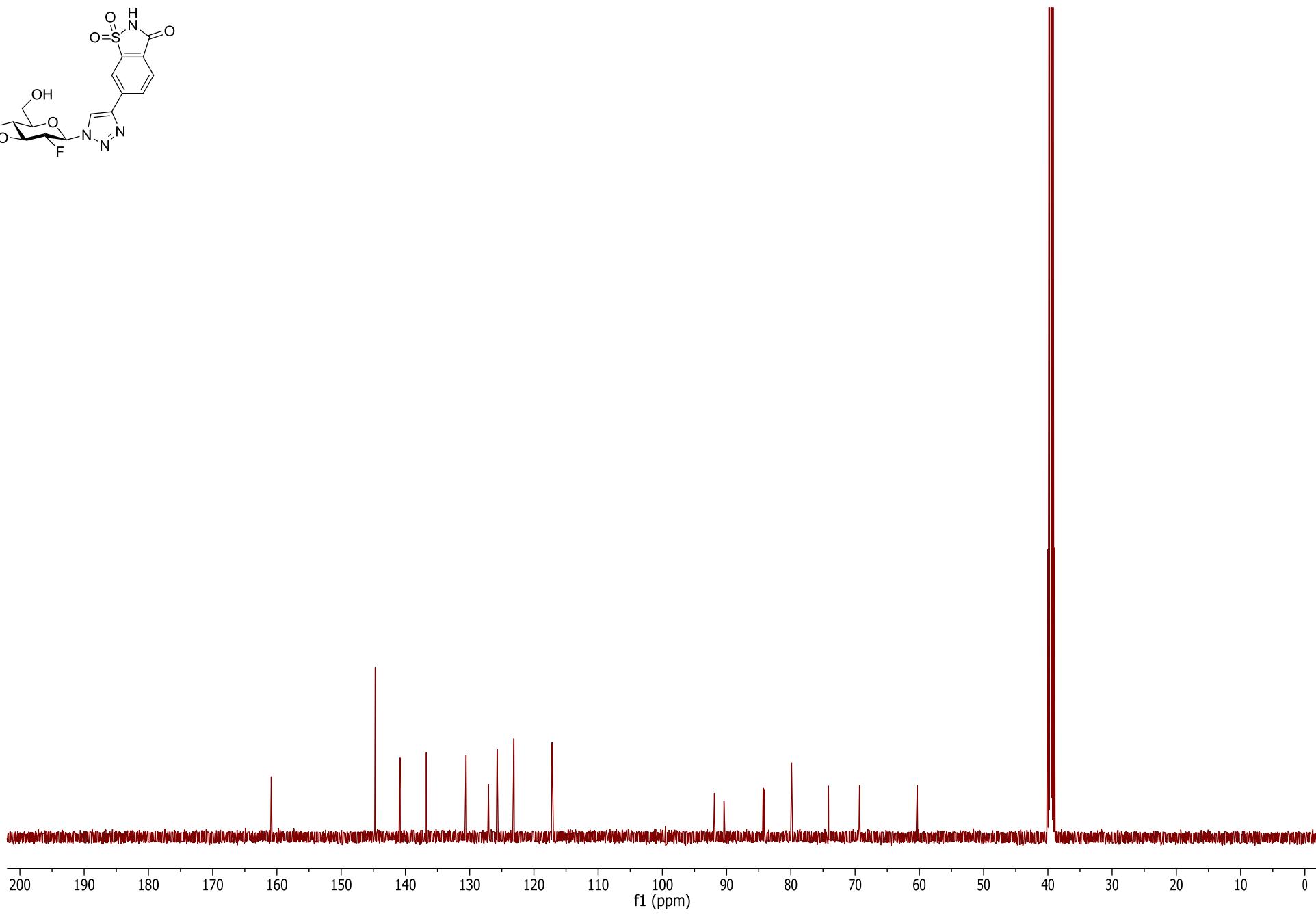
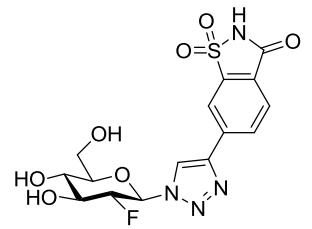
Compound **13** 125 MHz ^{13}C NMR (CD_3SO)



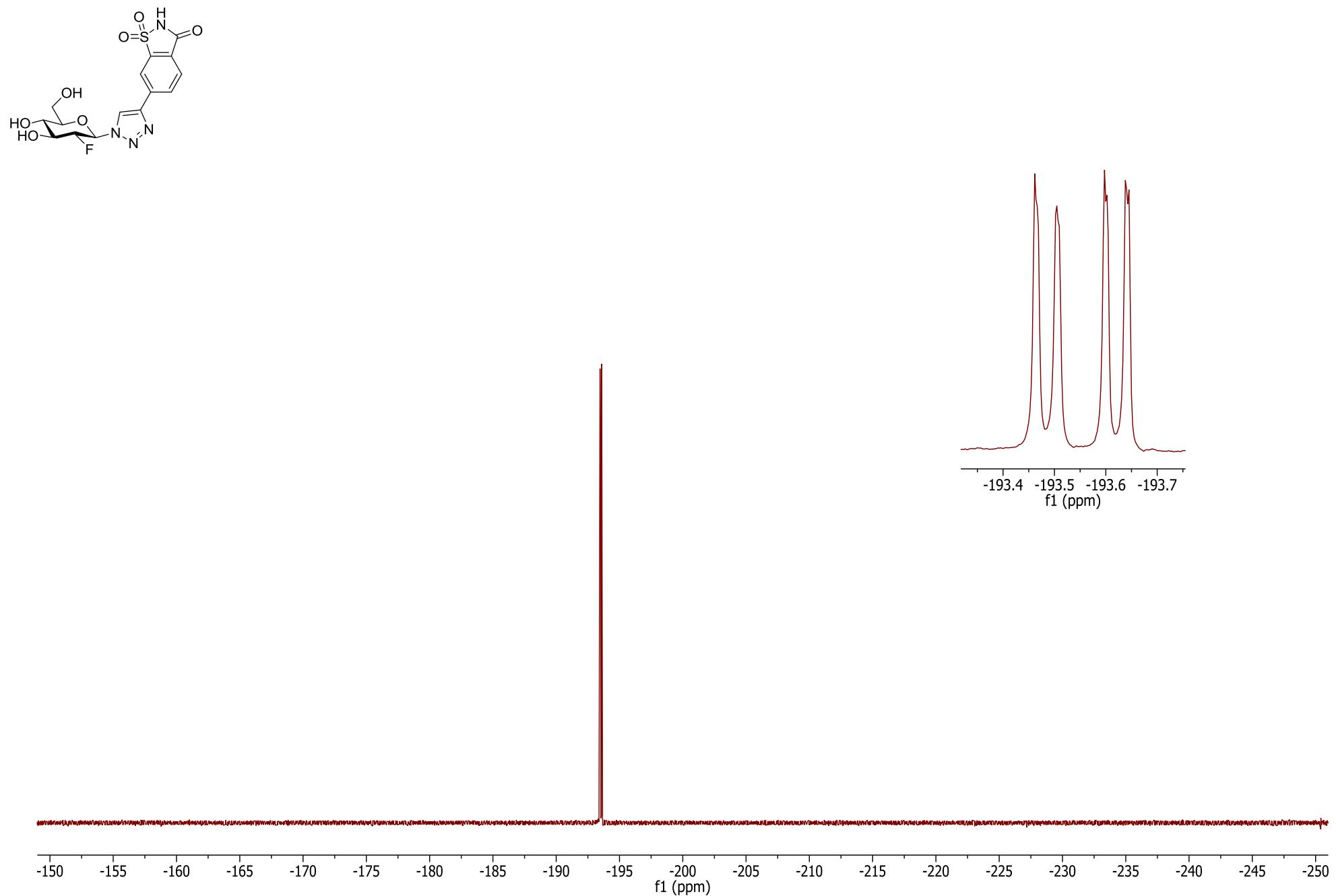
Compound **14** 500 MHz ^1H NMR (CD_3SO)



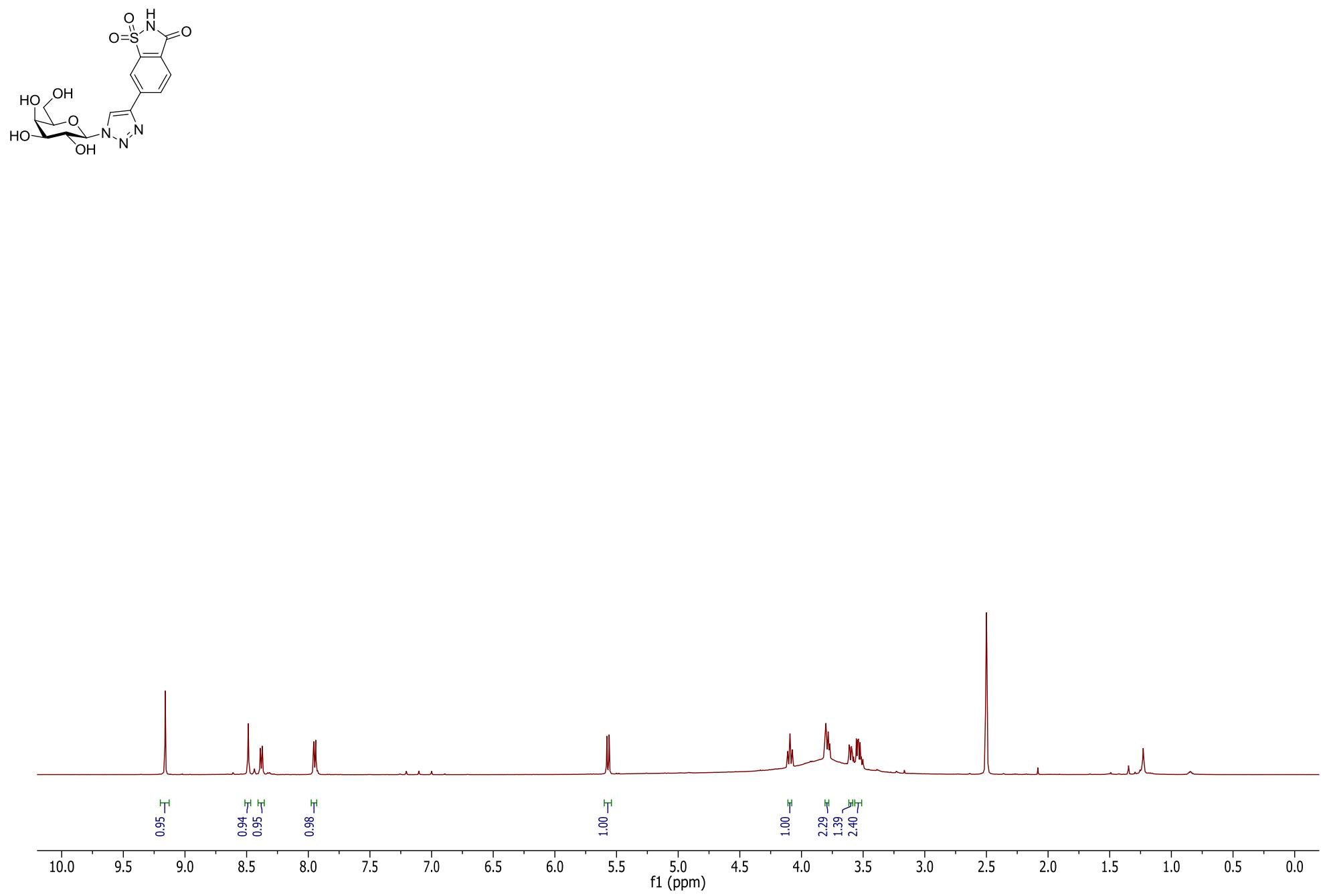
Compound **14** 125 MHz ^{13}C NMR (CD_3SO_2)



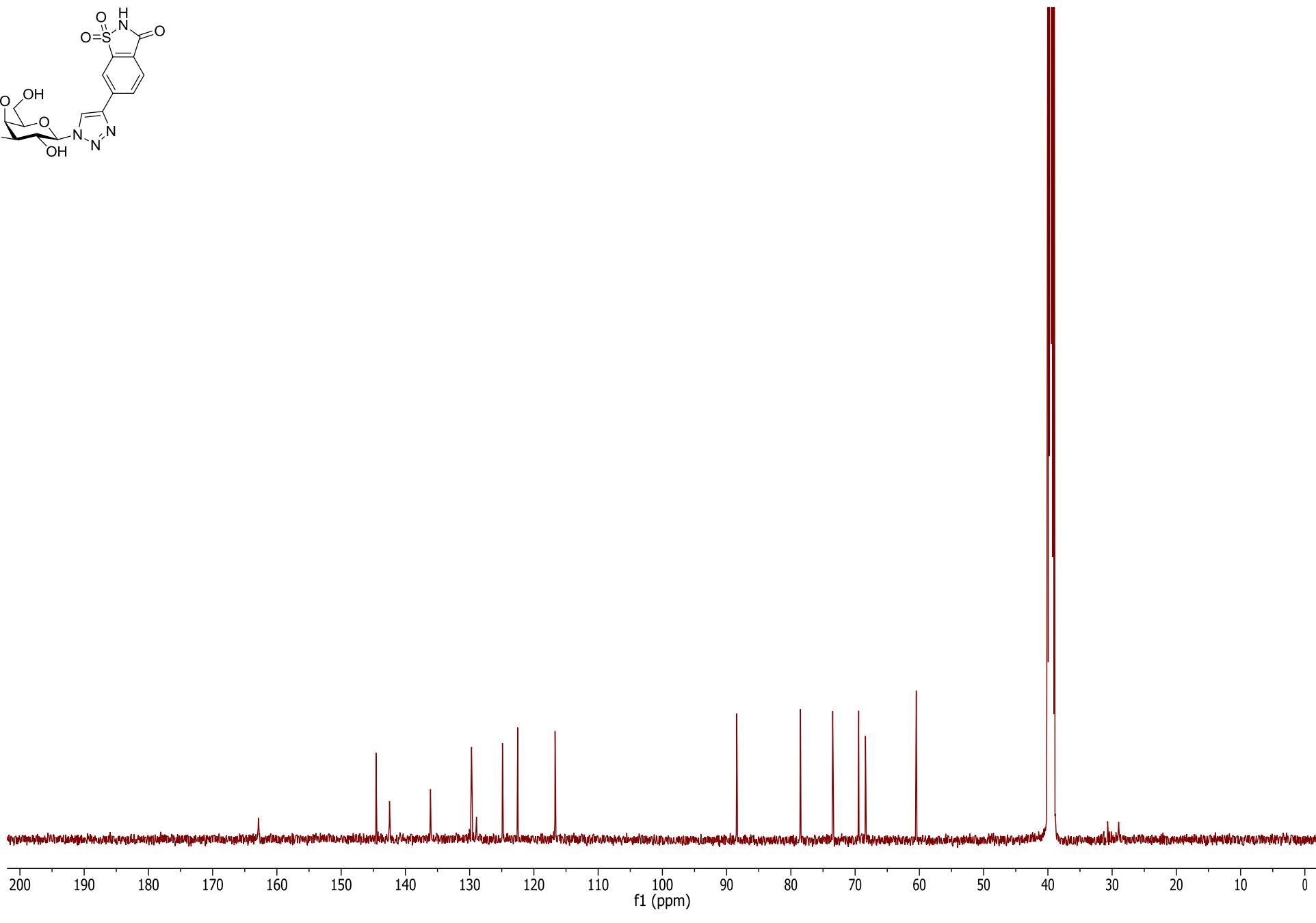
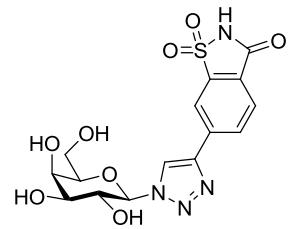
Compound **14** 376 MHz ^{19}F NMR (CD_3SO)



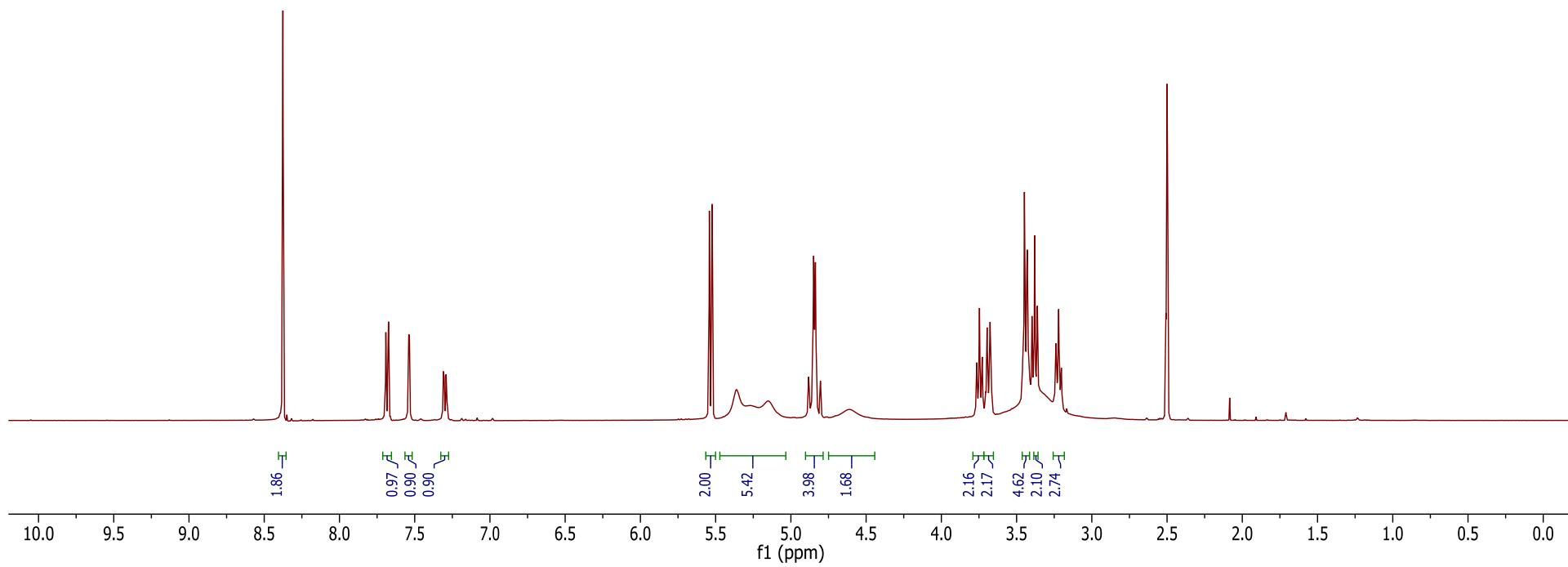
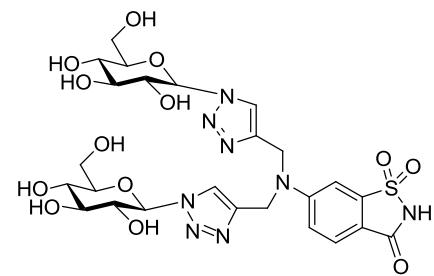
Compound **15** 500 MHz ^1H NMR (CD_3SO)



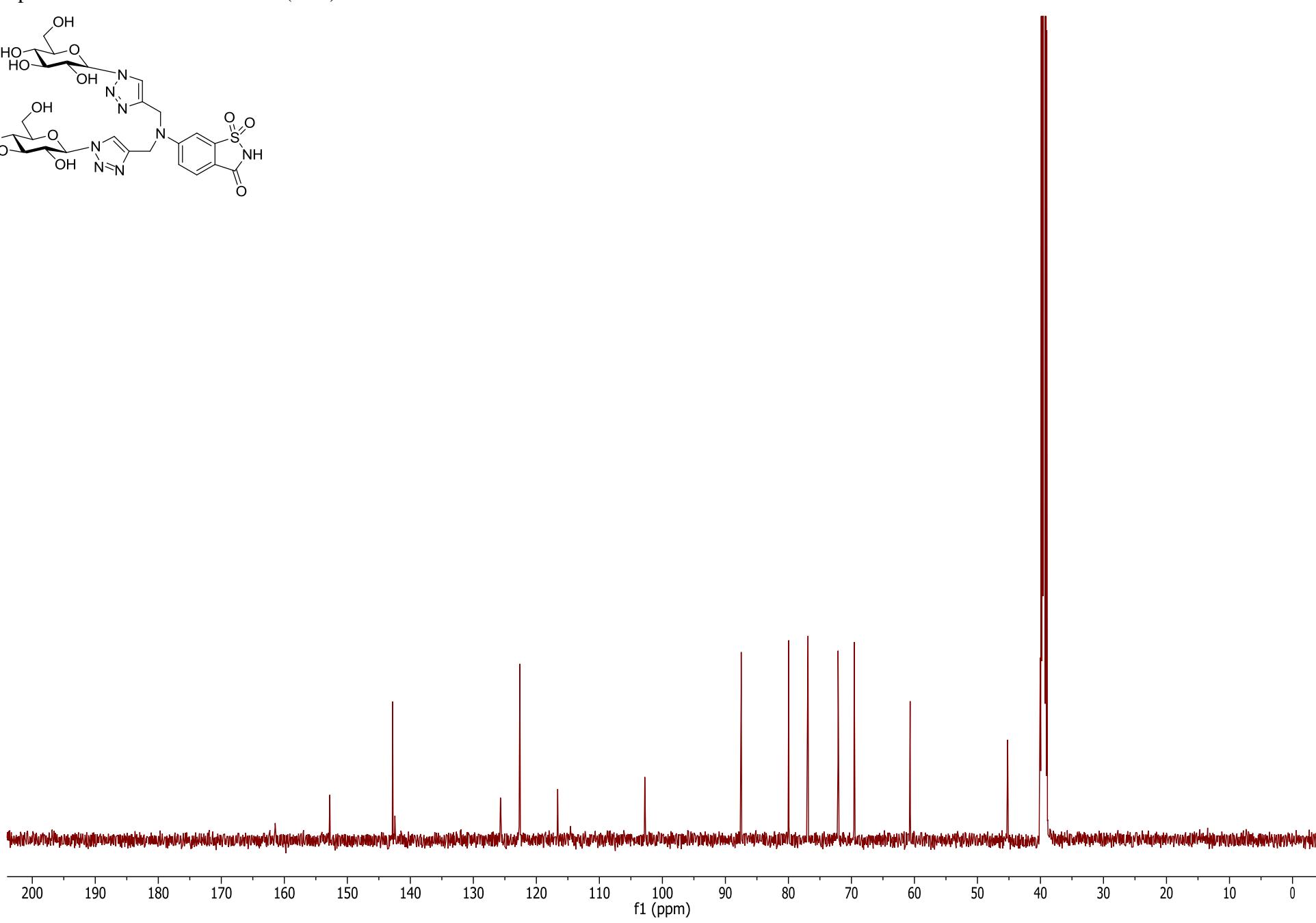
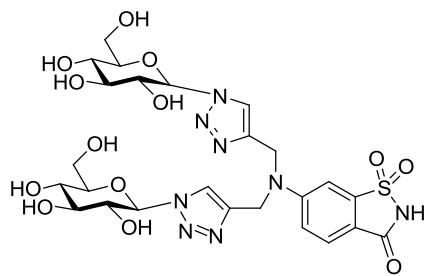
Compound **15** 125 MHz ^{13}C NMR (CD_3SO)



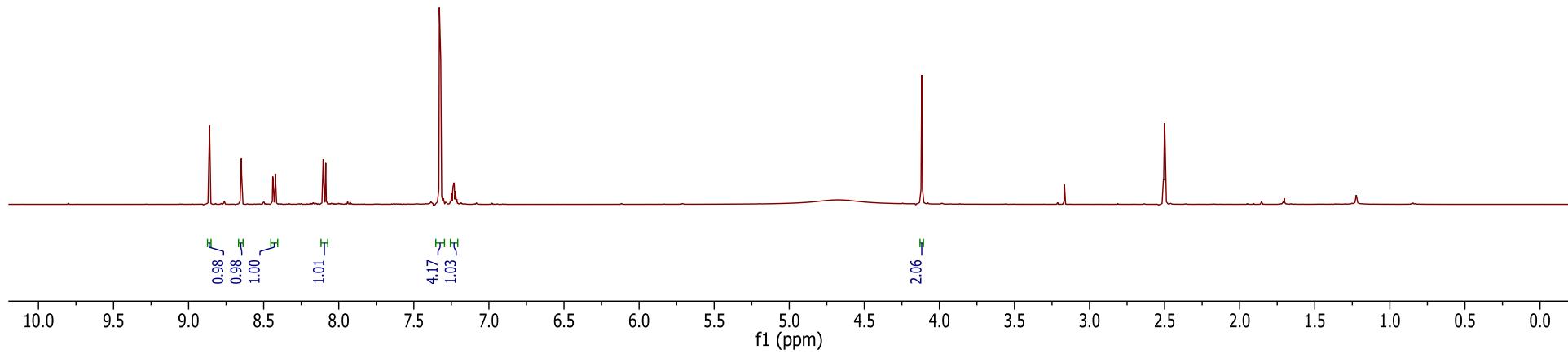
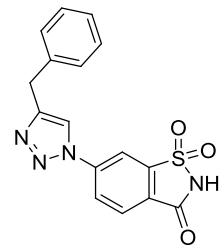
Compound **17** 500 MHz ^1H NMR (CD_3SO)



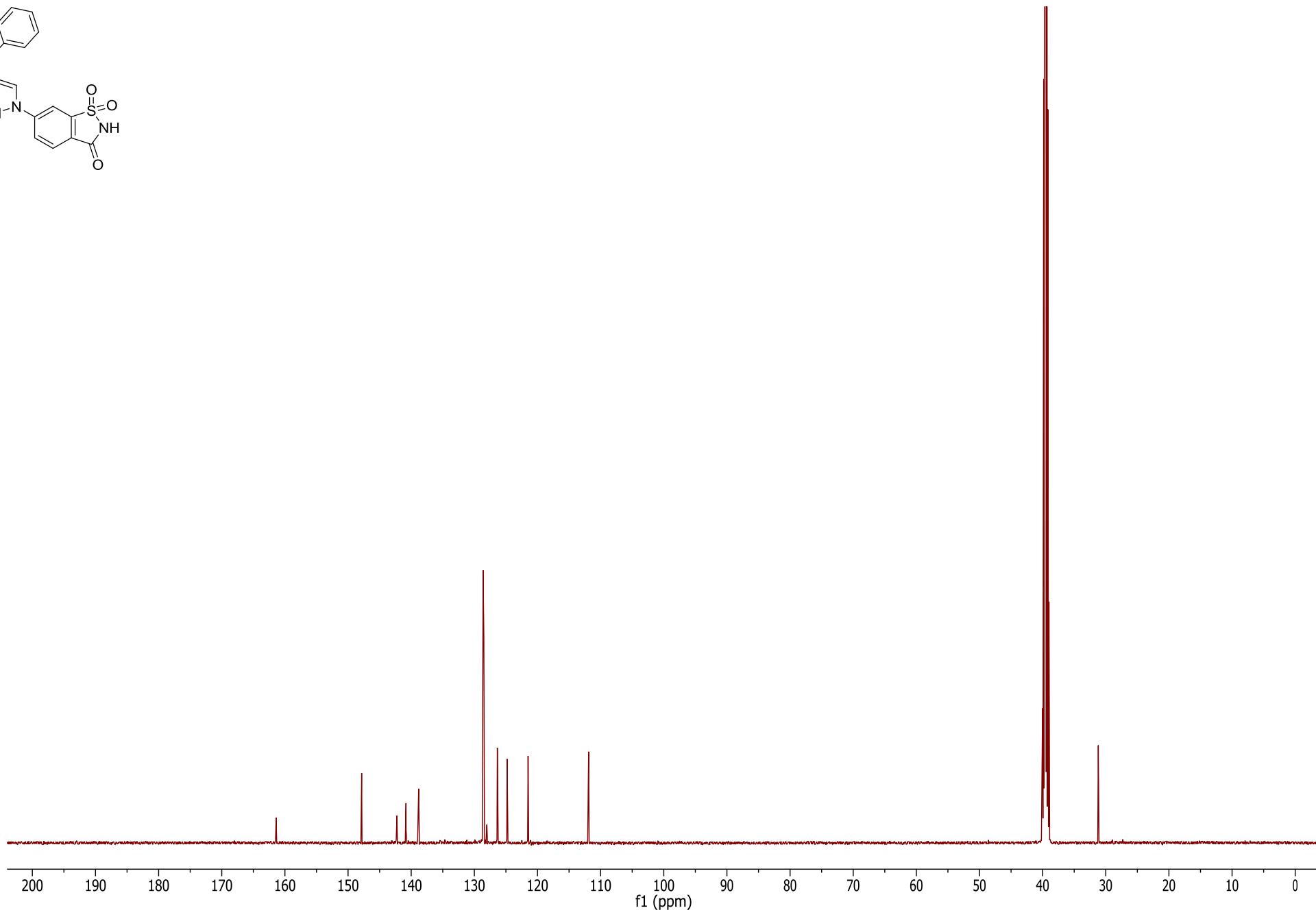
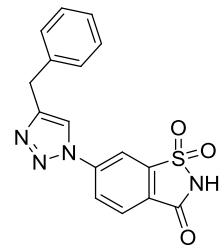
Compound **17** 125 MHz ^{13}C NMR (CD_3SO)



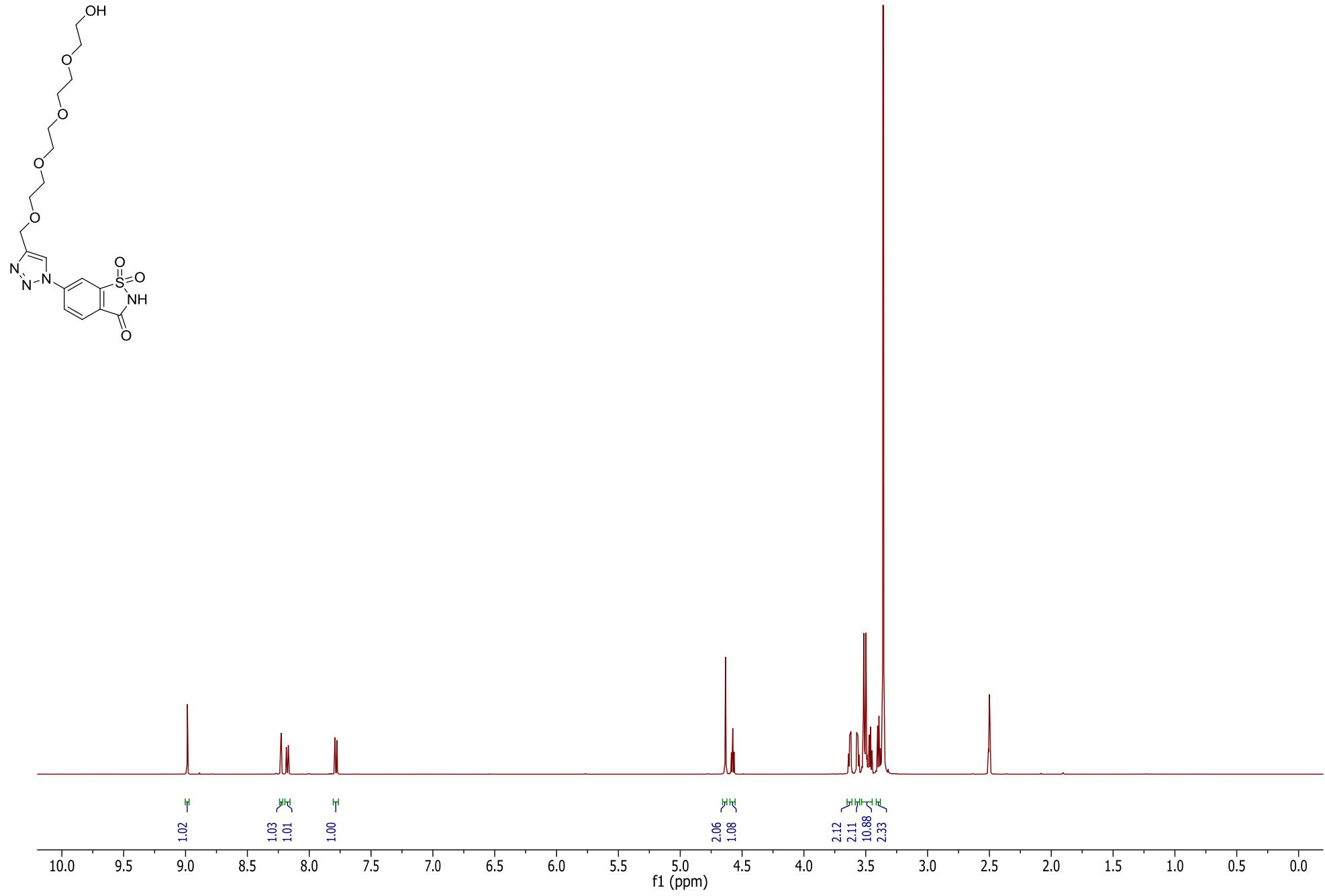
Compound **19** 500 MHz ^1H NMR (CD_3SO_2)



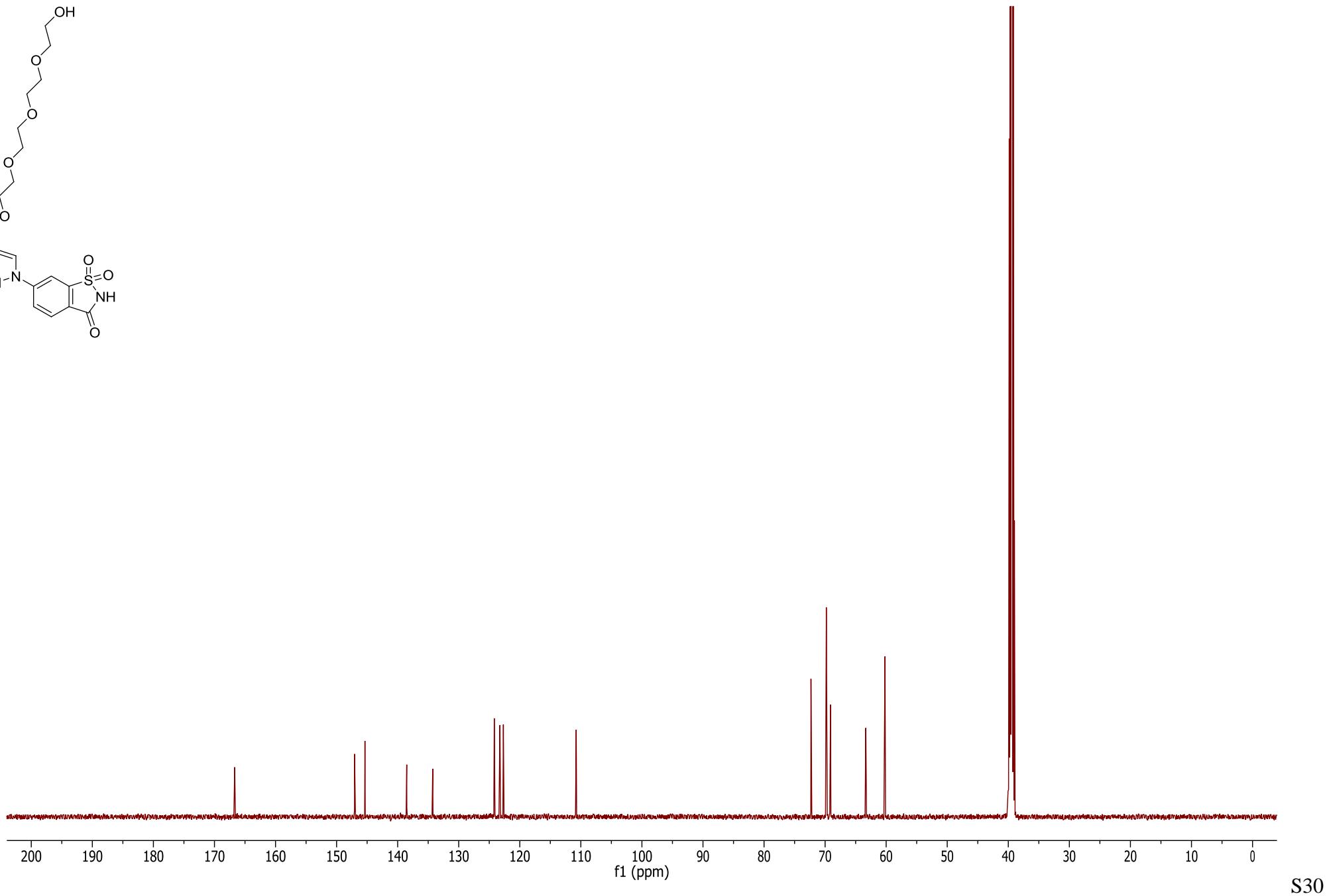
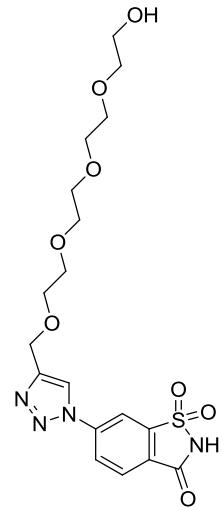
Compound **19** 125 MHz ^{13}C NMR (CD_3SO_2)



Compound **20** 500 MHz ^1H NMR (CD_3SO)

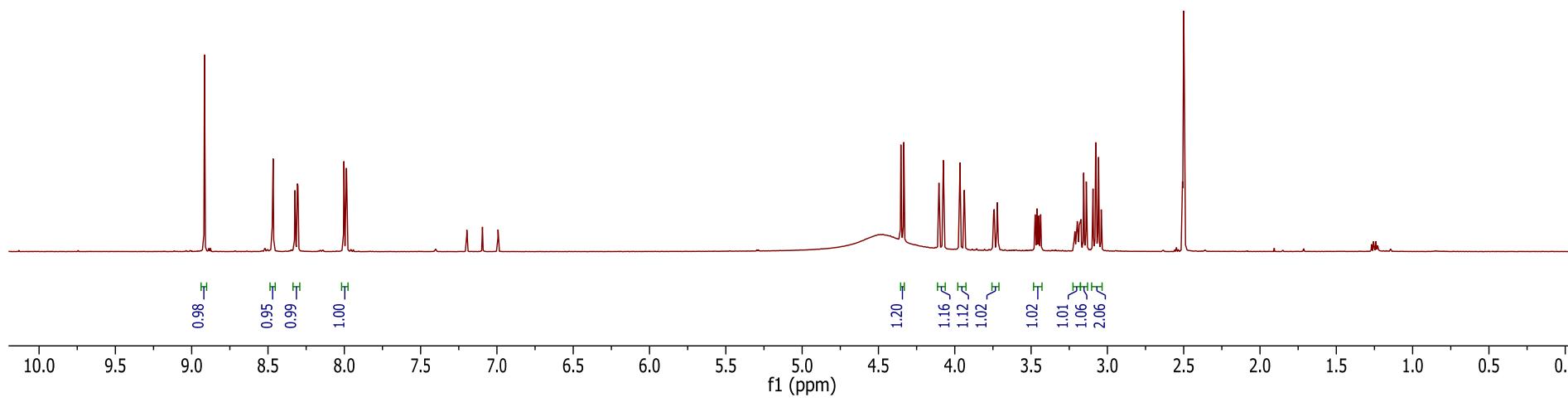
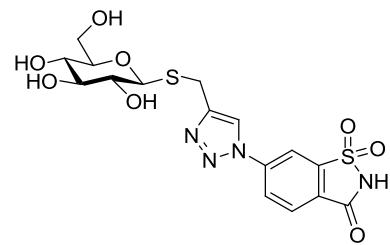


Compound **20** 125 MHz ^{13}C NMR (CD_3SO_2)

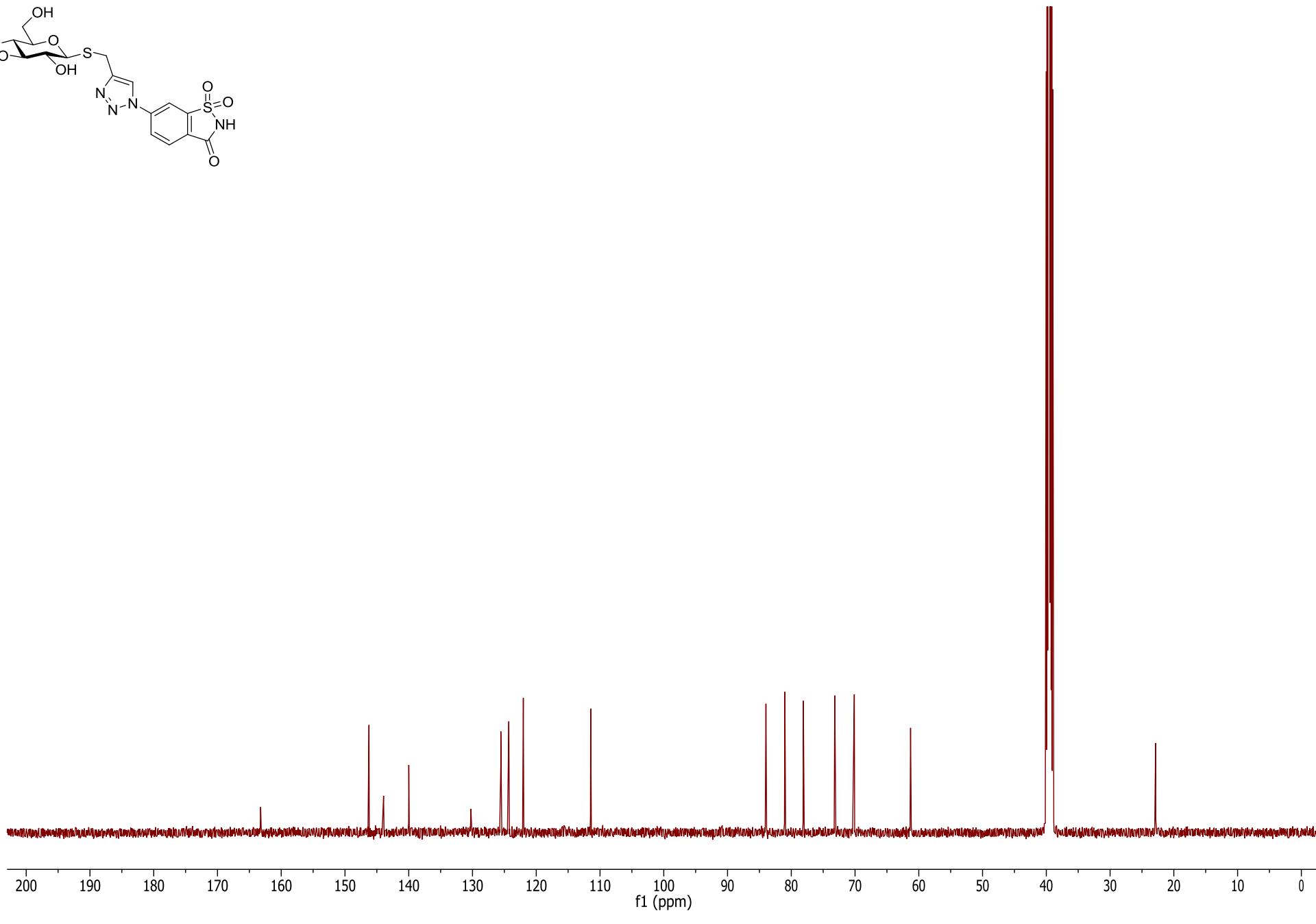
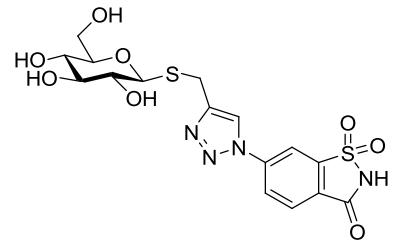


S30

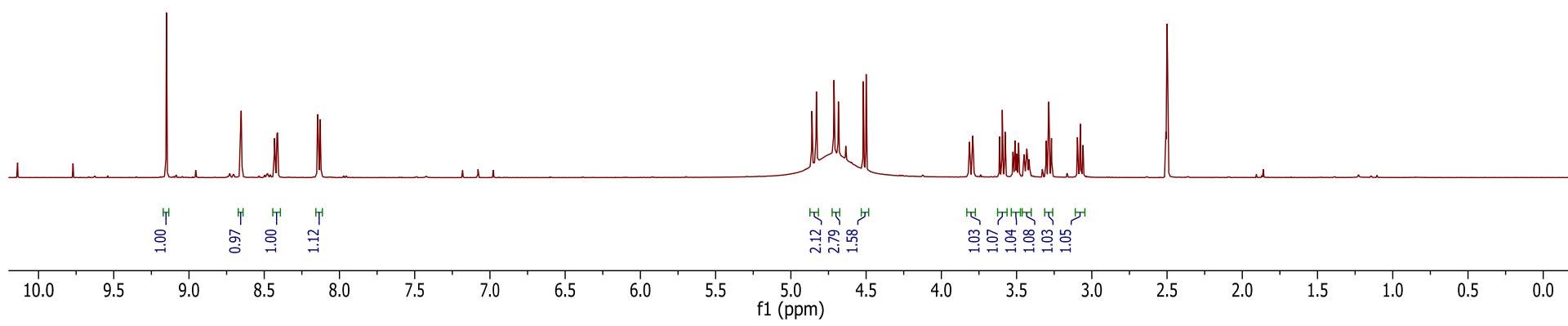
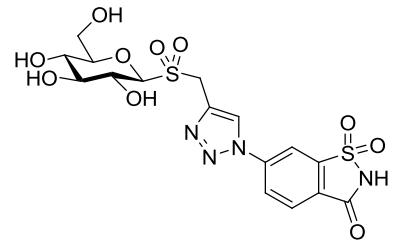
Compound 21 500 MHz ^1H NMR (CD_3SO)



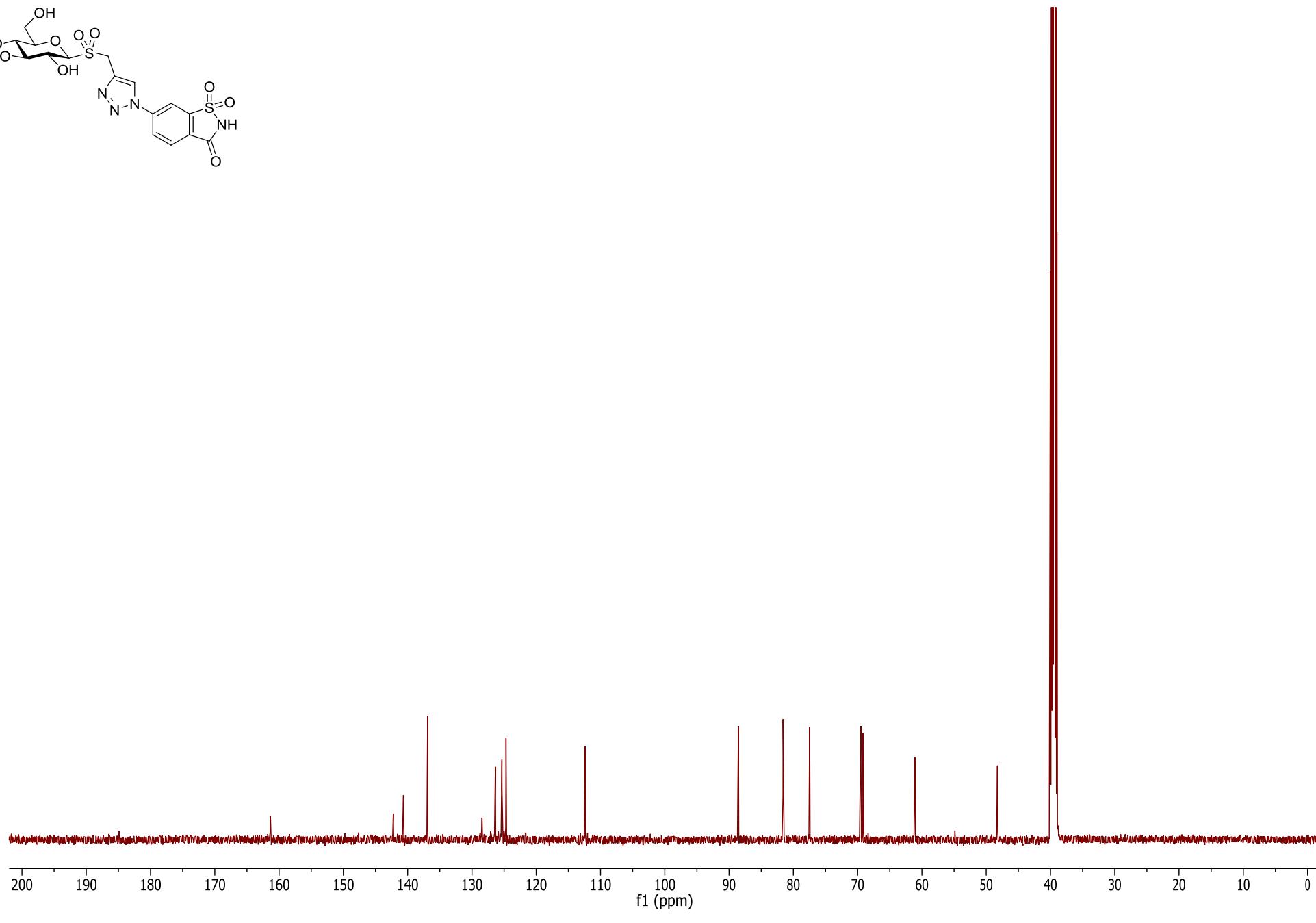
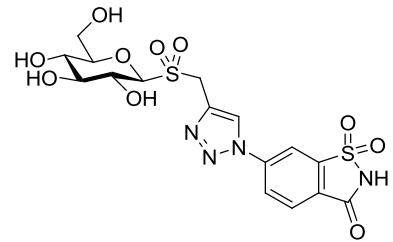
Compound **21** 125 MHz ^{13}C NMR (CD_3SO)



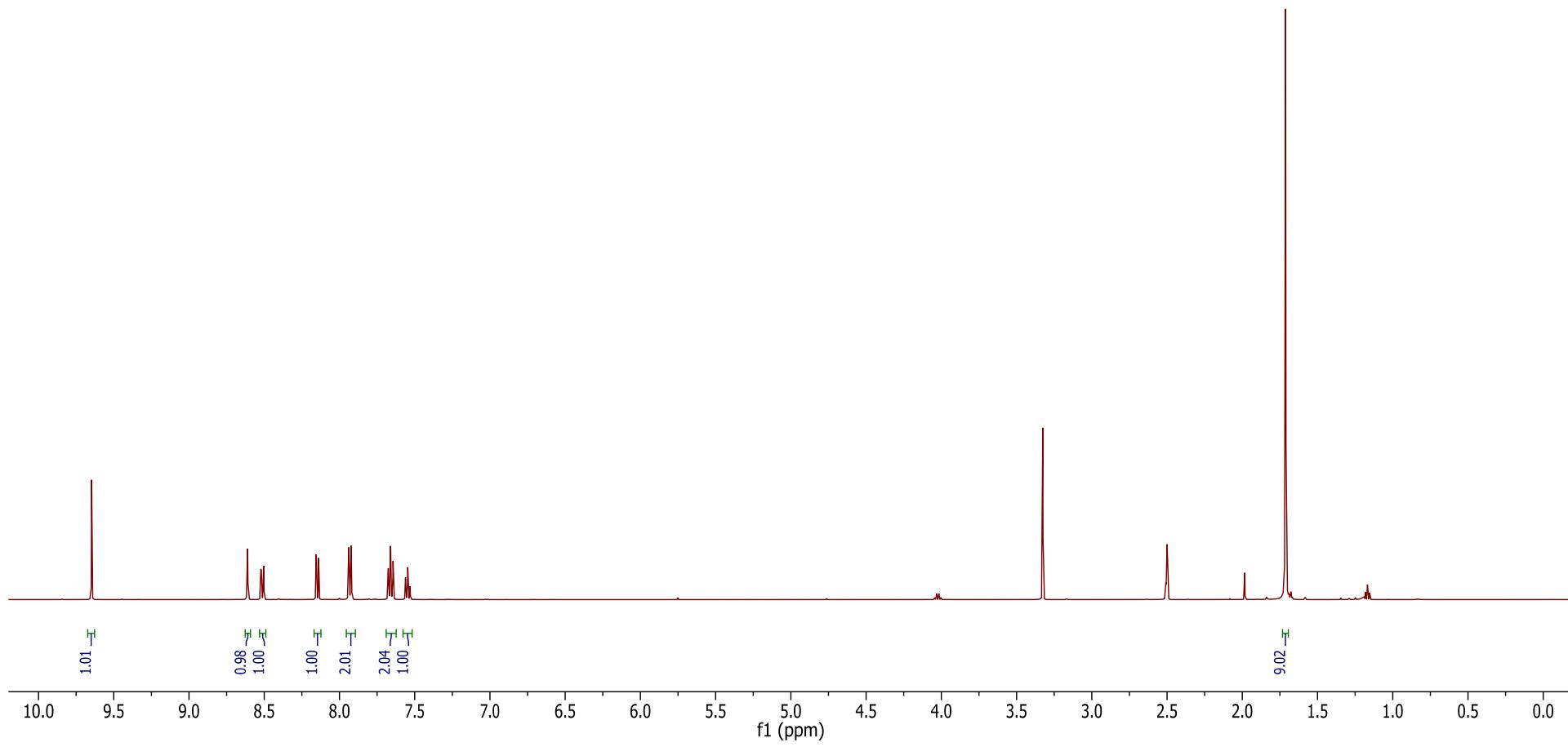
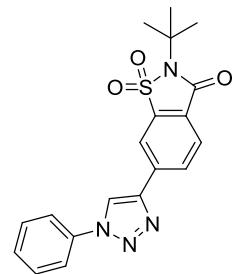
Compound 22 500 MHz ^1H NMR (CD_3SO)



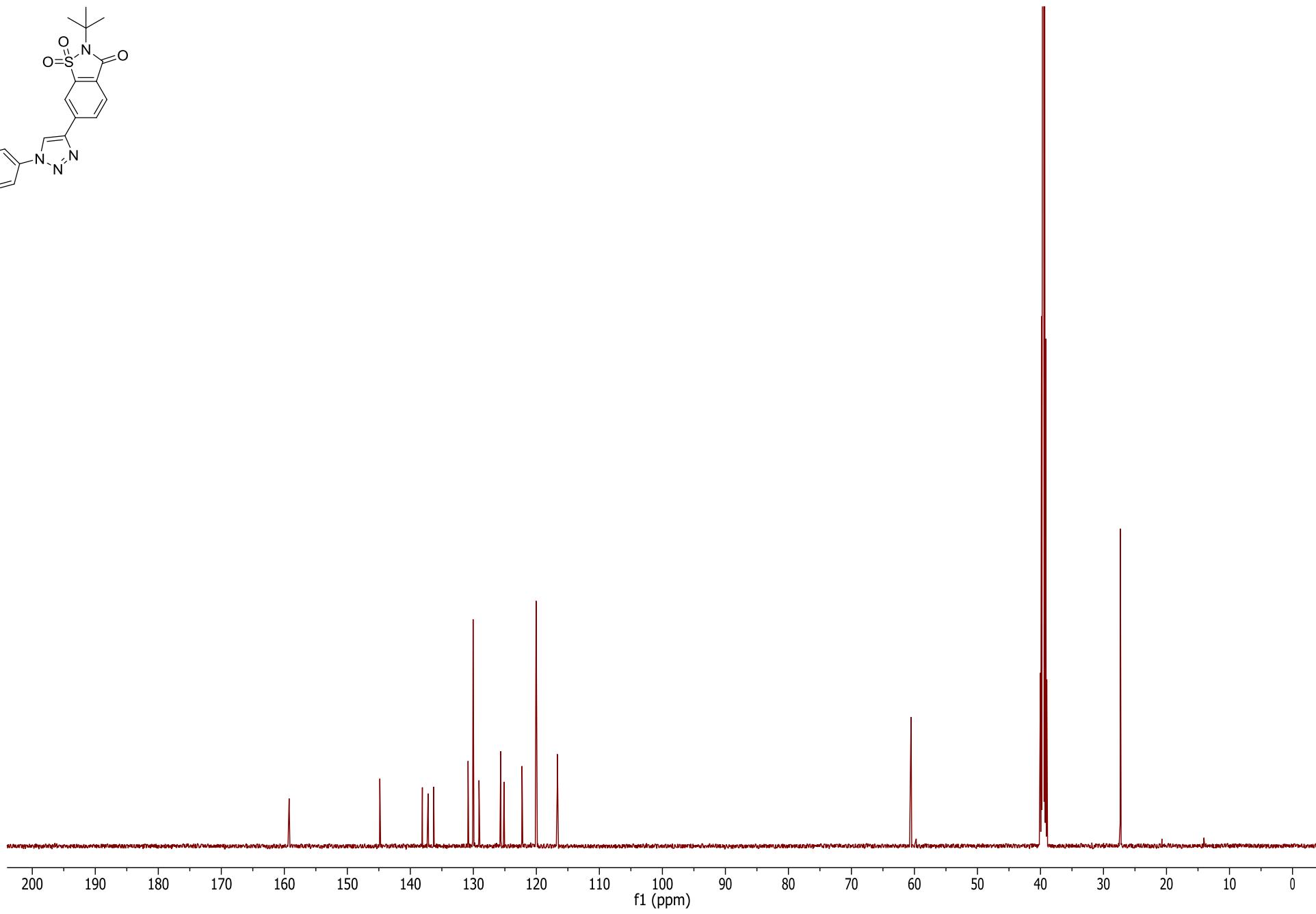
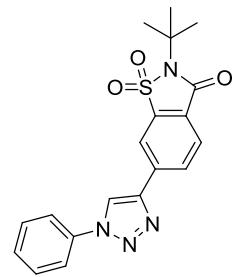
Compound 22 125 MHz ^{13}C NMR (CD_3SO)



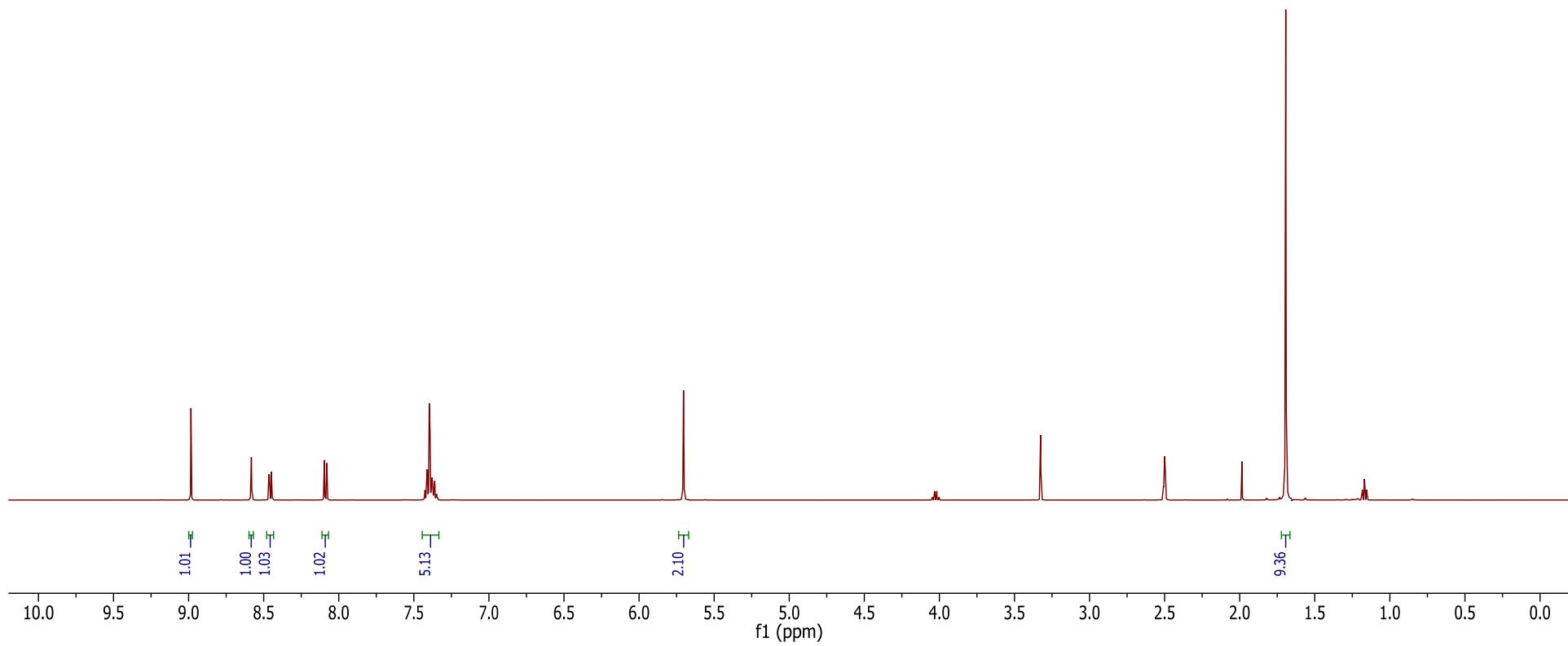
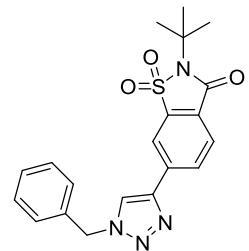
Compound **24** 500 MHz ^1H NMR (CD_3SO)



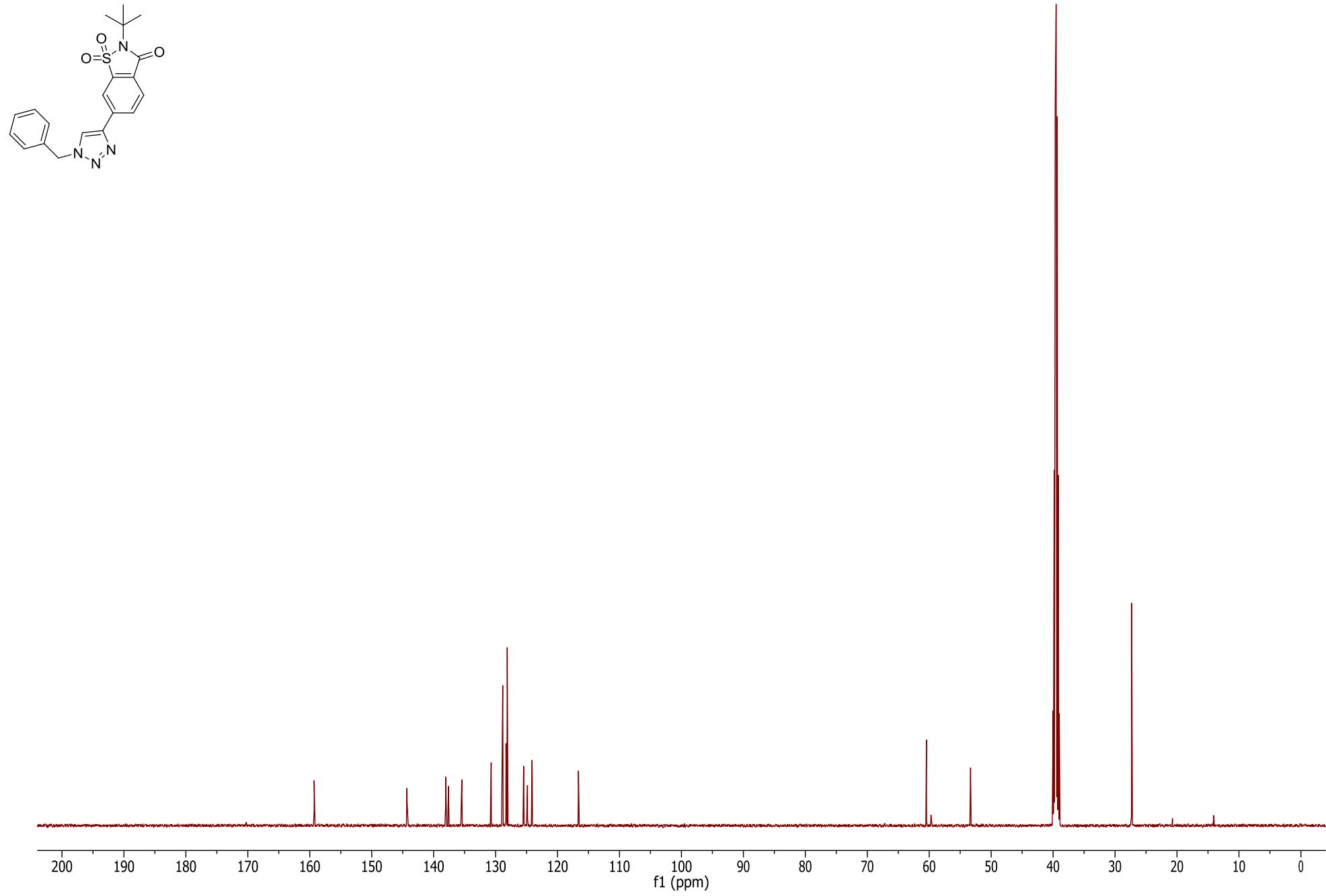
Compound **24** 125 MHz ^{13}C NMR (CD_3SO_2)



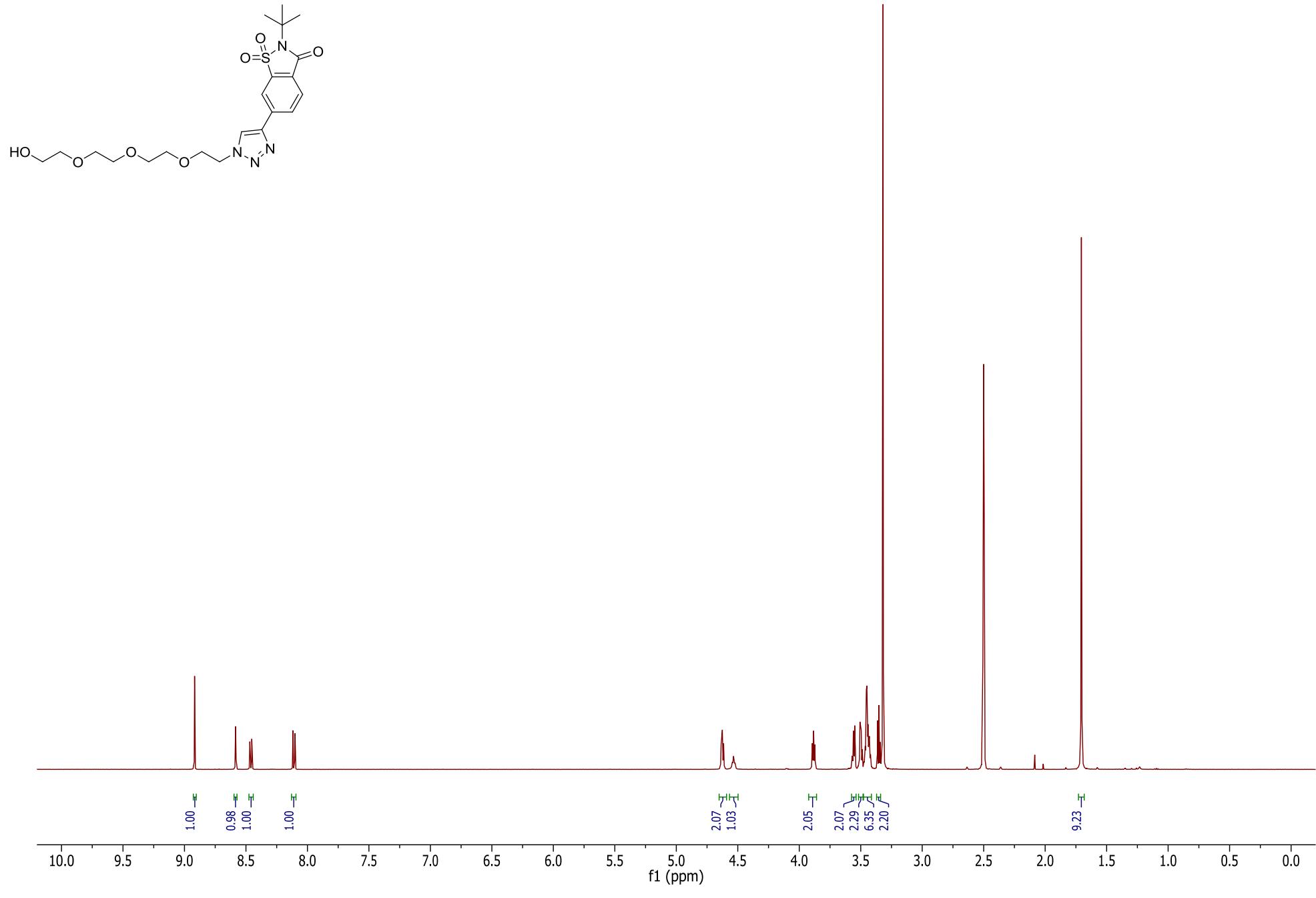
Compound **25** 500 MHz ^1H NMR (CD_3SO)



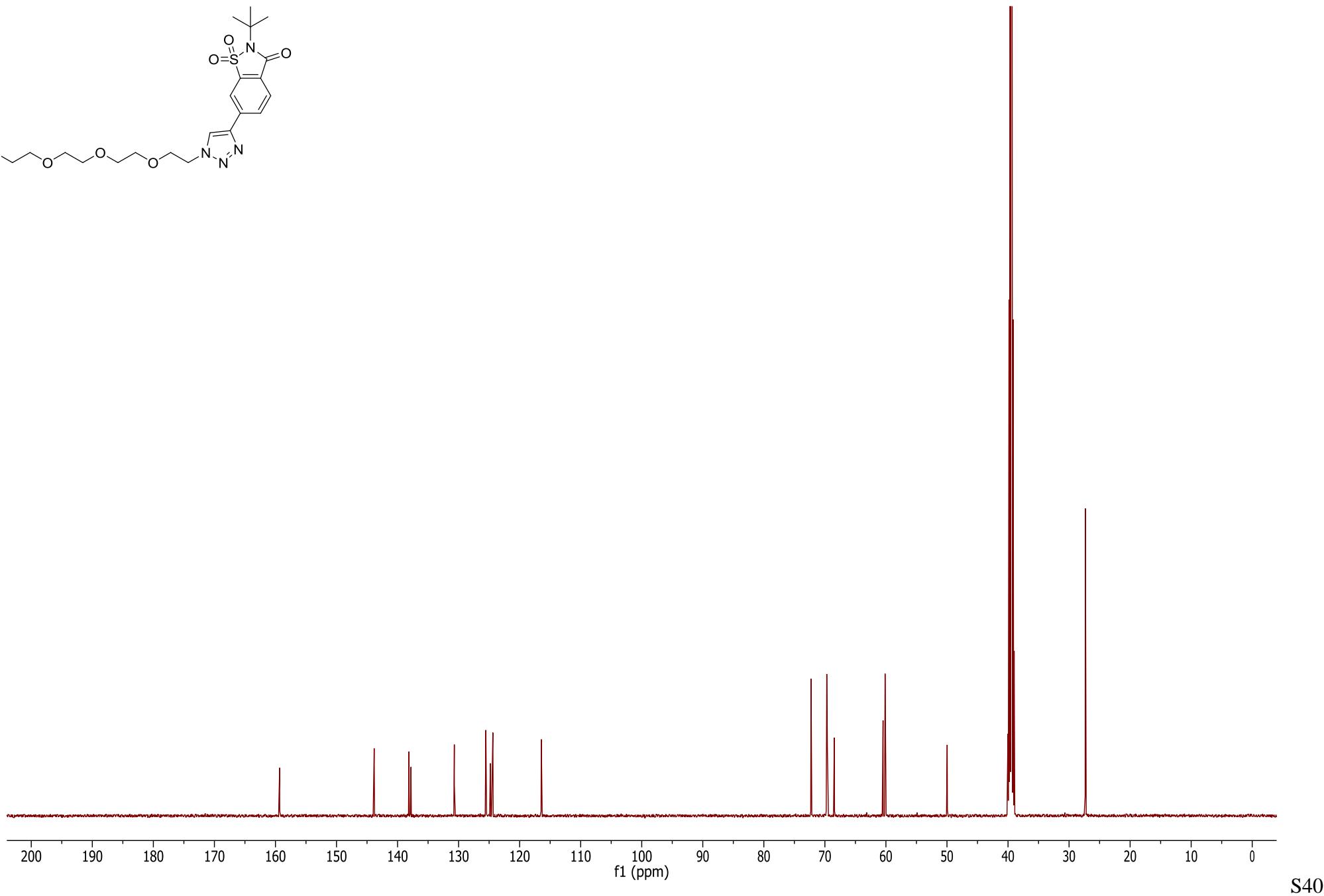
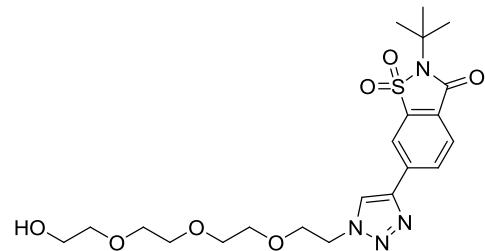
Compound **25** 125 MHz ^{13}C NMR (CD_3SO_2)



Compound **26** 500 MHz ^1H NMR (CD_3SO)

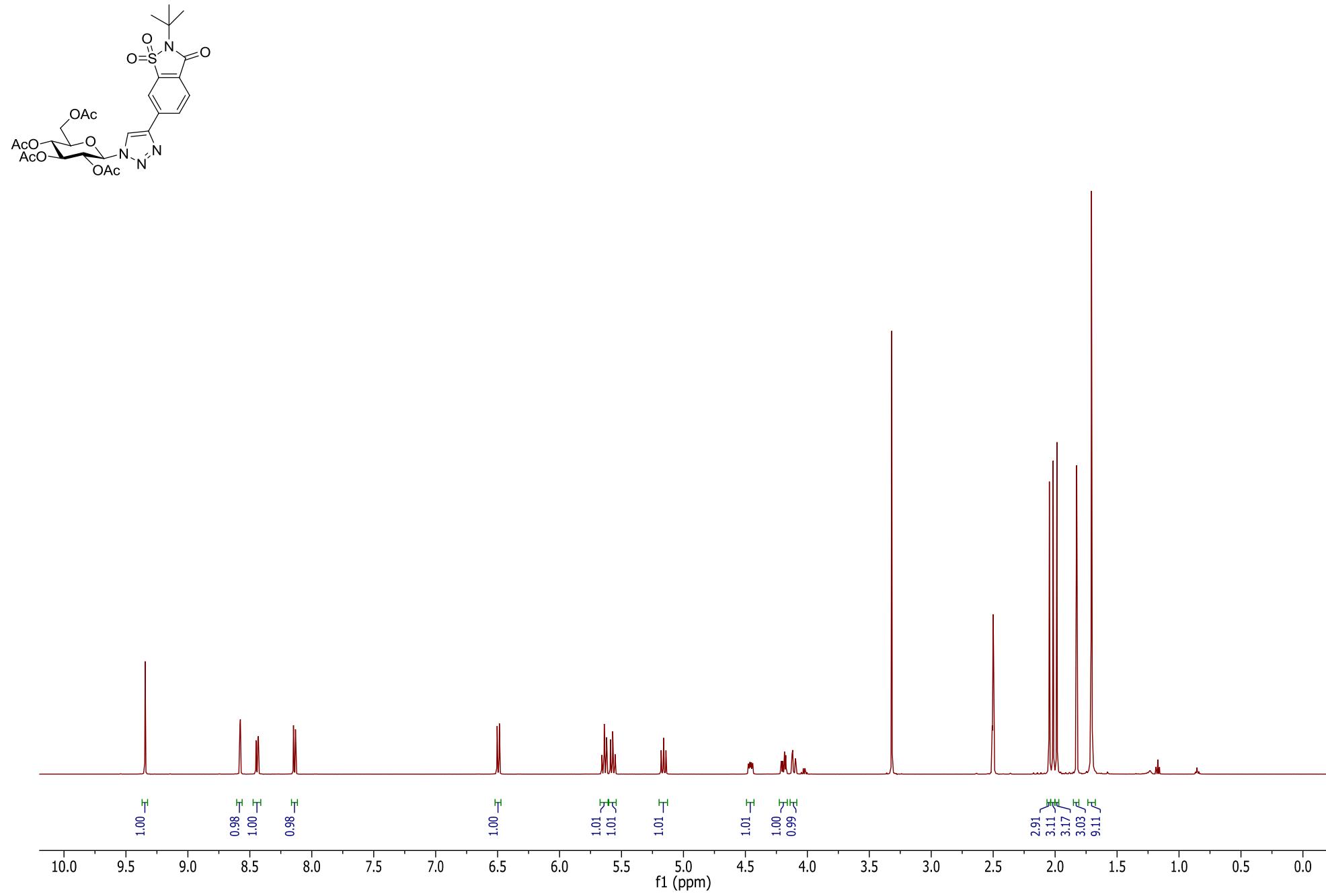


Compound **26** 125 MHz ^{13}C NMR (CD_3SO_2)

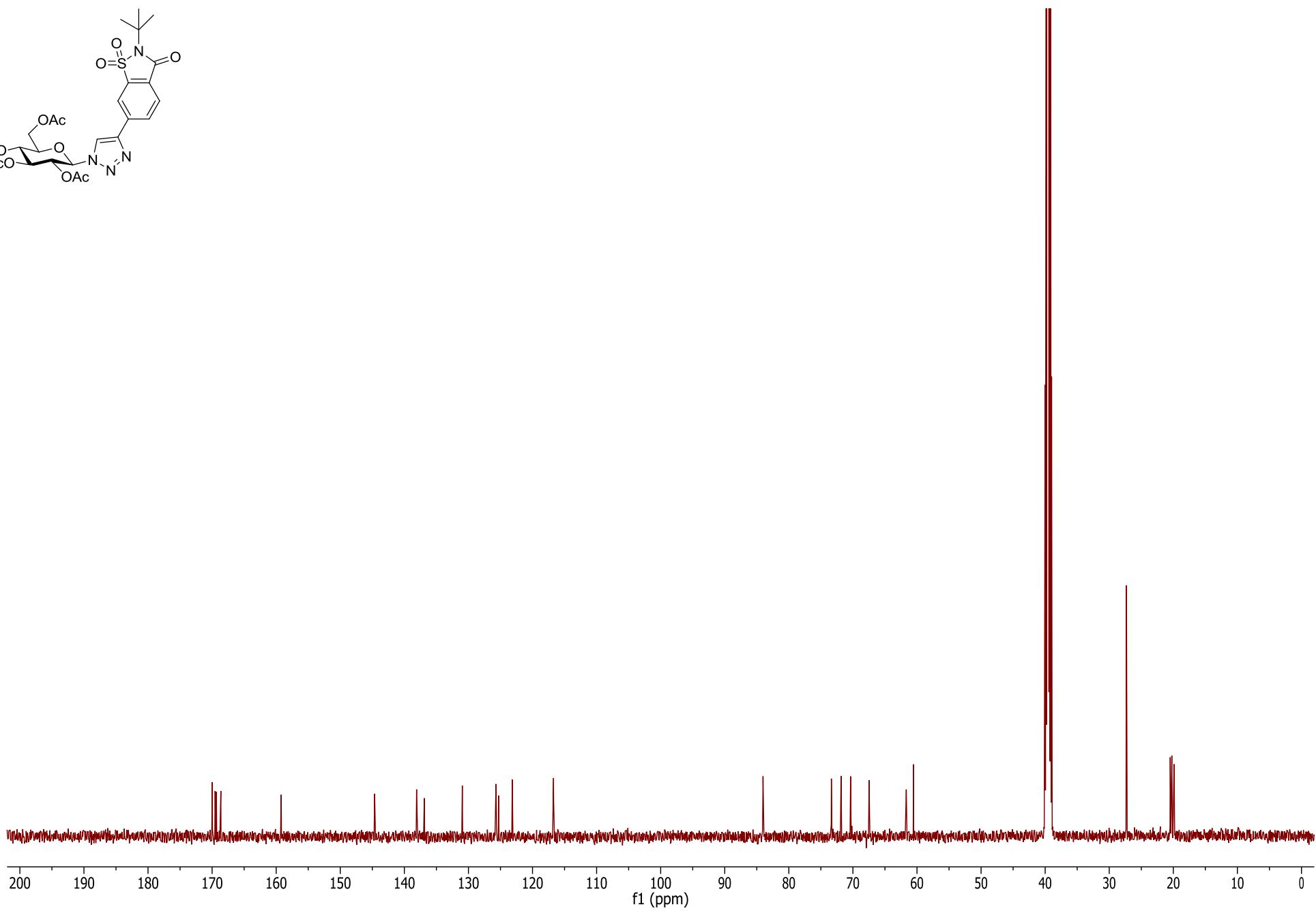
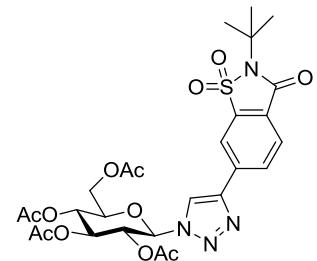


S40

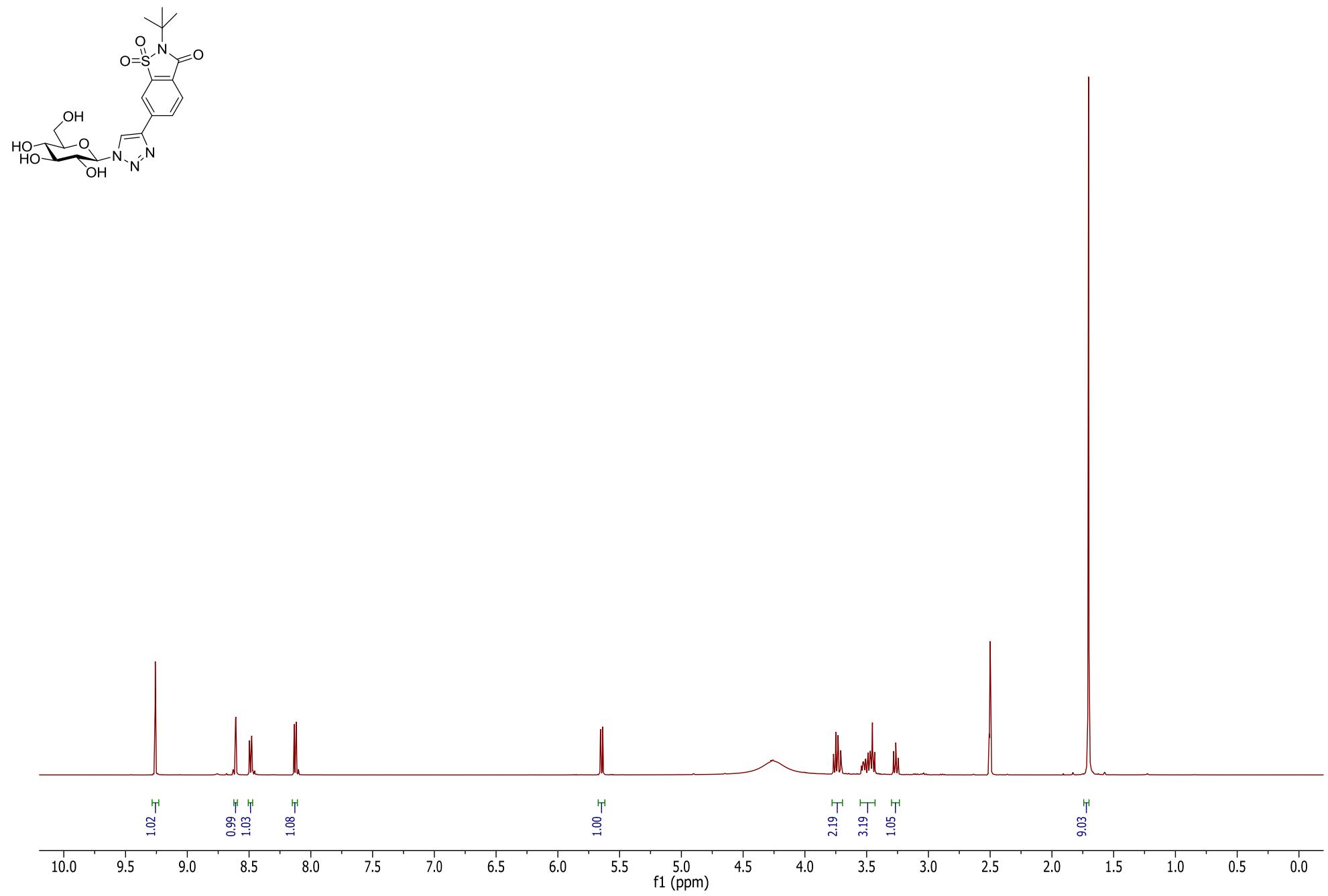
Compound 27 500 MHz ^1H NMR CDCl_3



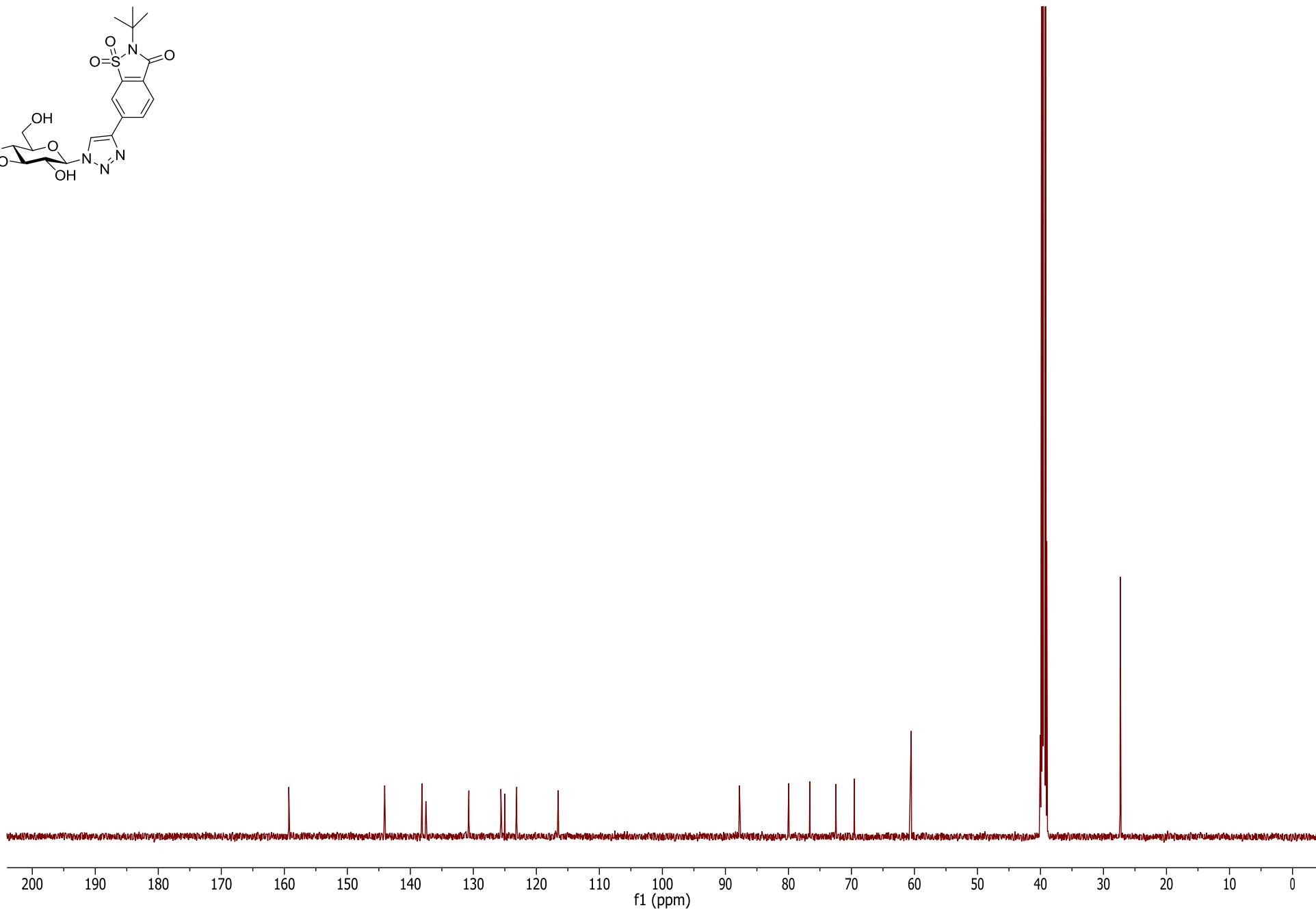
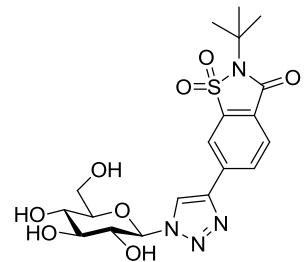
Compound 27 125 MHz ^{13}C NMR CDCl_3



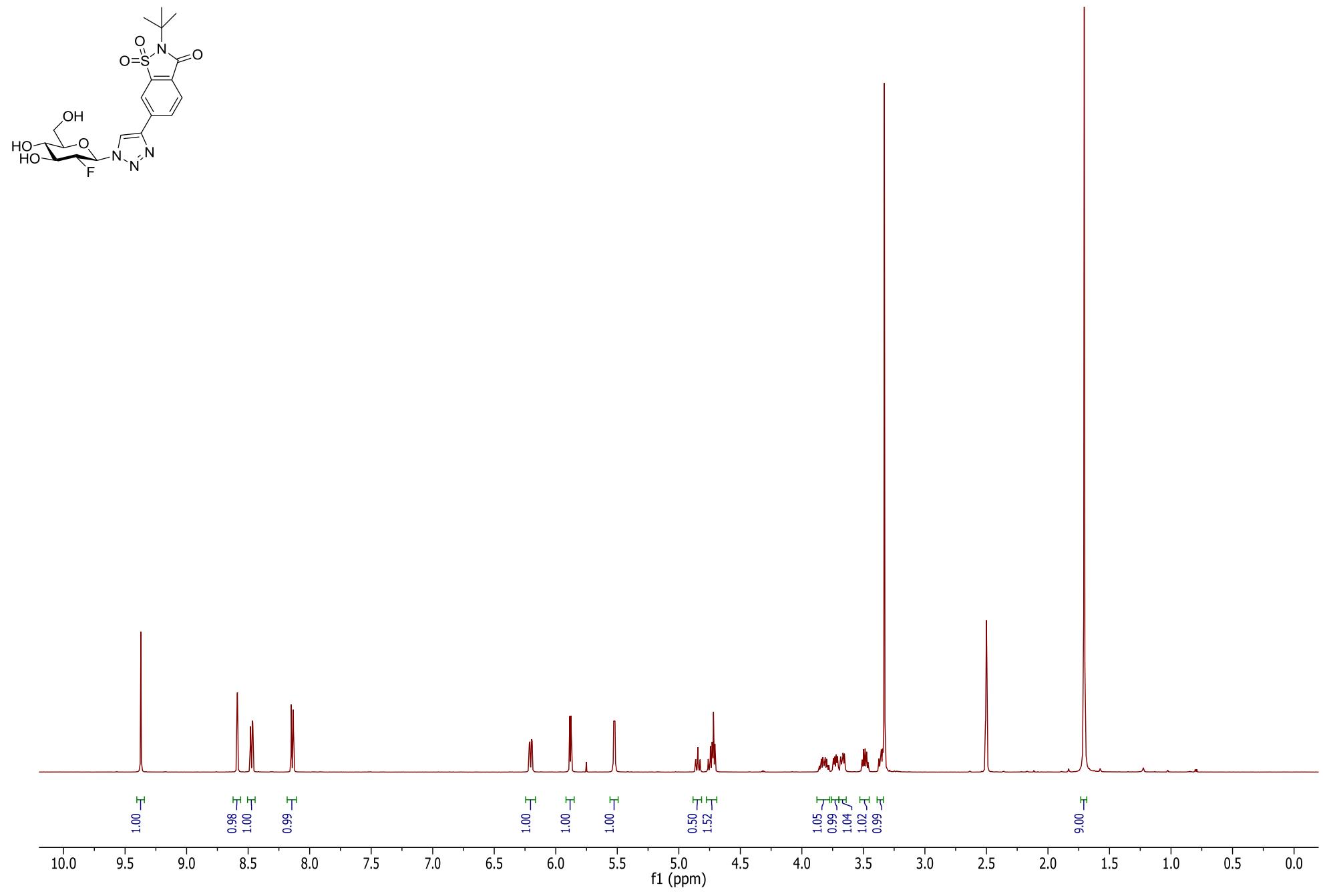
Compound 28 500 MHz ^1H NMR (CD_3SO)



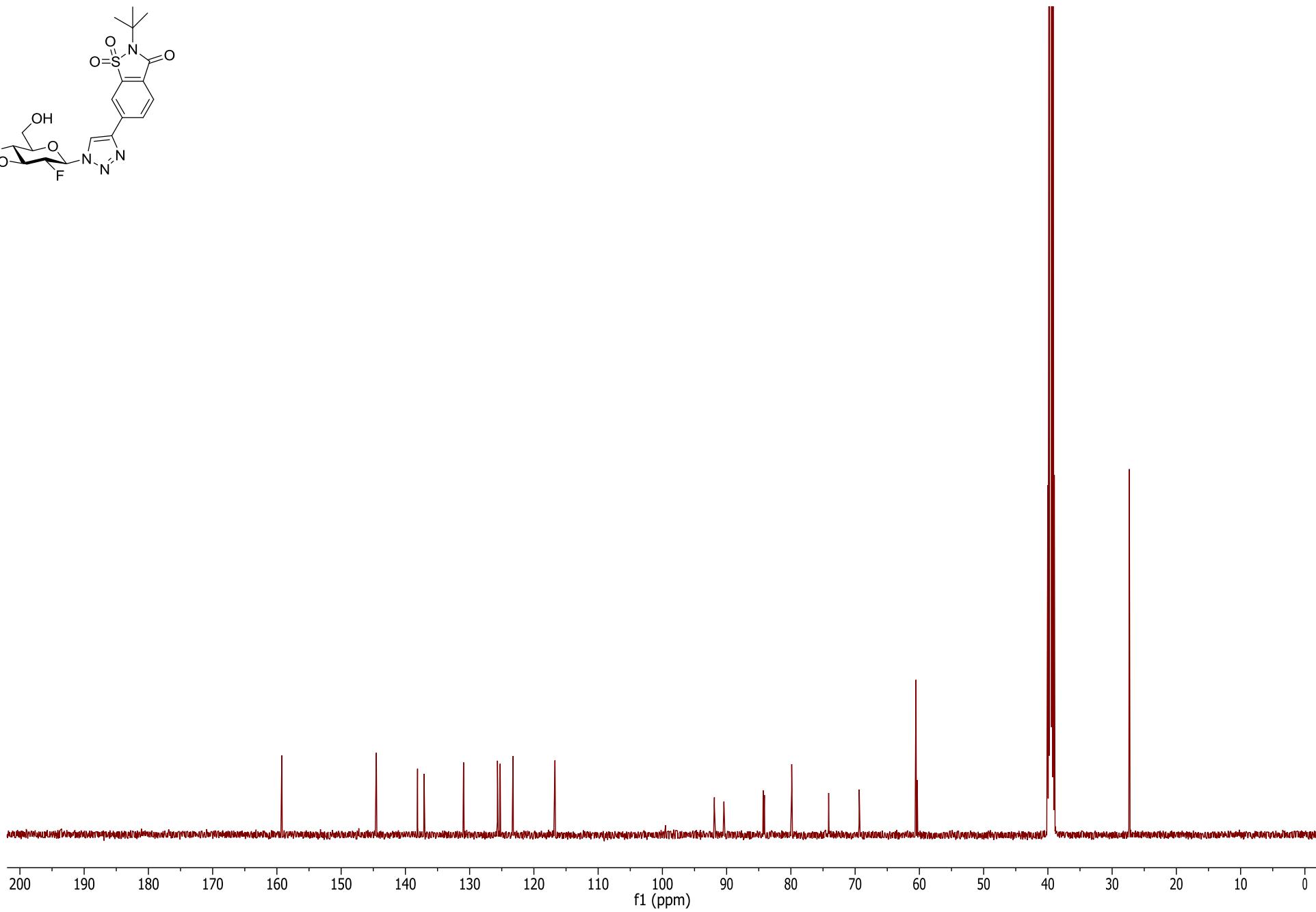
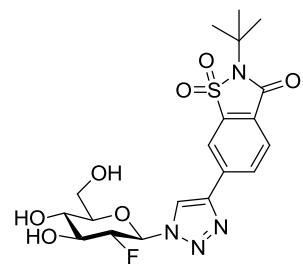
Compound **28** 125 MHz ^{13}C NMR (CD_3SO)



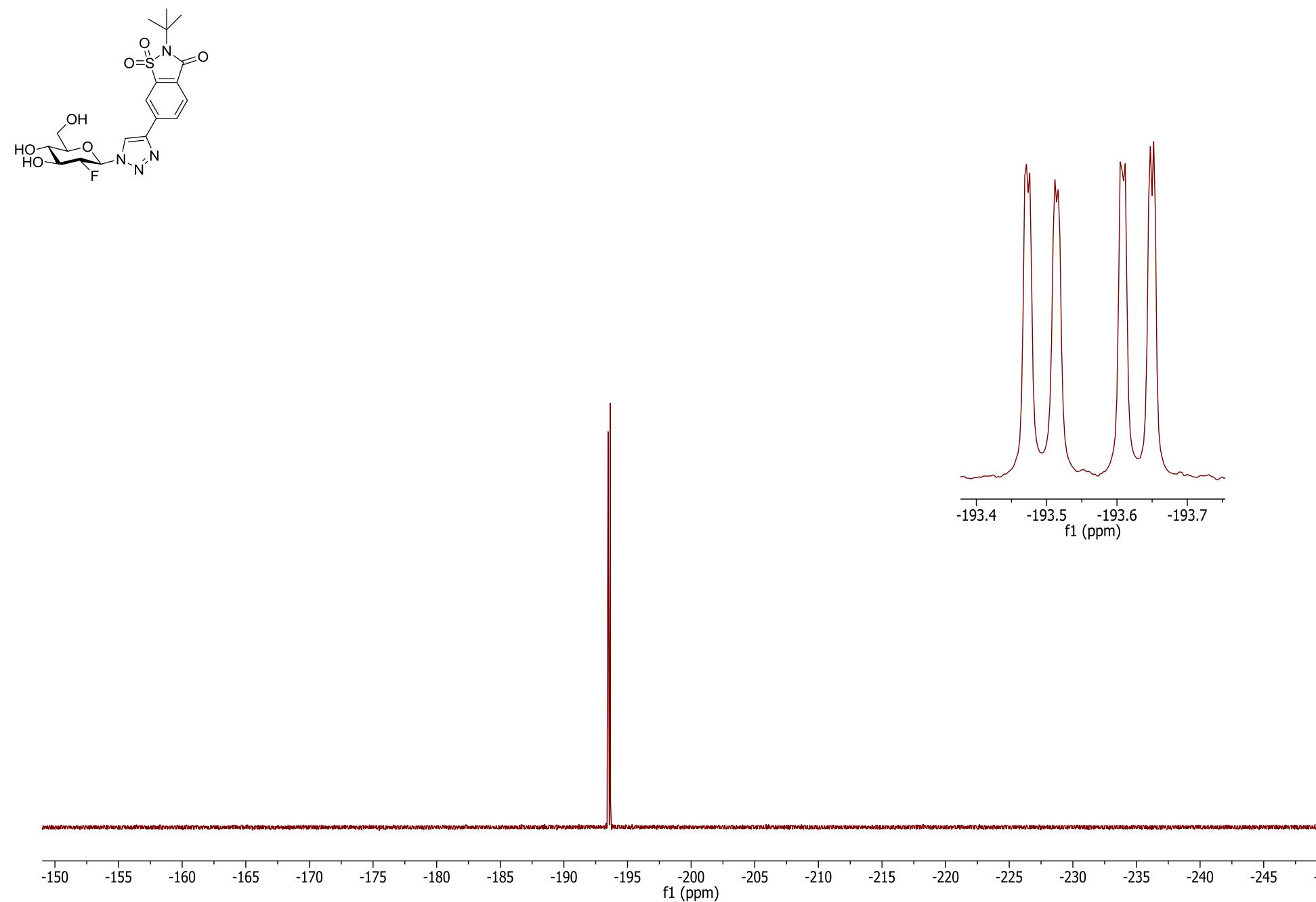
Compound 29 500 MHz ^1H NMR (CD_3SO)



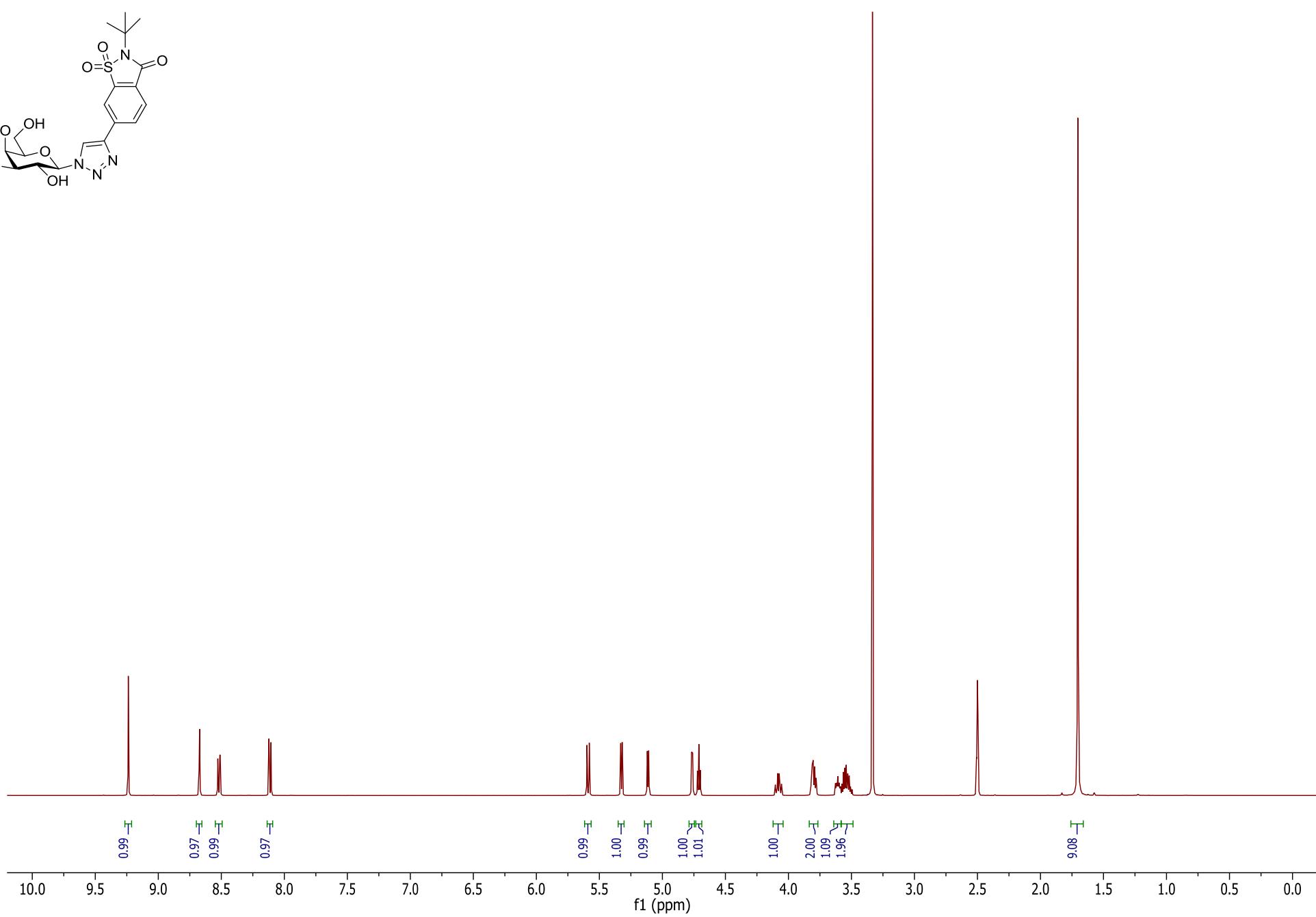
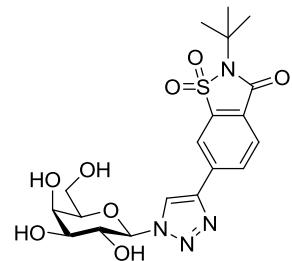
Compound 29 125 MHz ^{13}C NMR (CD_3SO)



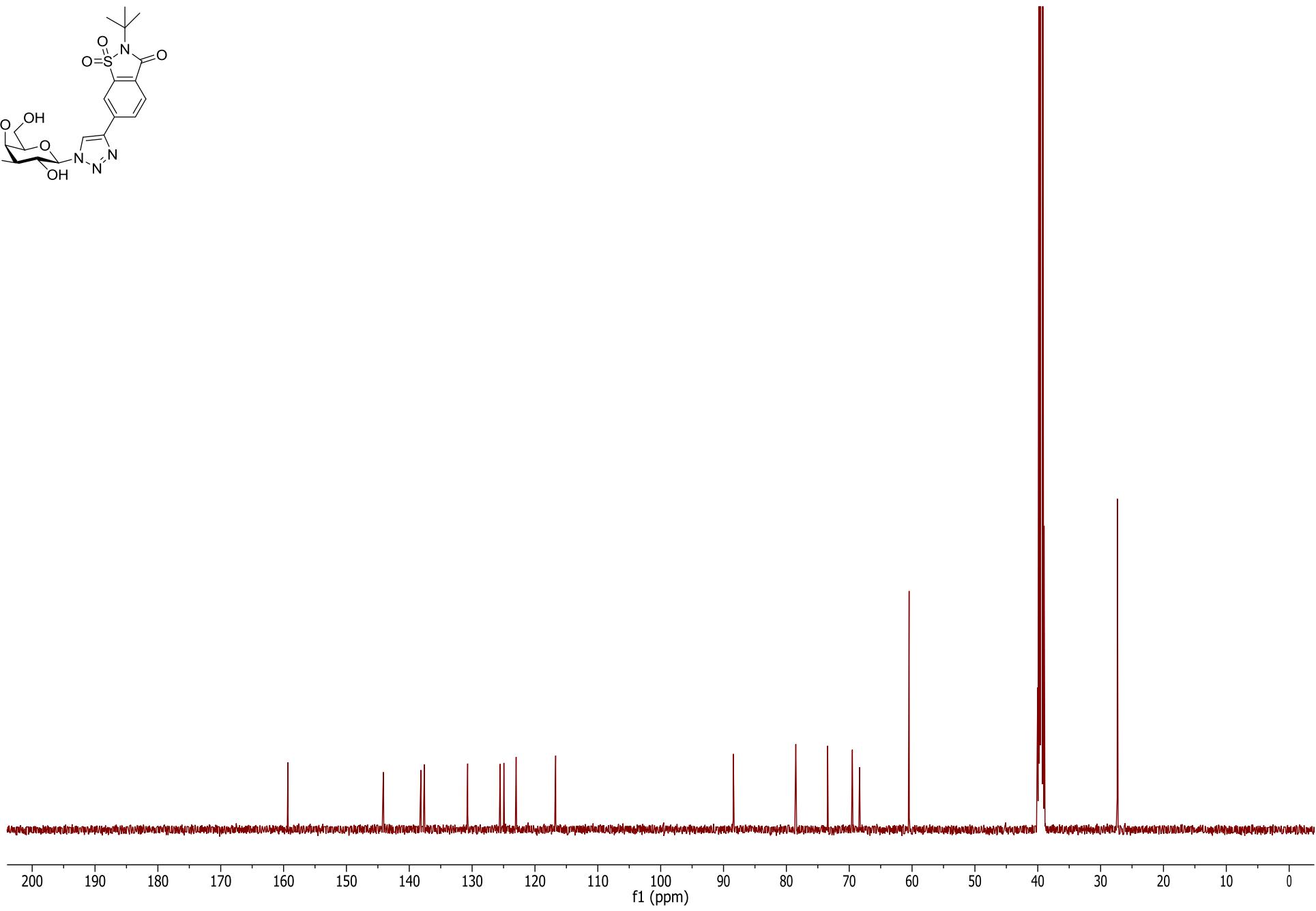
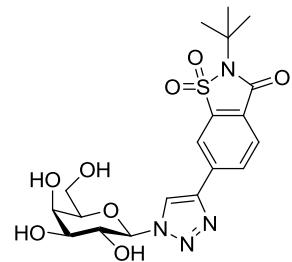
Compound 29 376 MHz ^{19}F NMR (CD_3SO_2)



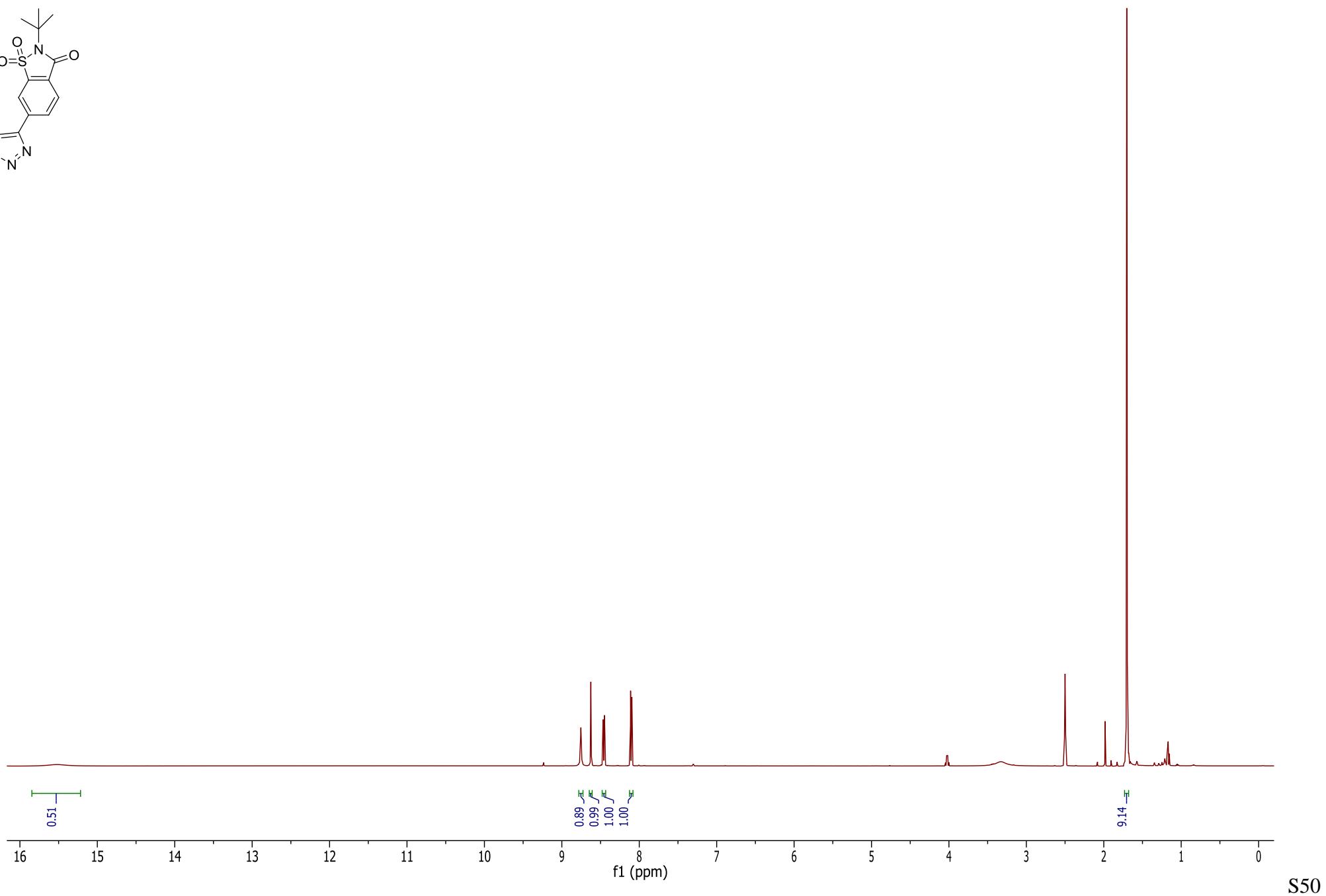
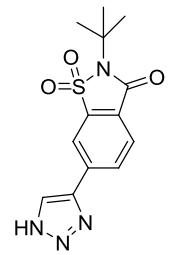
Compound **30** 500 MHz ^1H NMR (CD_3SO)



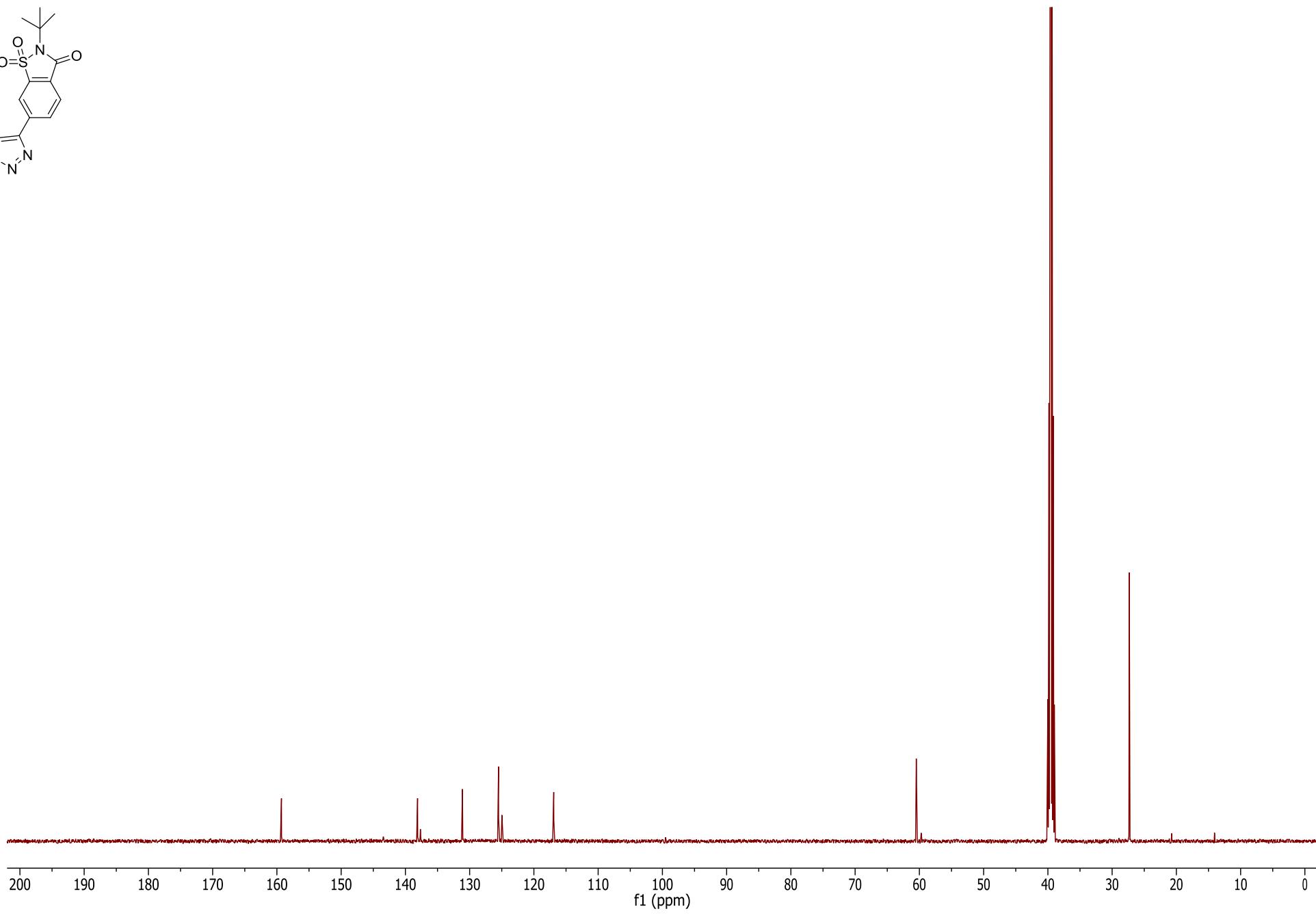
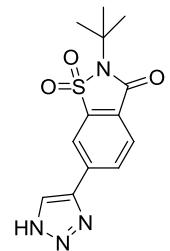
Compound **30** 125 MHz ^{13}C NMR (CD_3SO)



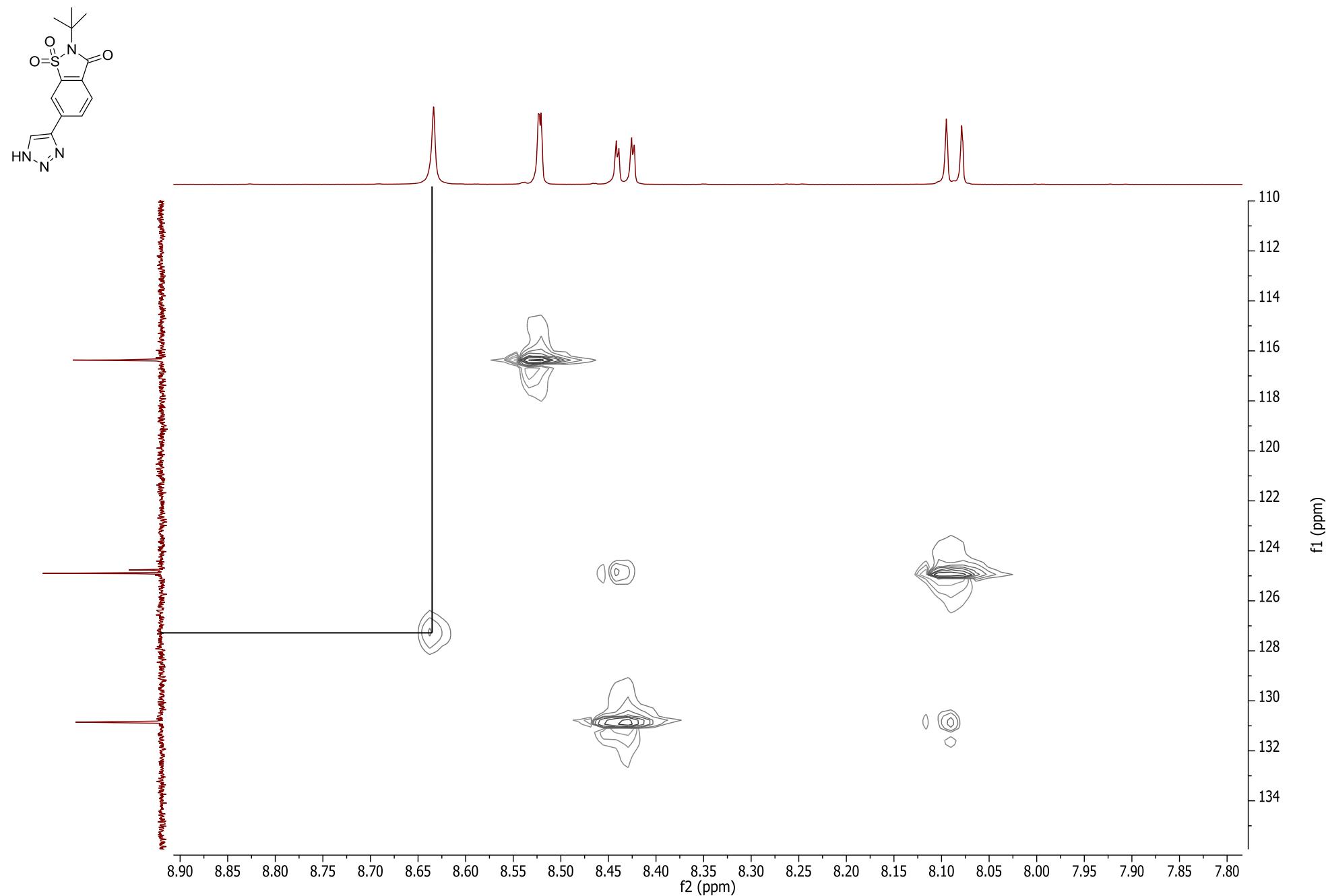
Compound **3I** 500 MHz ^1H NMR (CD_3SO)



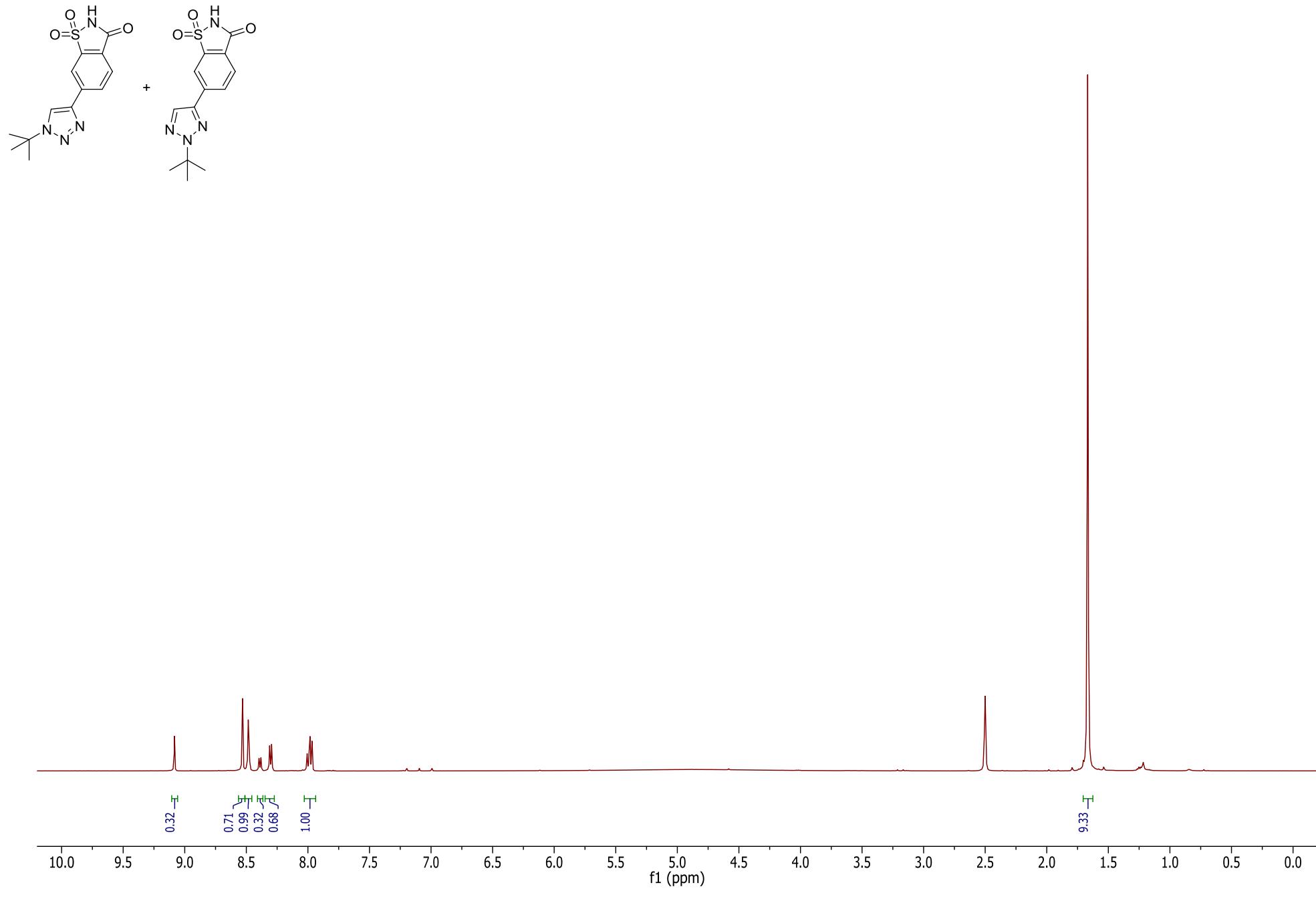
Compound **3I** 125 MHz ^{13}C NMR (CD_3SO)



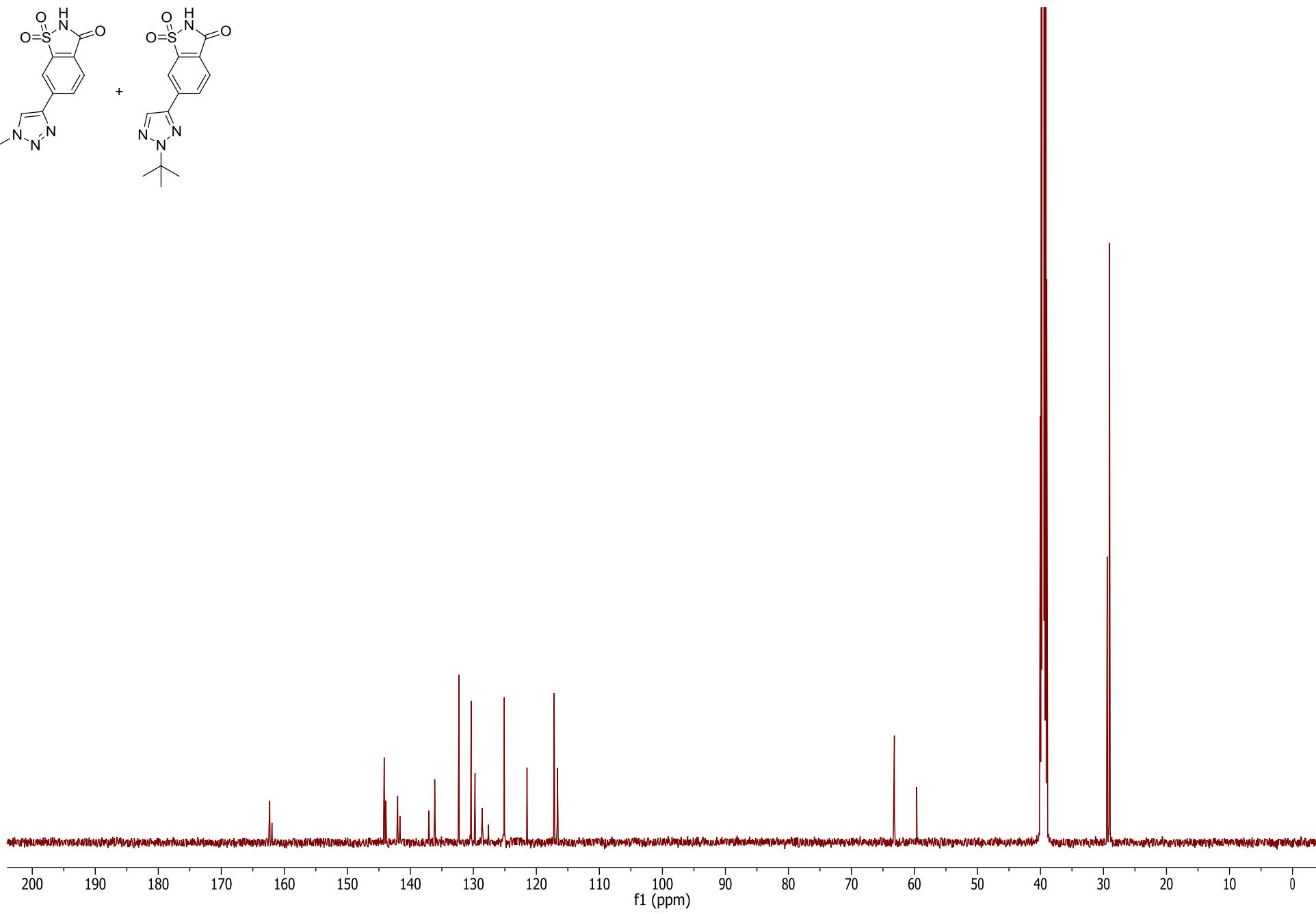
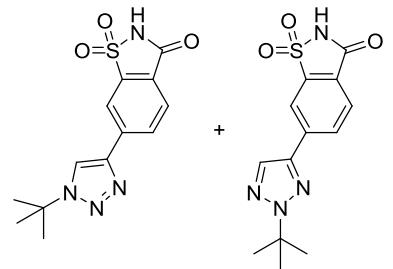
Compound 31 HSQC NMR (CD_3SO_2 , 90 °C, coupling constant 160 Hz)



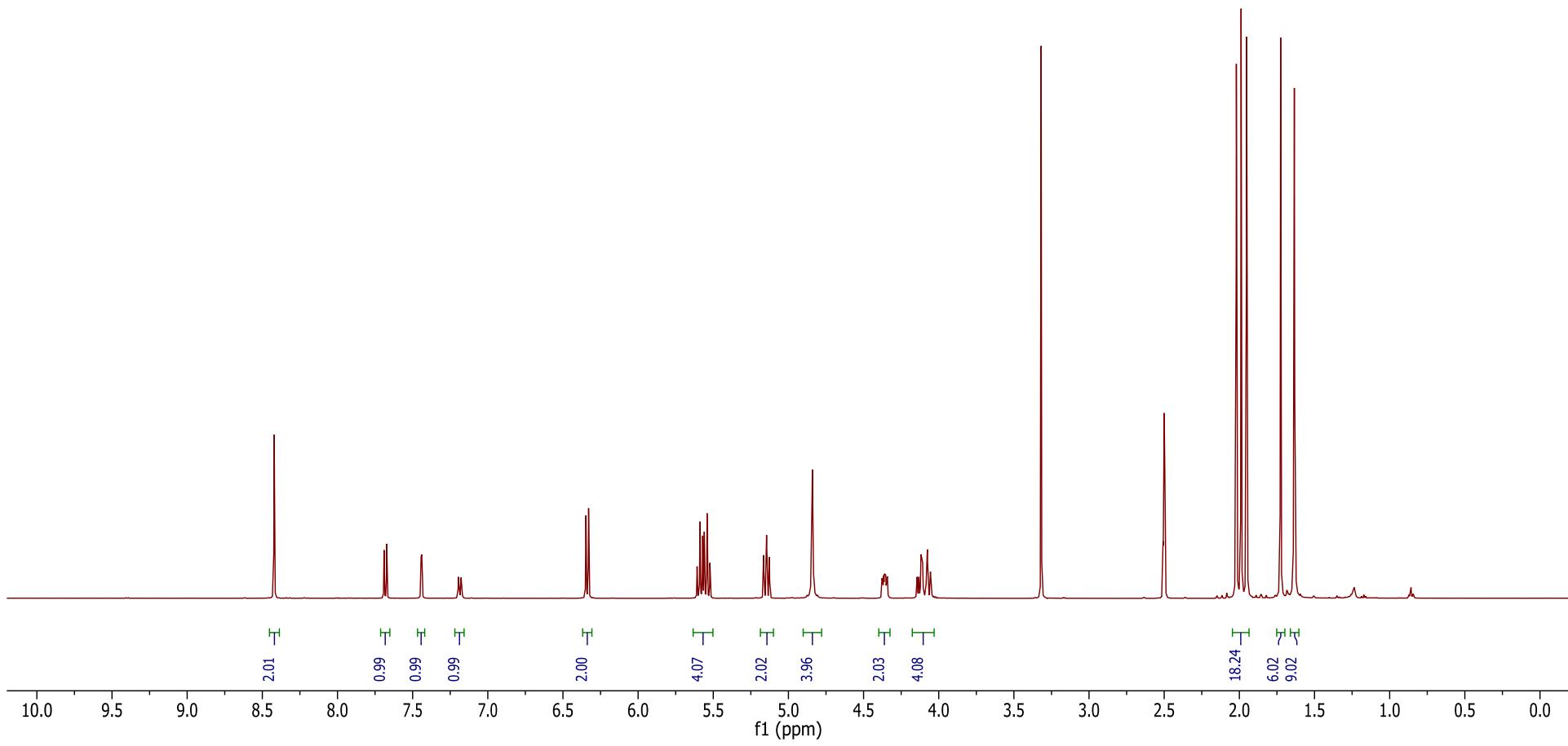
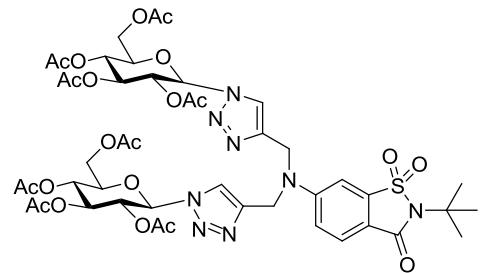
Compound **32a+32b** 500 MHz ^1H NMR (CD_3SO)



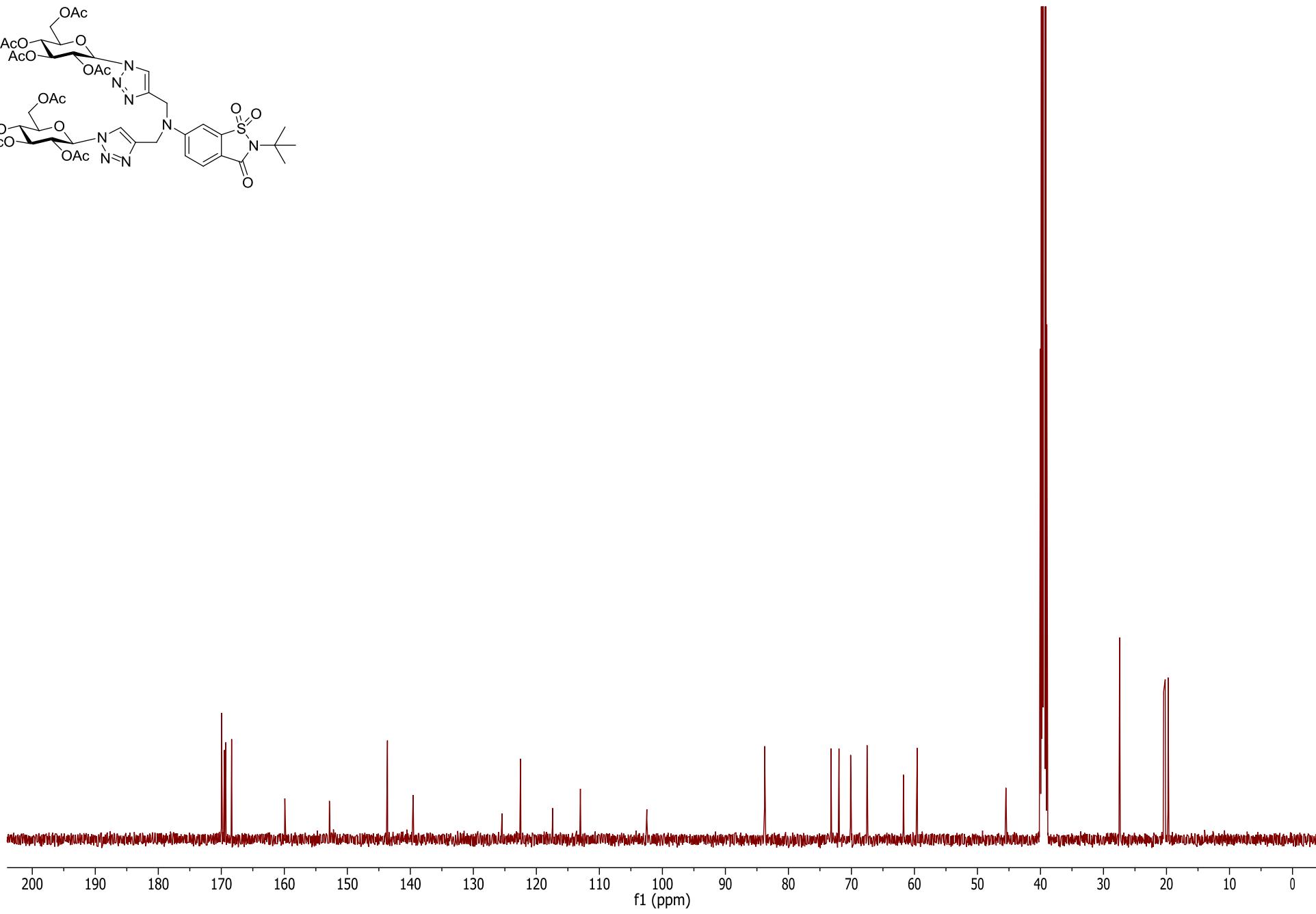
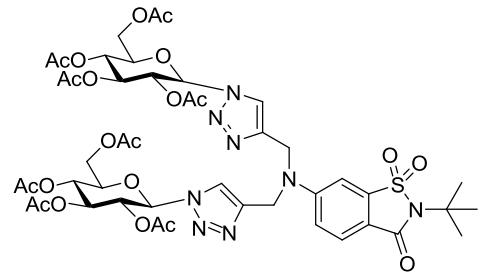
Compound 32a+32b 125 MHz ^{13}C NMR (CD_3SO_2)



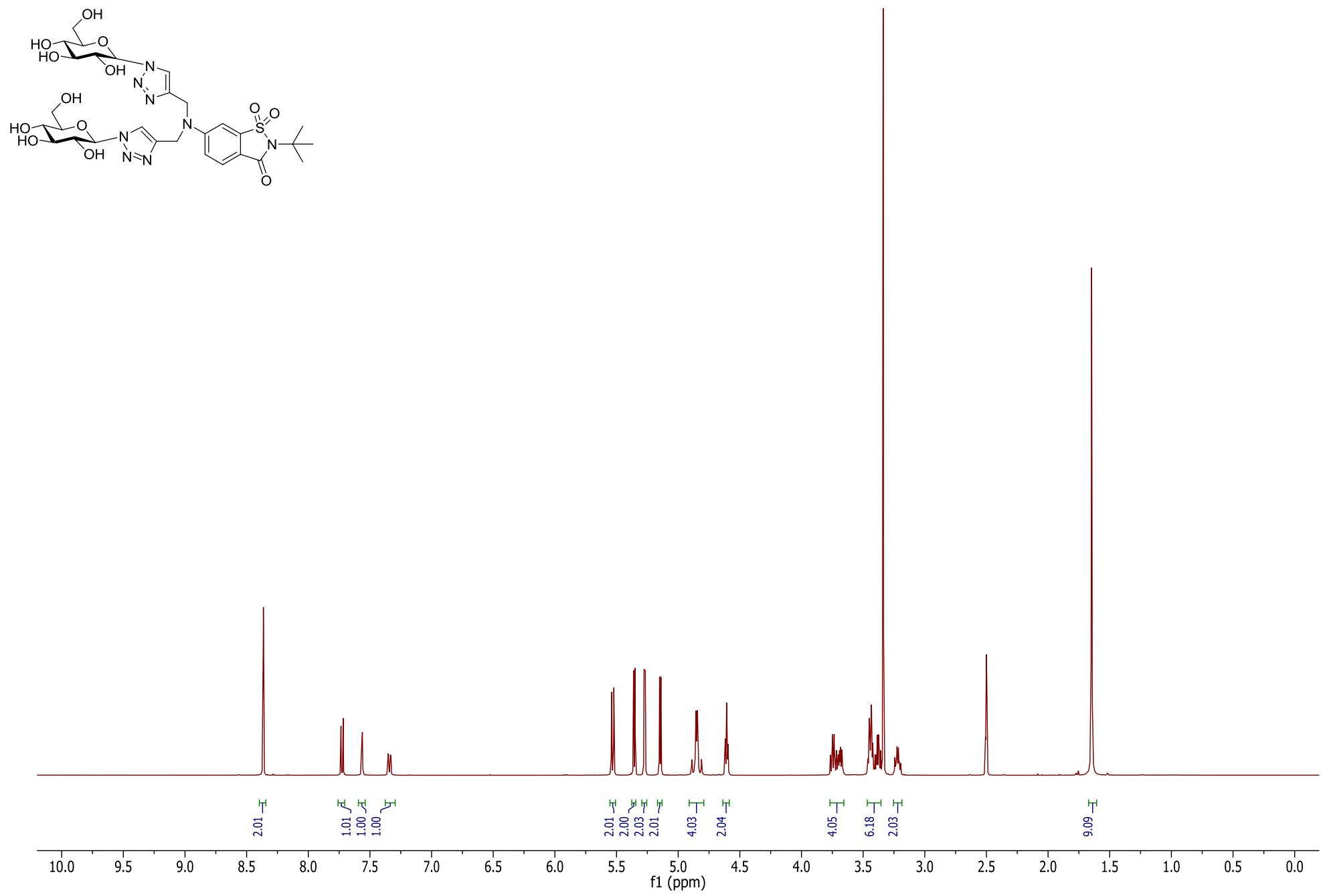
Compound 33 500 MHz ^1H NMR (CD_3SO)



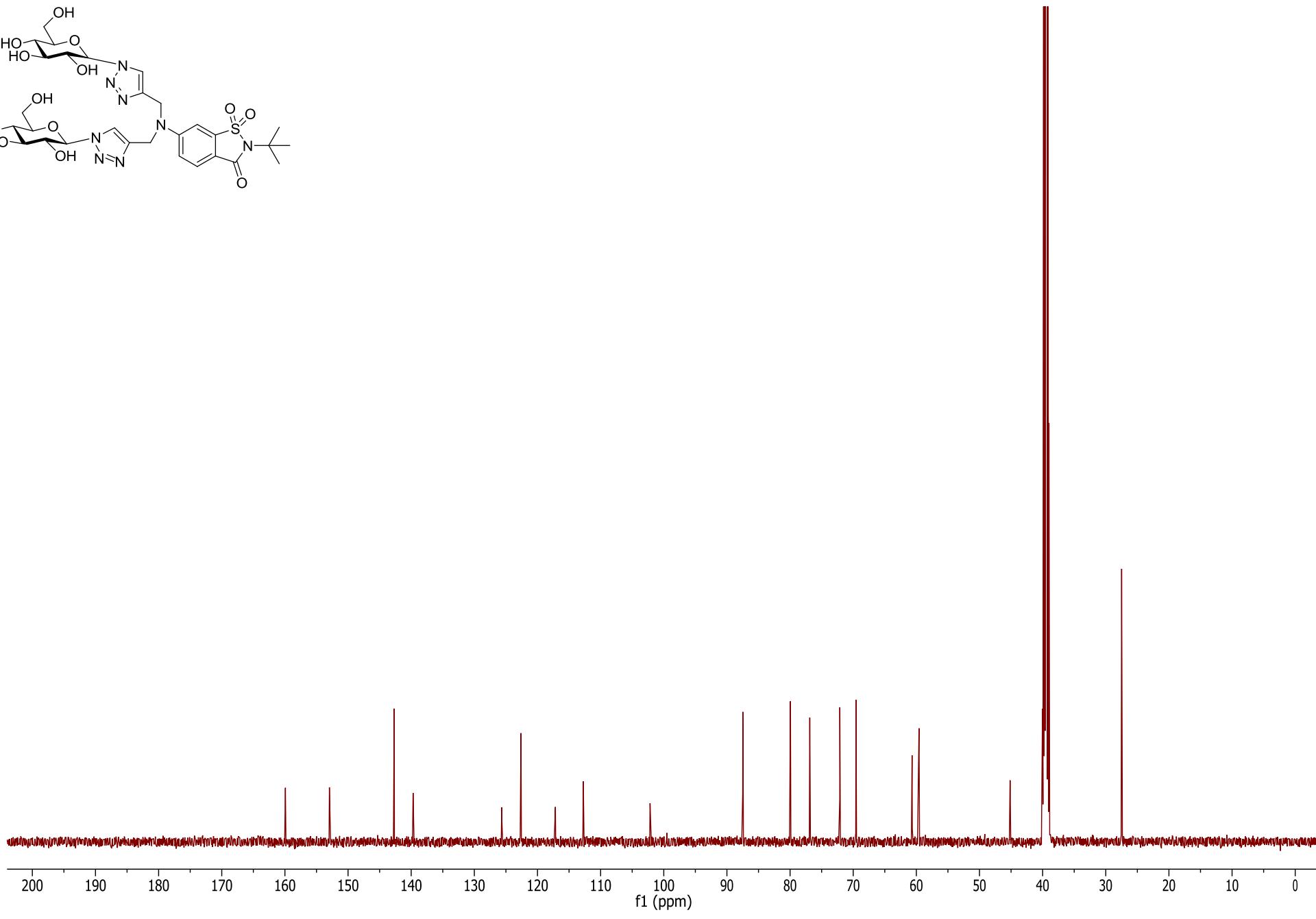
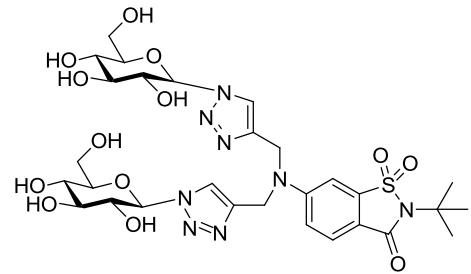
Compound 33 125 MHz ^{13}C NMR (CD_3SO)



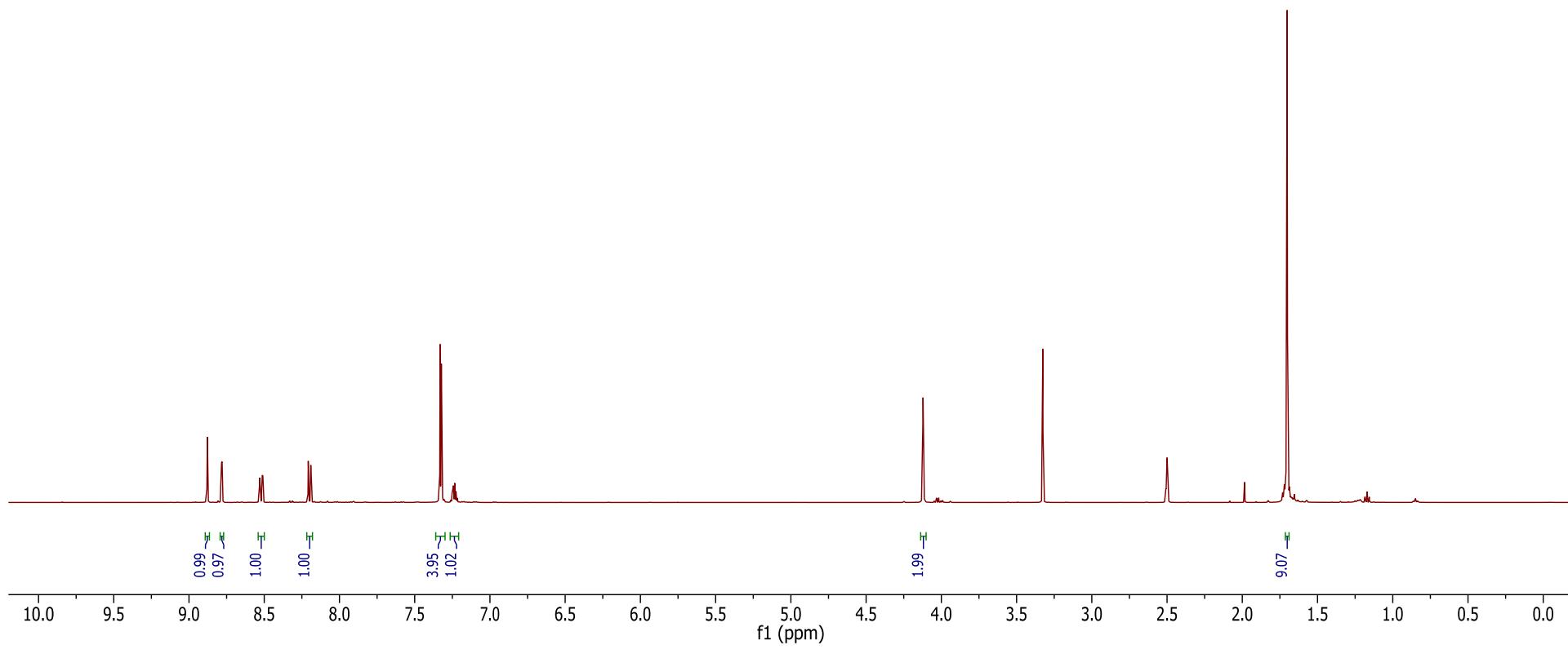
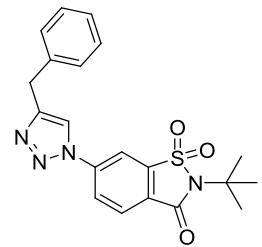
Compound 34 500 MHz ^1H NMR (CD_3SO)



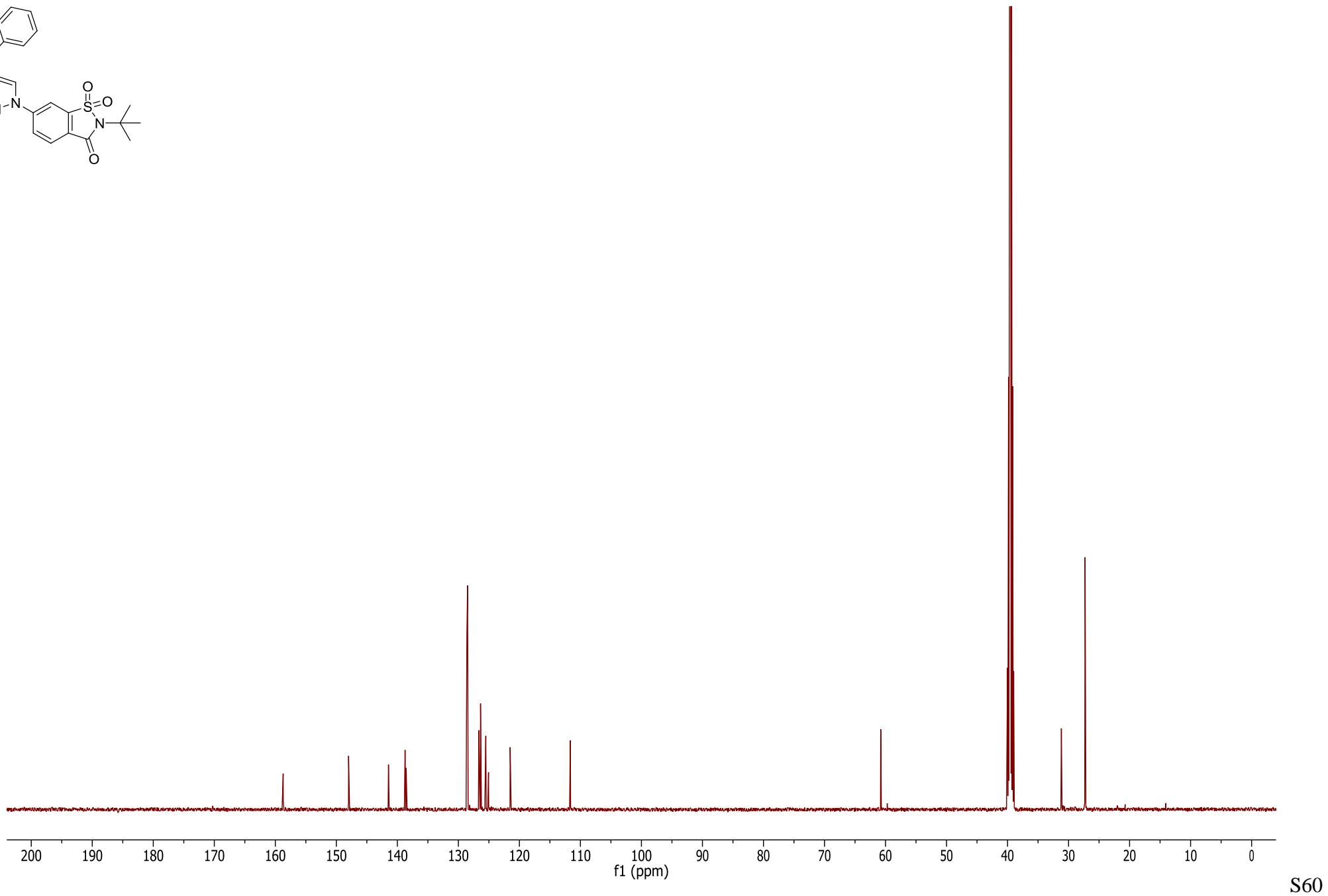
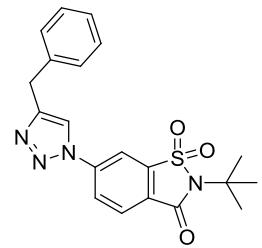
Compound 34 125 MHz ^{13}C NMR (CD_3SO)



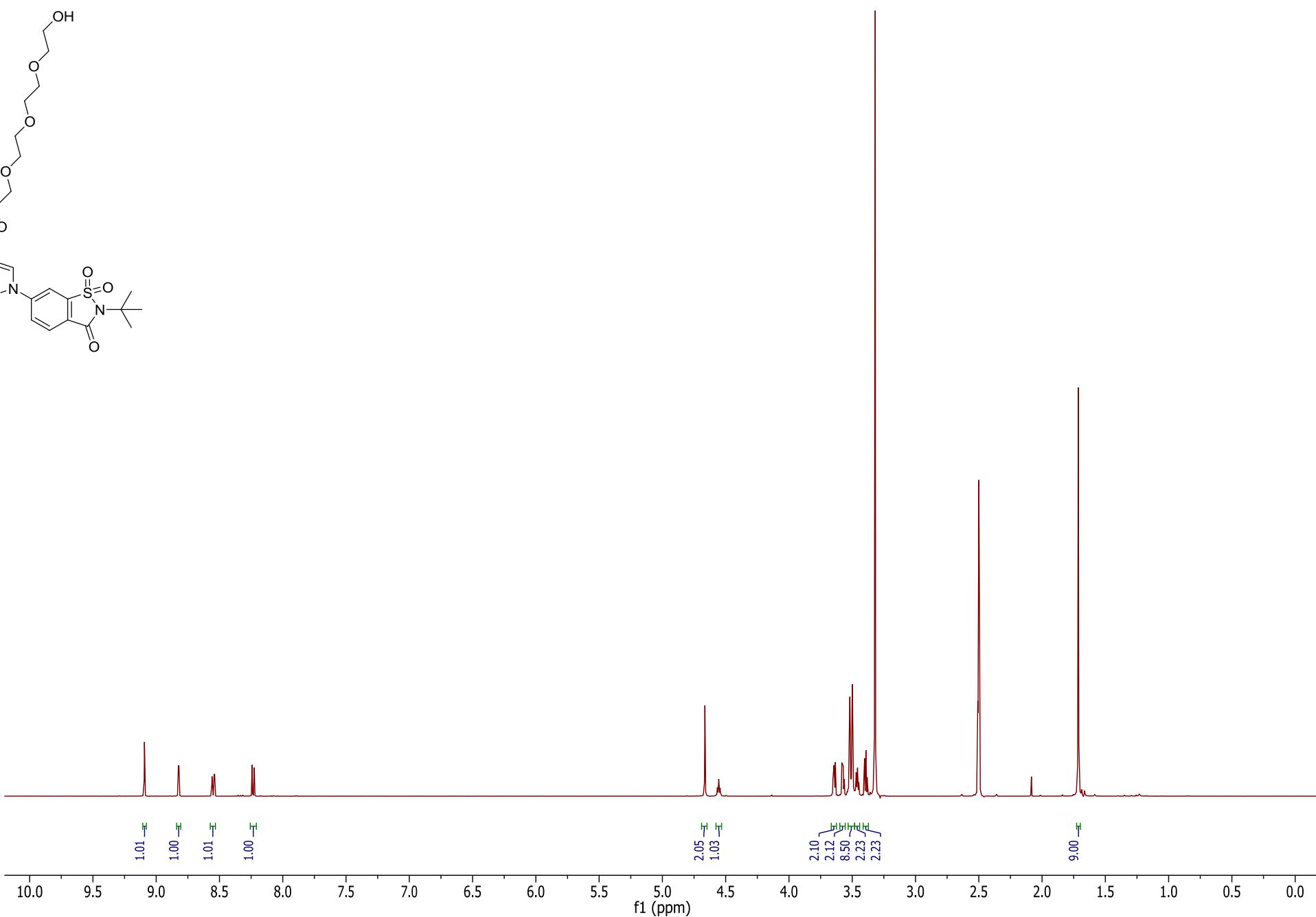
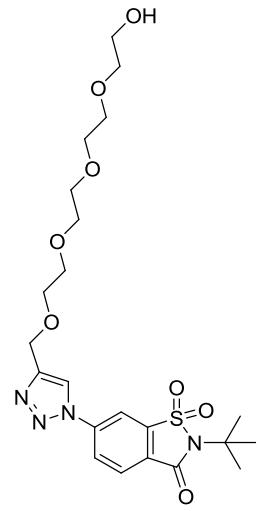
Compound 35 500 MHz ^1H NMR (CD_3SO)



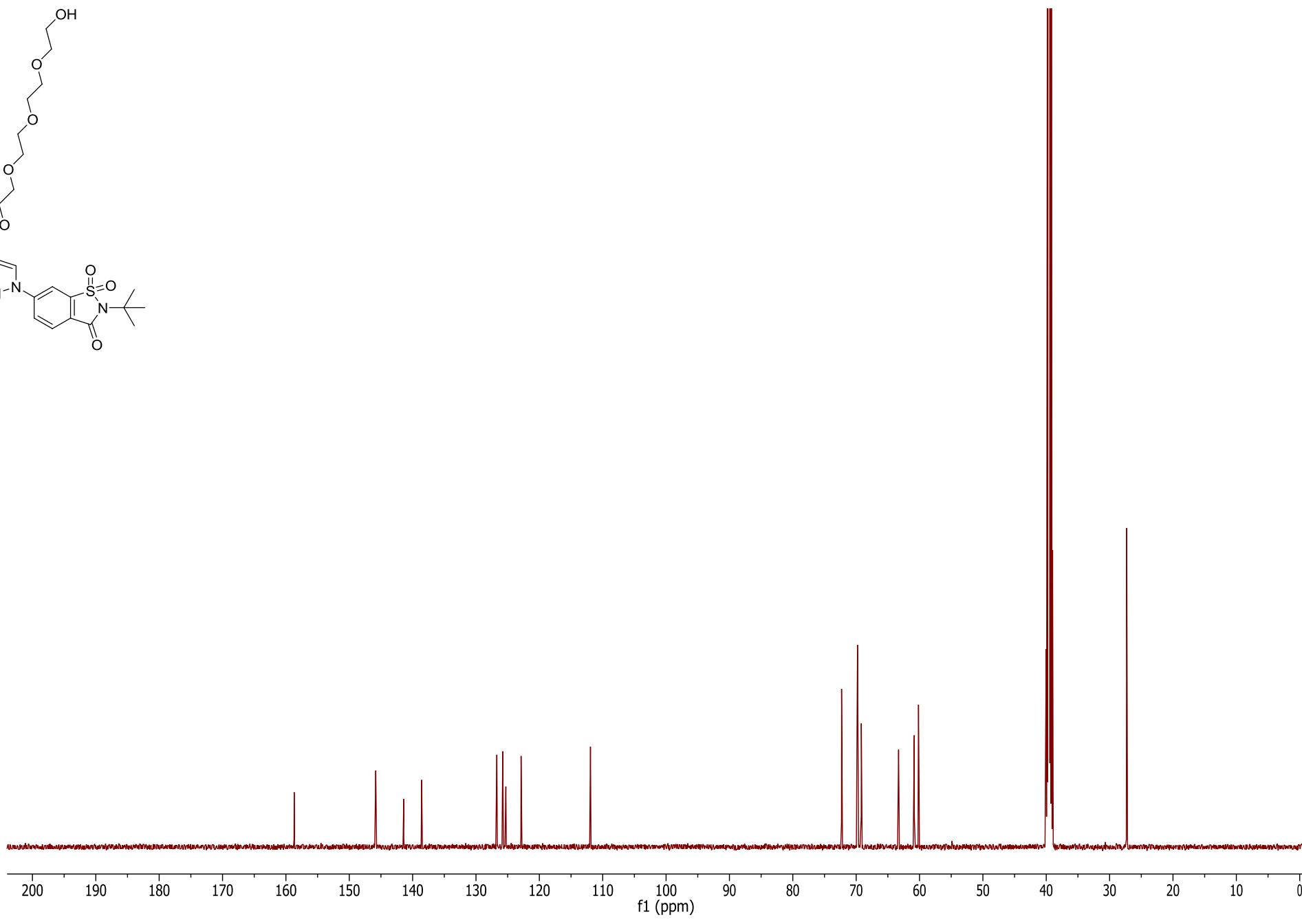
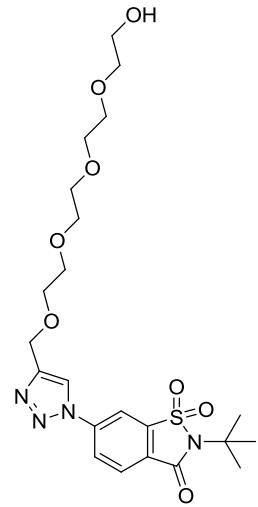
Compound 35 125 MHz ^{13}C NMR (CD_3SO_2)



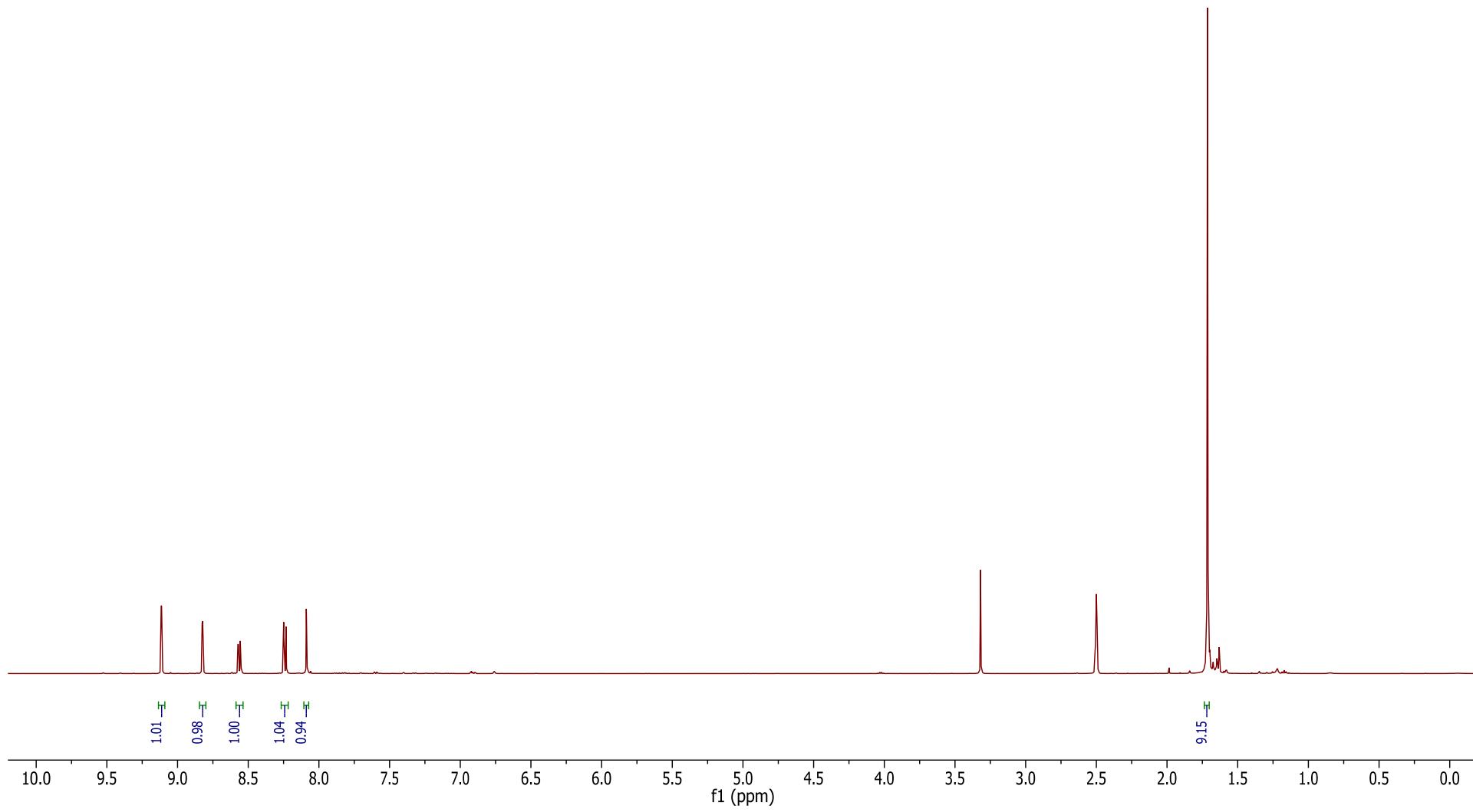
Compound 36 500 MHz ^1H NMR (CD_3SO)



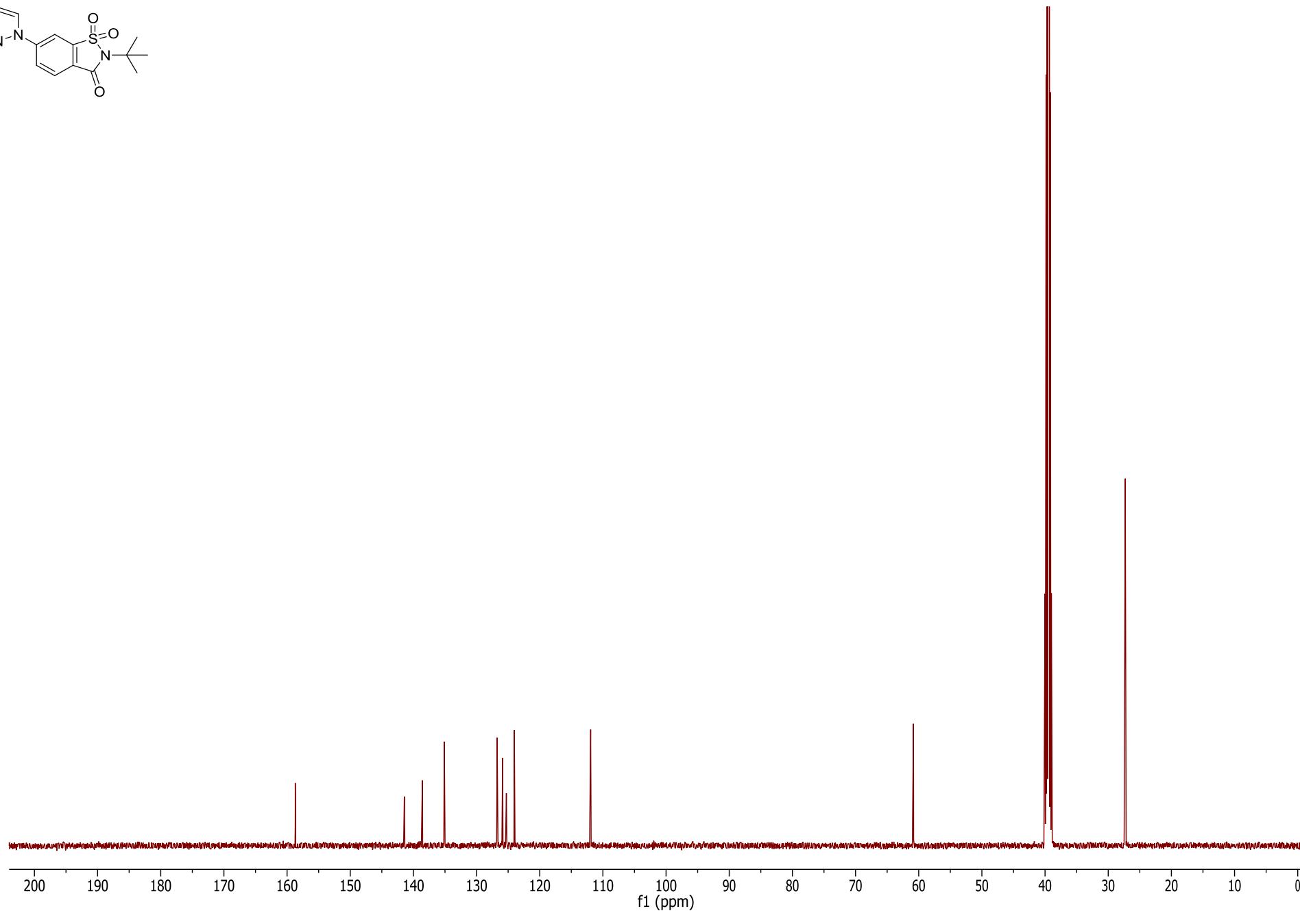
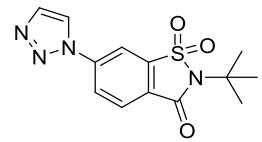
Compound 36 125 MHz ^{13}C NMR (CD_3SO_2)



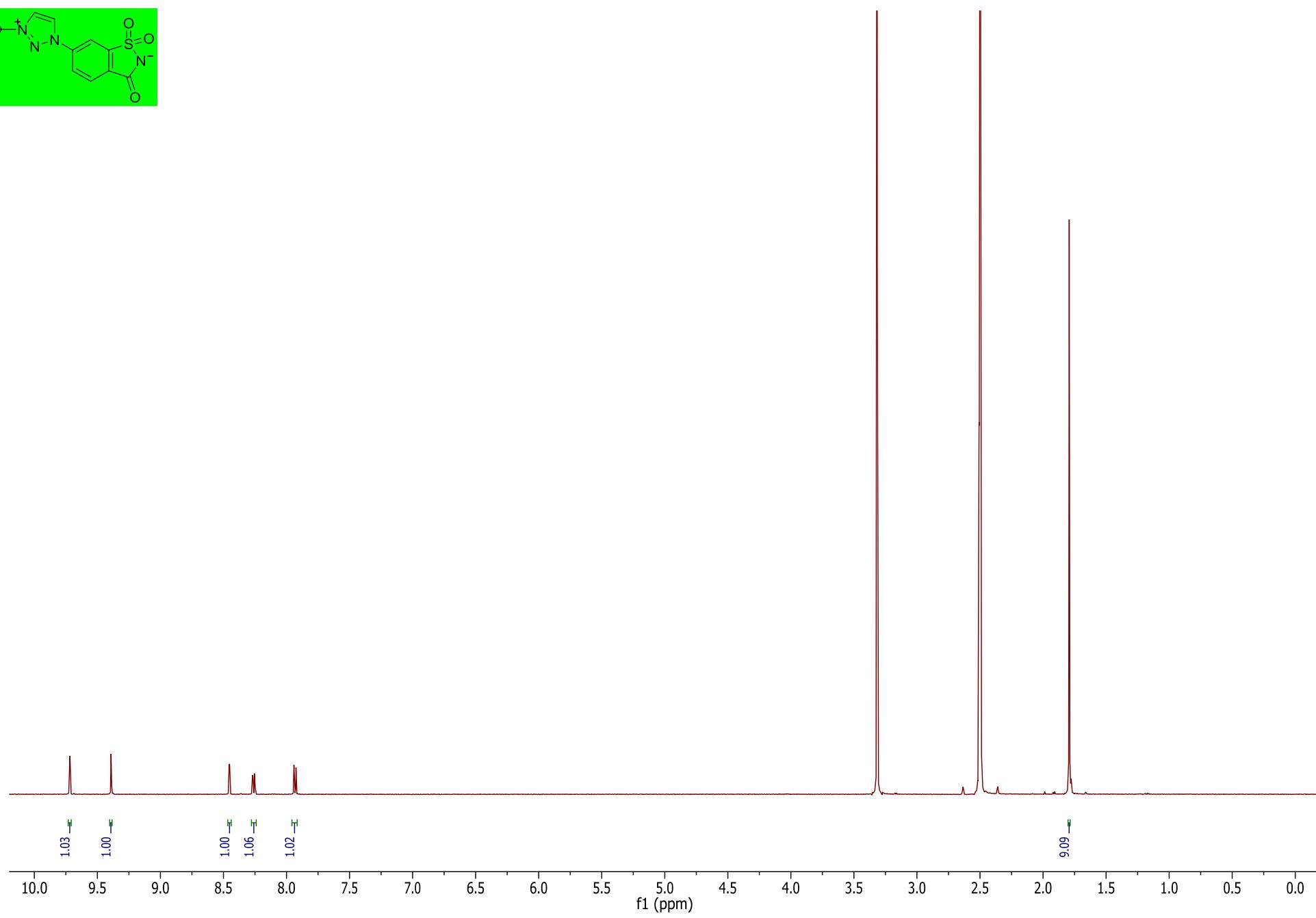
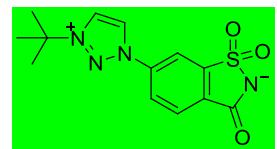
Compound 37 500 MHz ^1H NMR (CD_3SO)



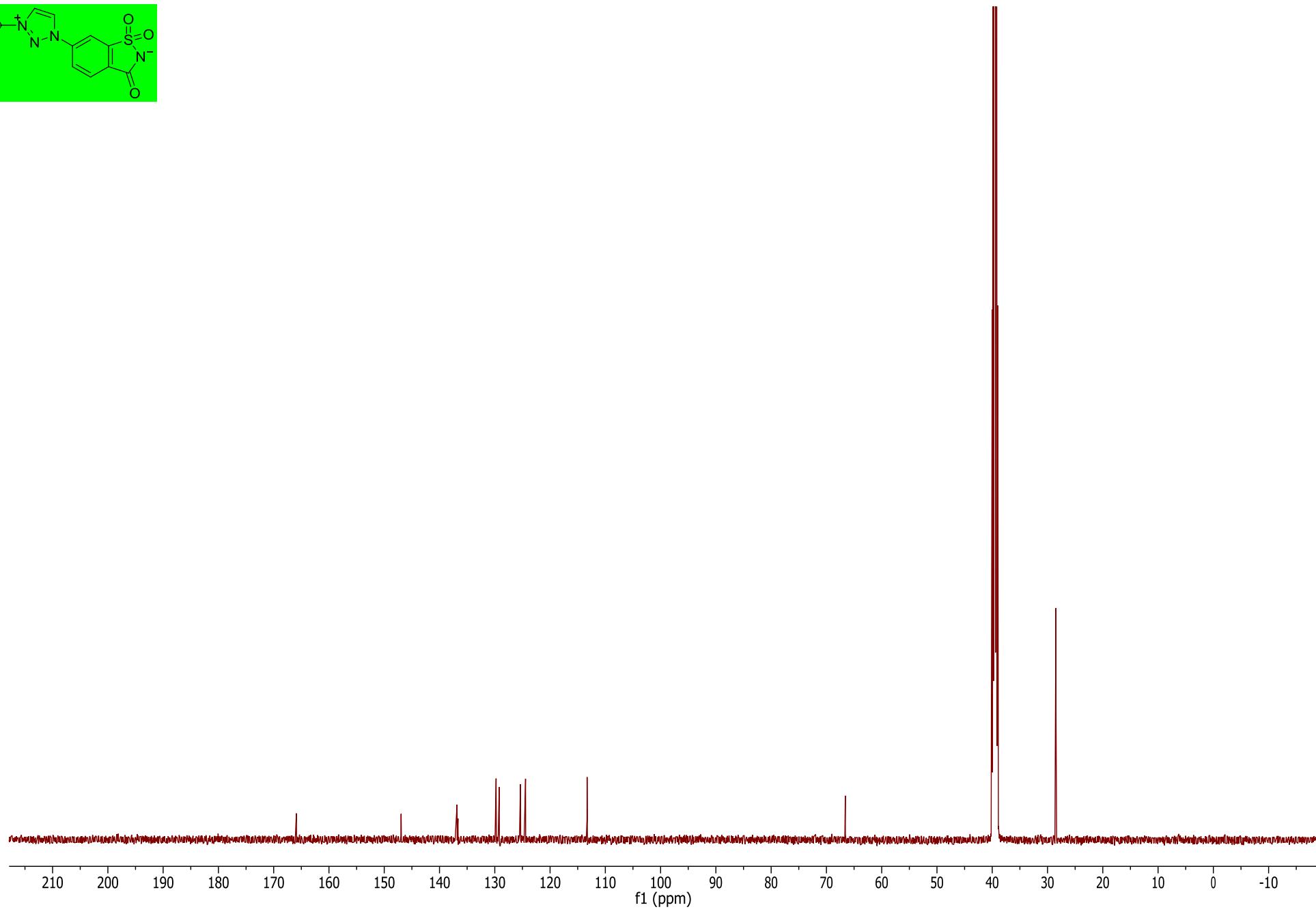
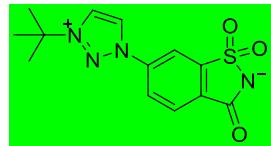
Compound 37 125 MHz ^{13}C NMR (CD_3SO_2)



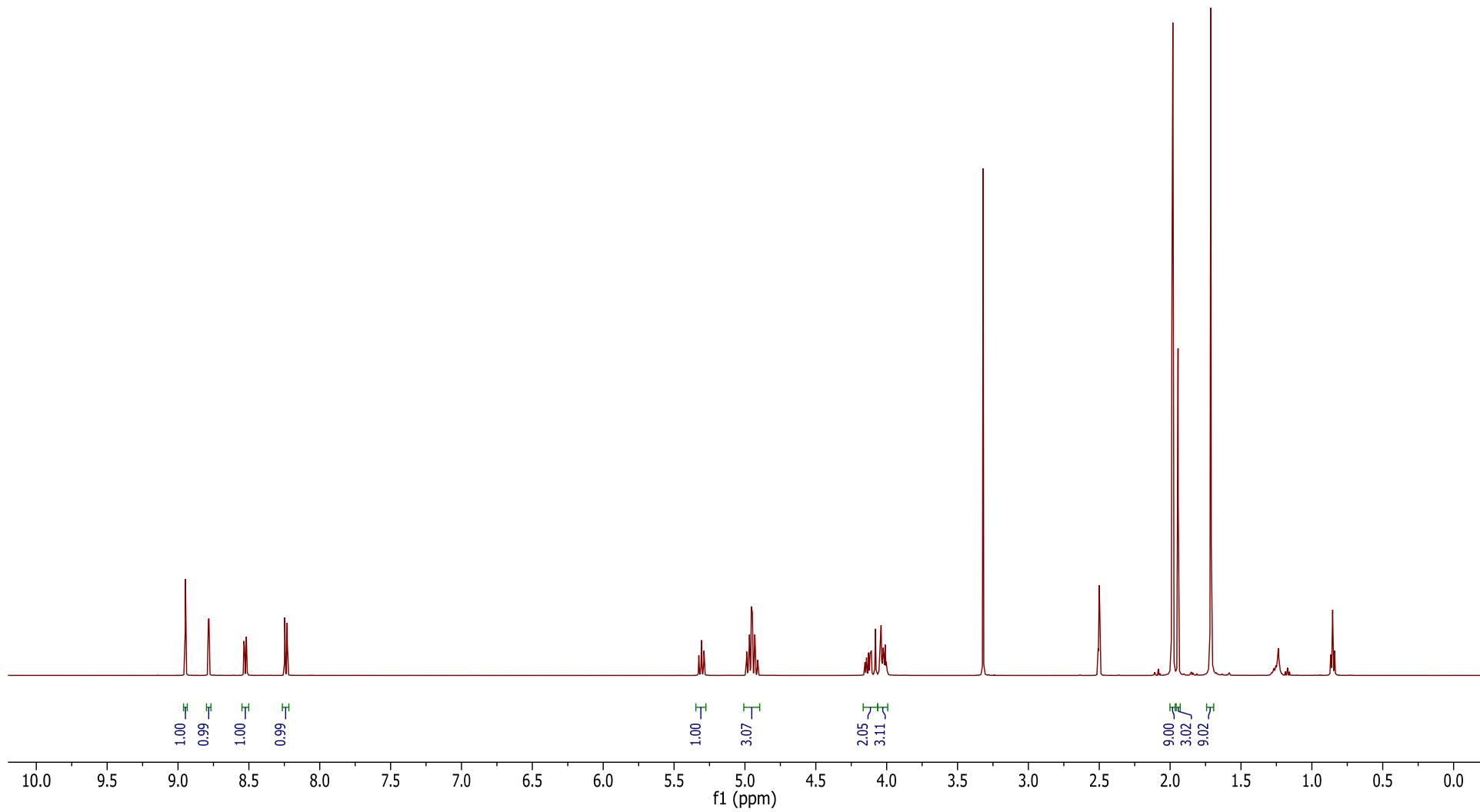
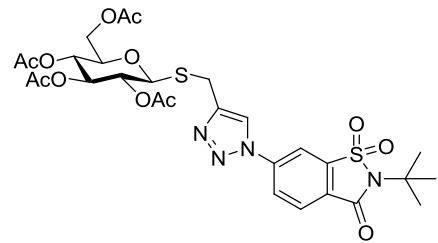
Compound 38 500 MHz ^1H NMR (CD_3SO)



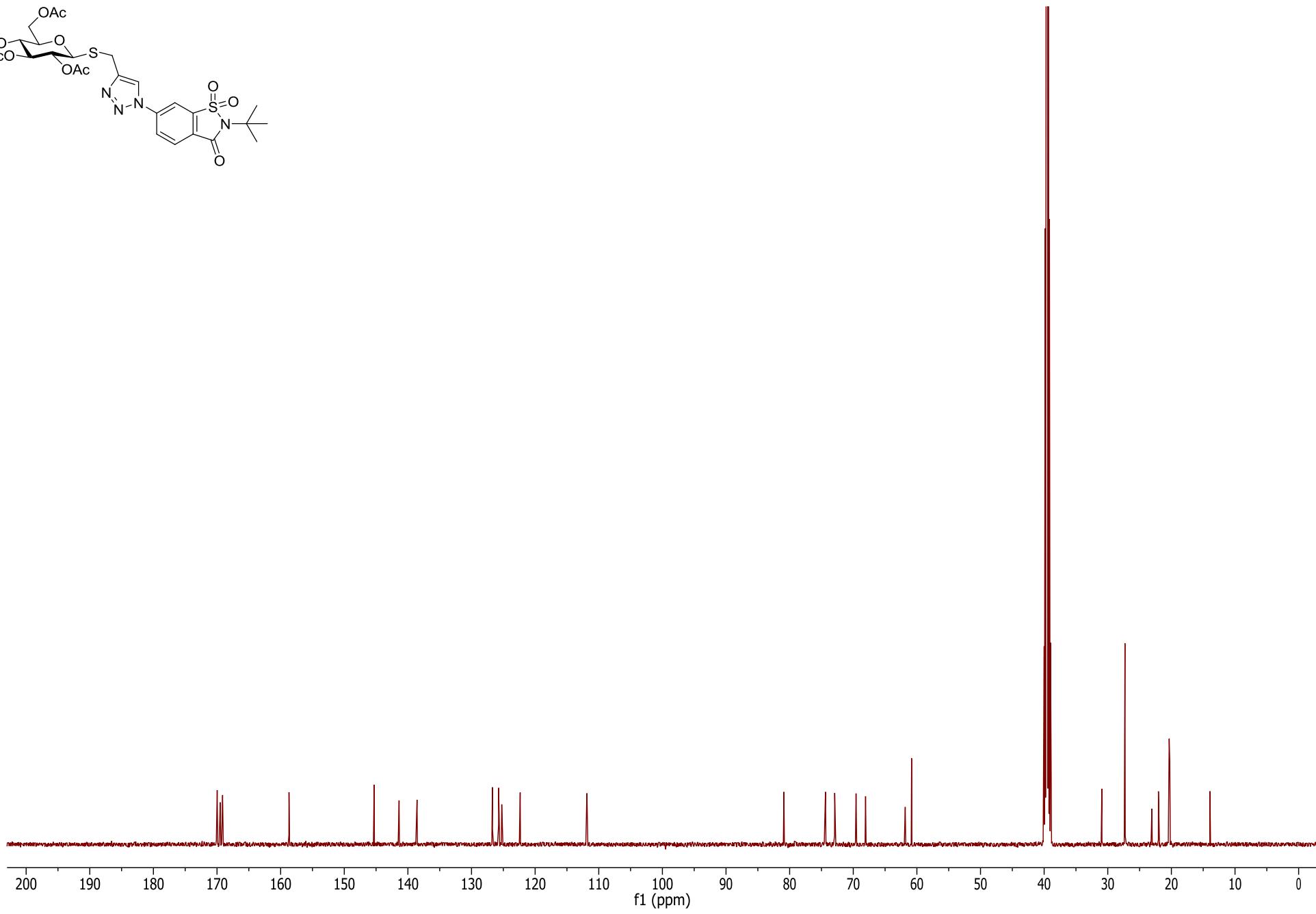
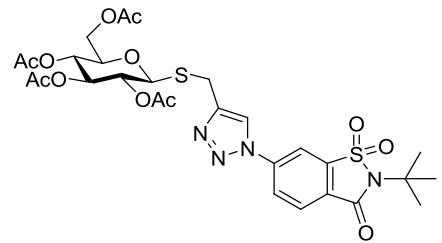
Compound **38** 125 MHz ^{13}C NMR (CD_3SO_2)



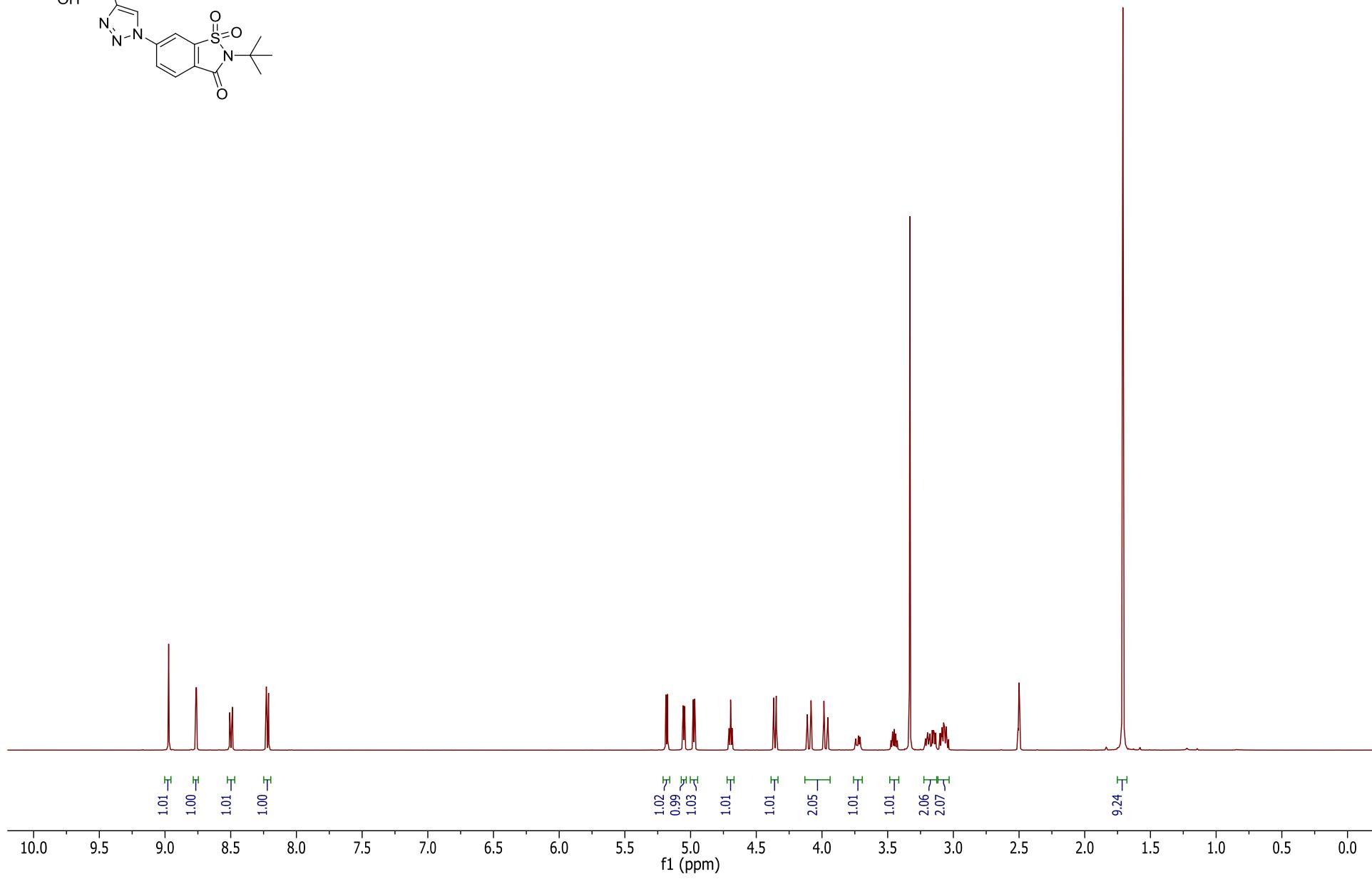
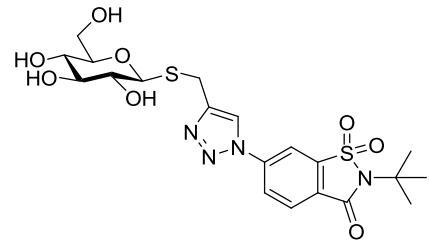
Compound 39 500 MHz ^1H NMR (CD_3SO)



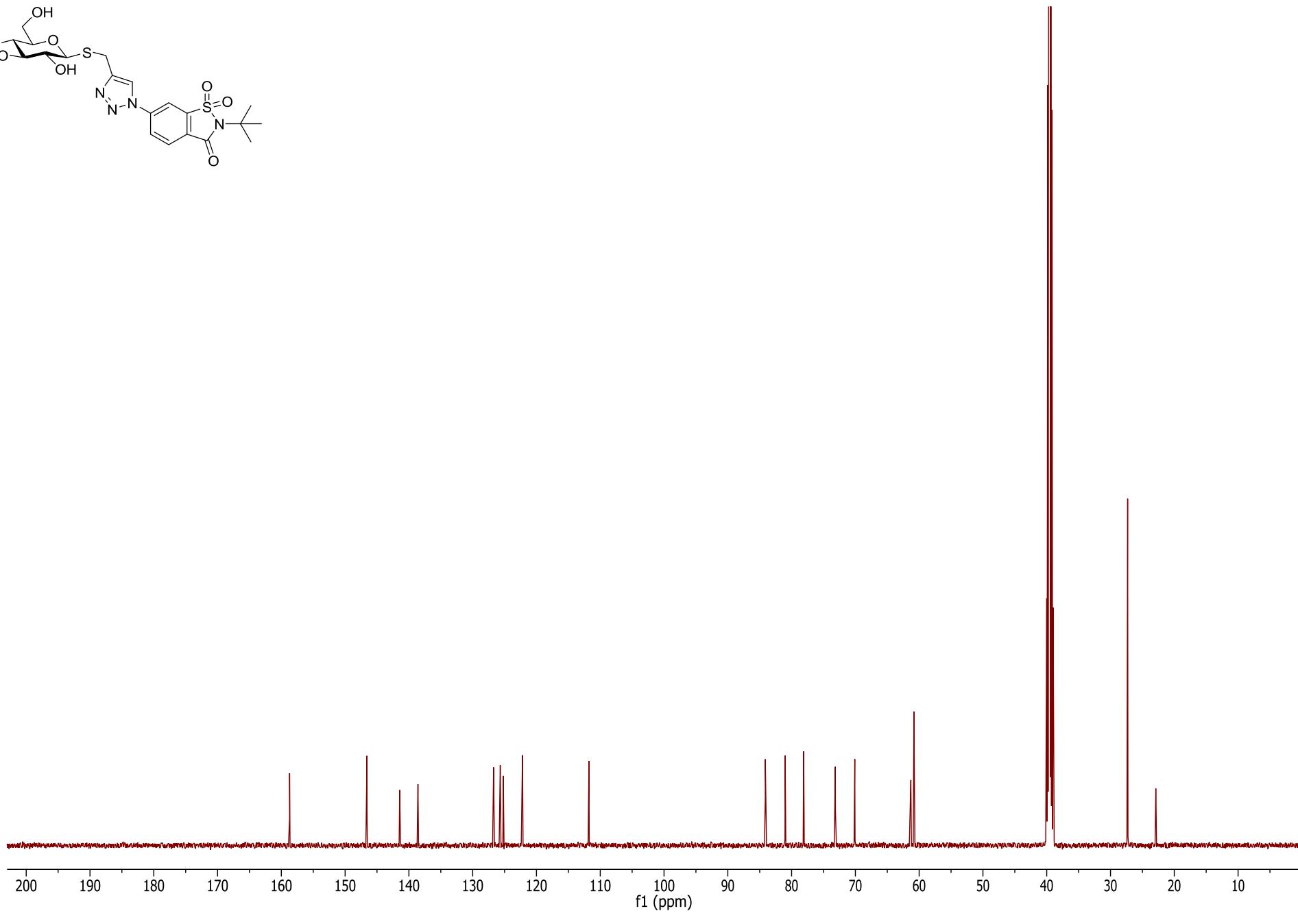
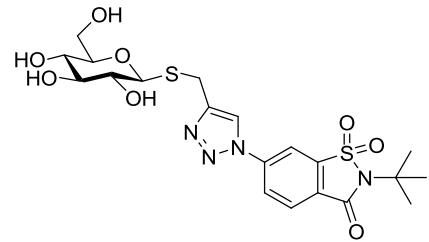
Compound 39 125 MHz ^{13}C NMR (CD_3SO_2)



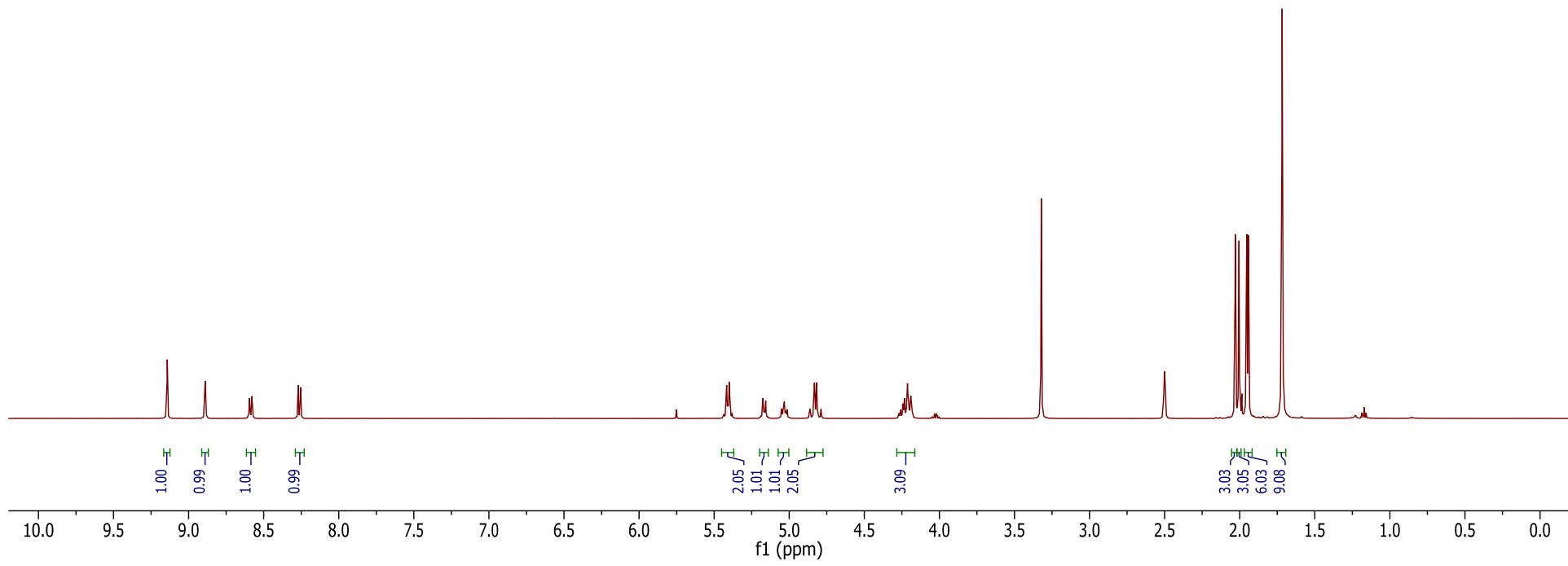
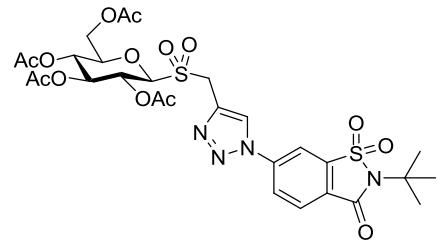
Compound **40** 500 MHz ^1H NMR (CD_3SO)



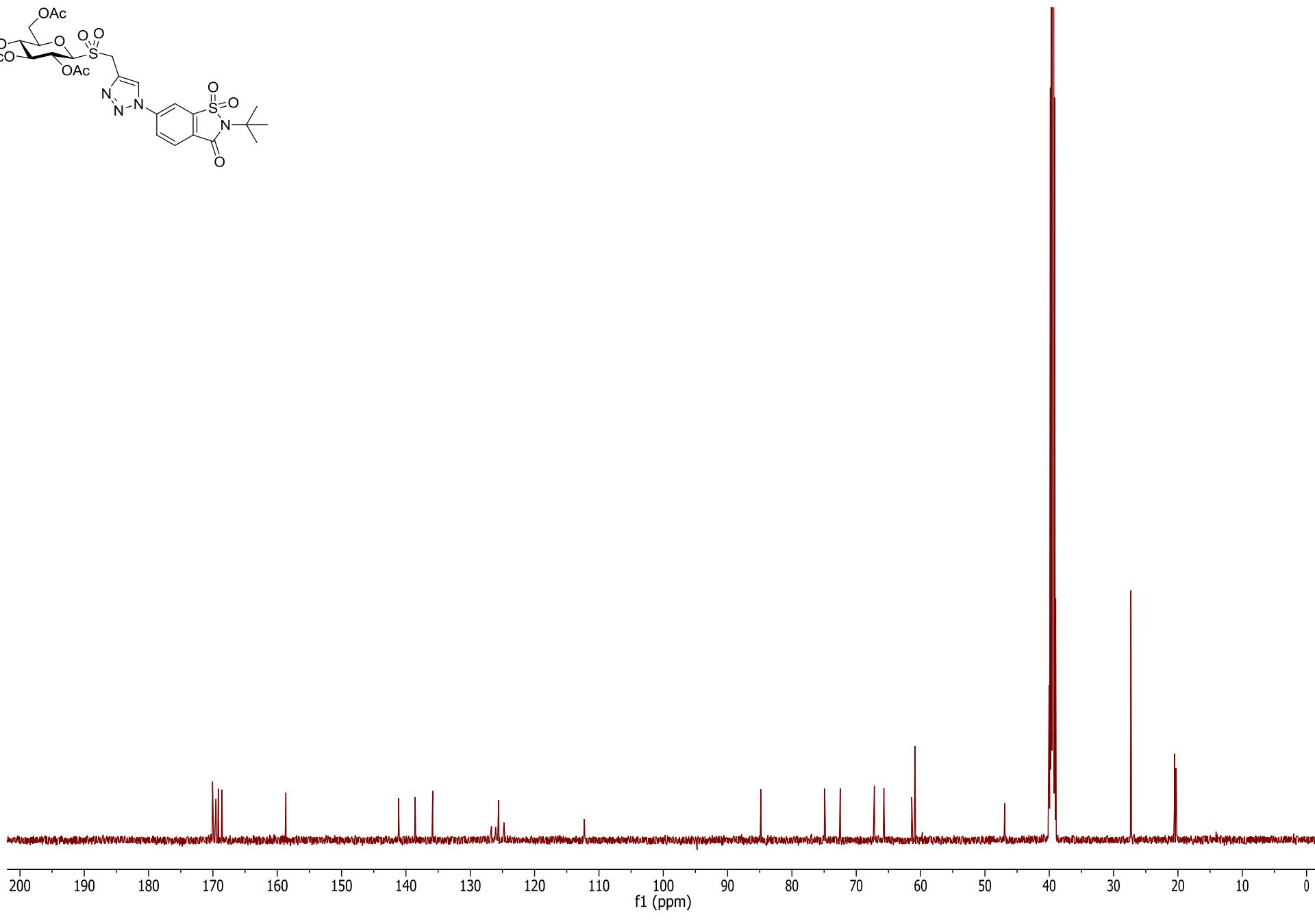
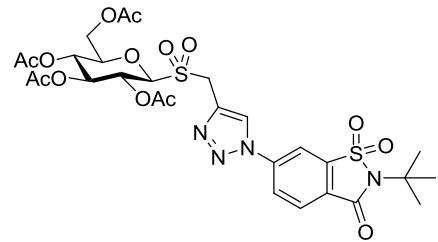
Compound **40** 125 MHz ^{13}C NMR (CD_3SO)



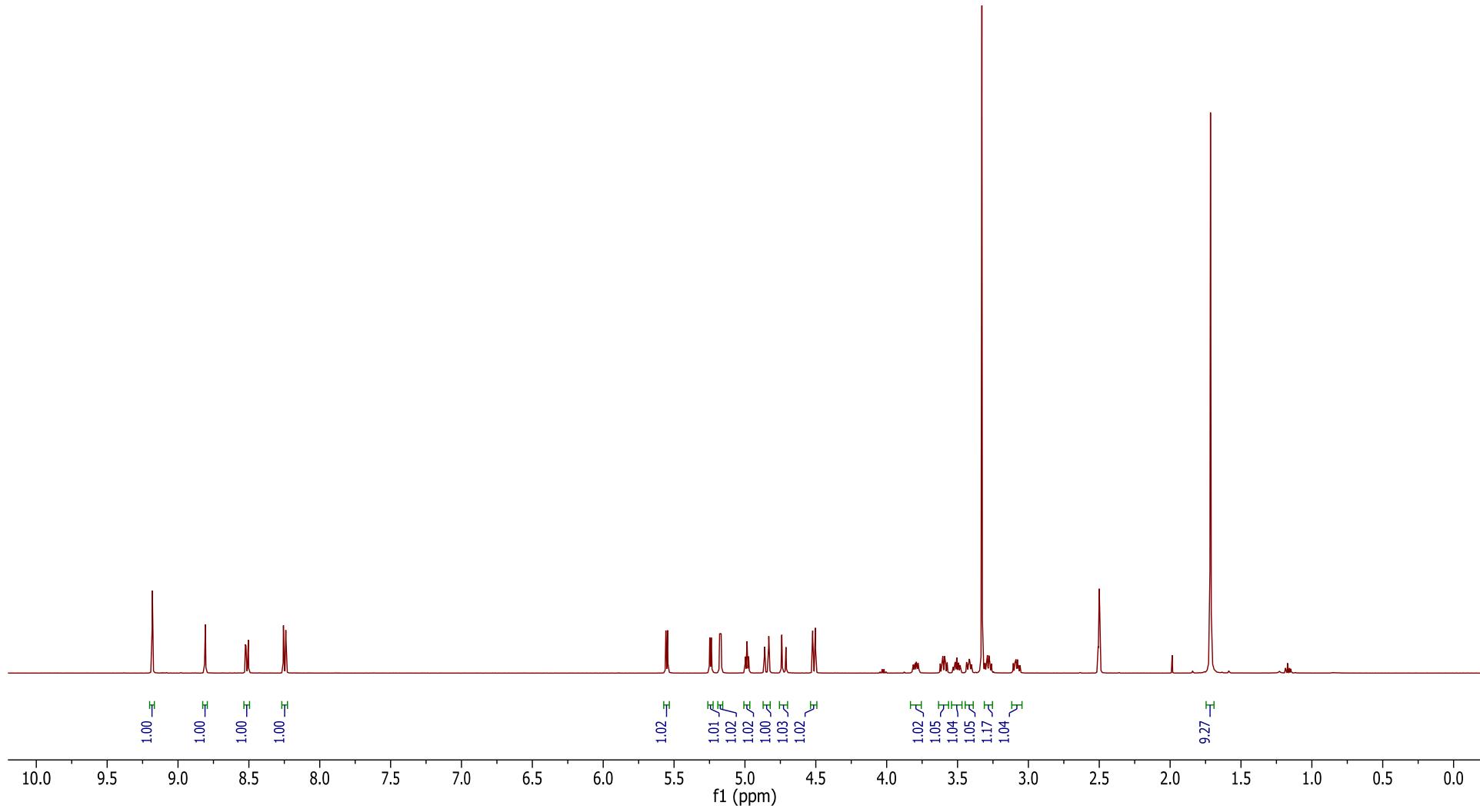
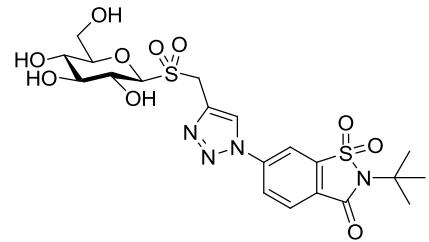
Compound 41 500 MHz ^1H NMR (CD_3SO)



Compound 41 125 MHz ^{13}C NMR (CD_3SO_2)



Compound 42 500 MHz ^1H NMR (CD_3SO)



Compound 42 125 MHz ^{13}C NMR (CD_3SO)

