Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information
For

Synthesis of indenofurans, benzofurans and spiro-lactones *via* Hauser-Kraus annulation involving 1,6-addition of phthalide to quinone methides

Pallabita Basu, Nishikant Satam and Irishi N. N. Namboothiri*

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400 076, INDIA
irishi@iitb.ac.in

Table of Contents

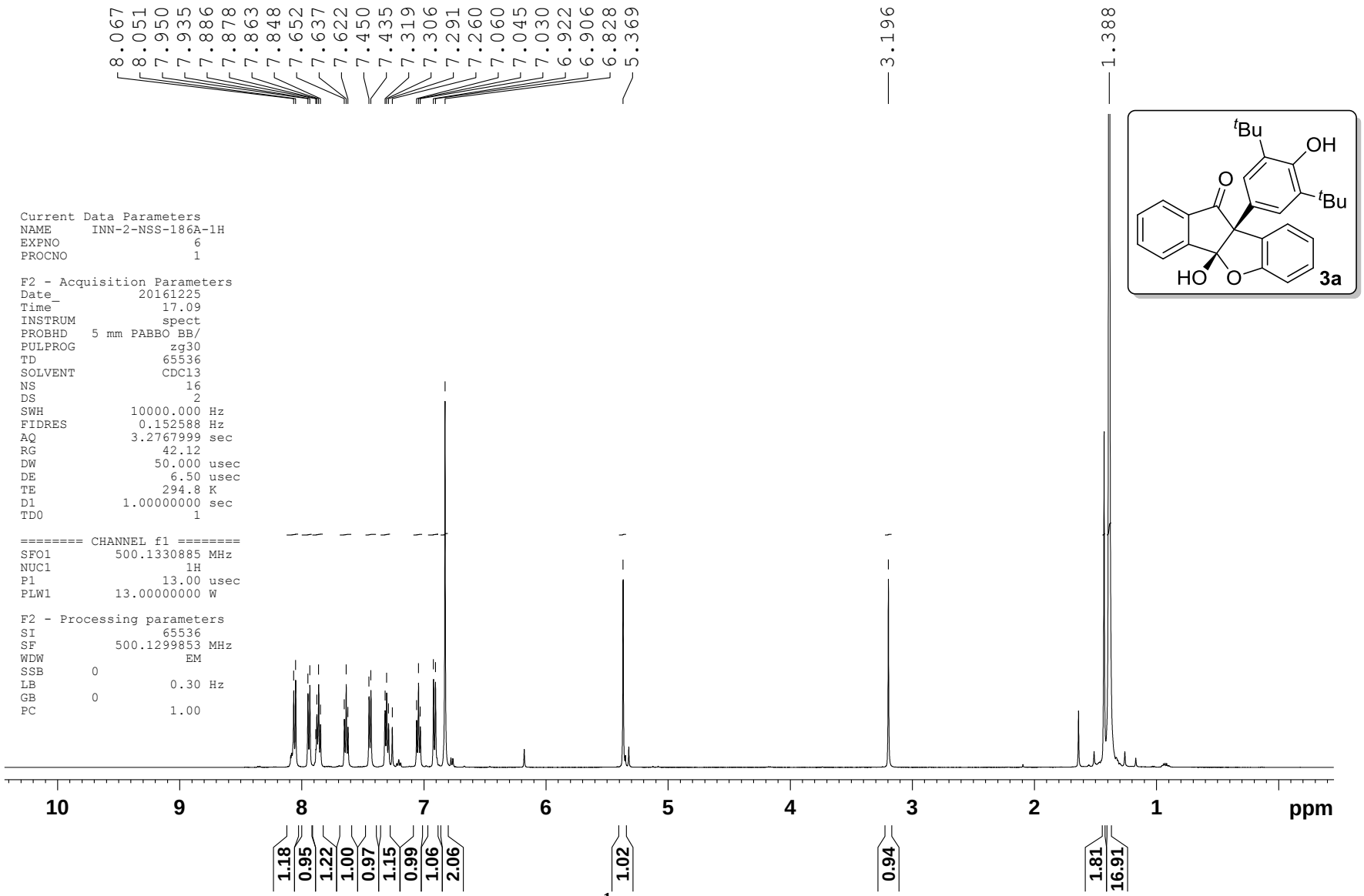


Figure S01. ^{1}H NMR Spectrum of 3a

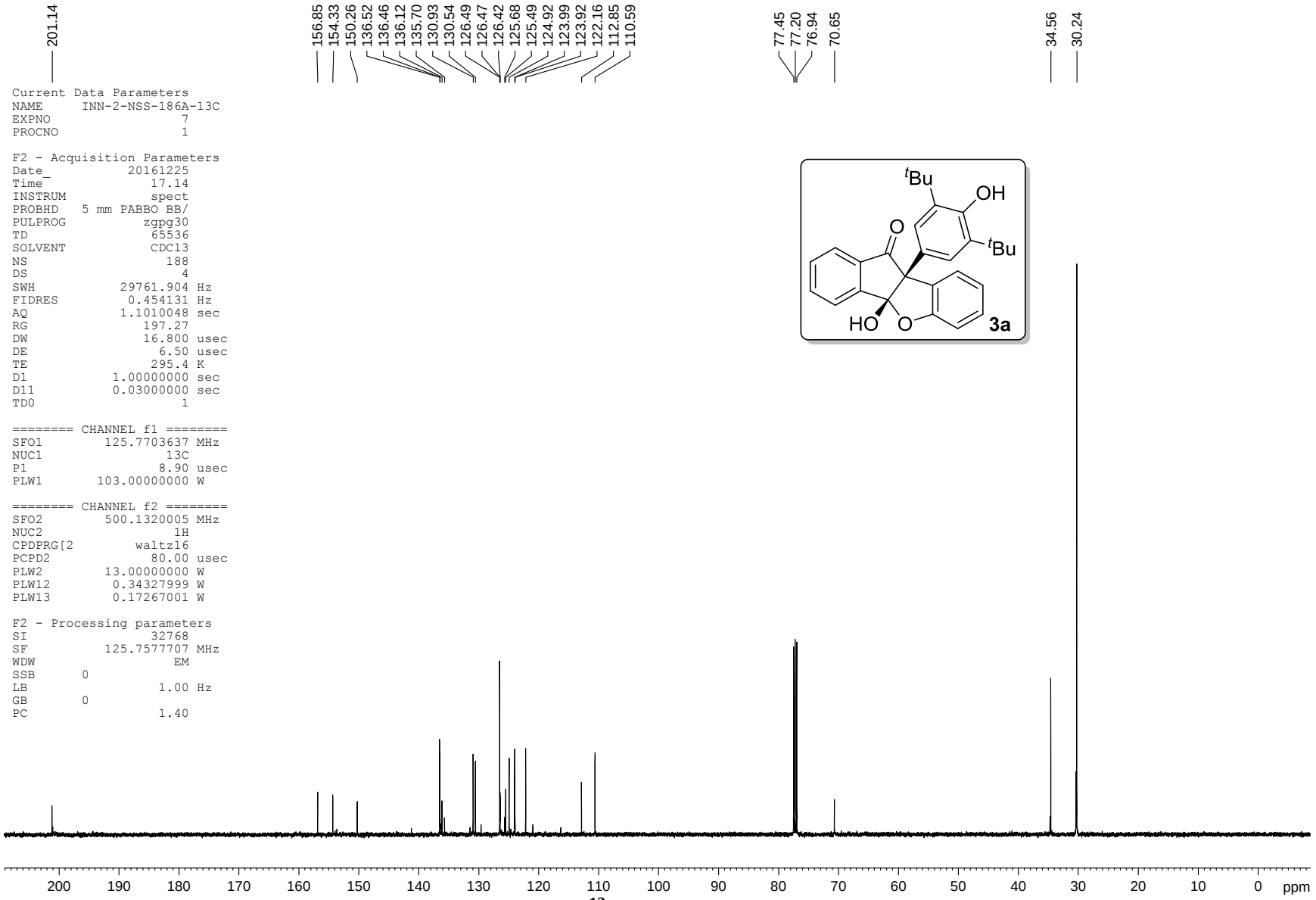


Figure S02. ^{13}C NMR Spectrum of 3a

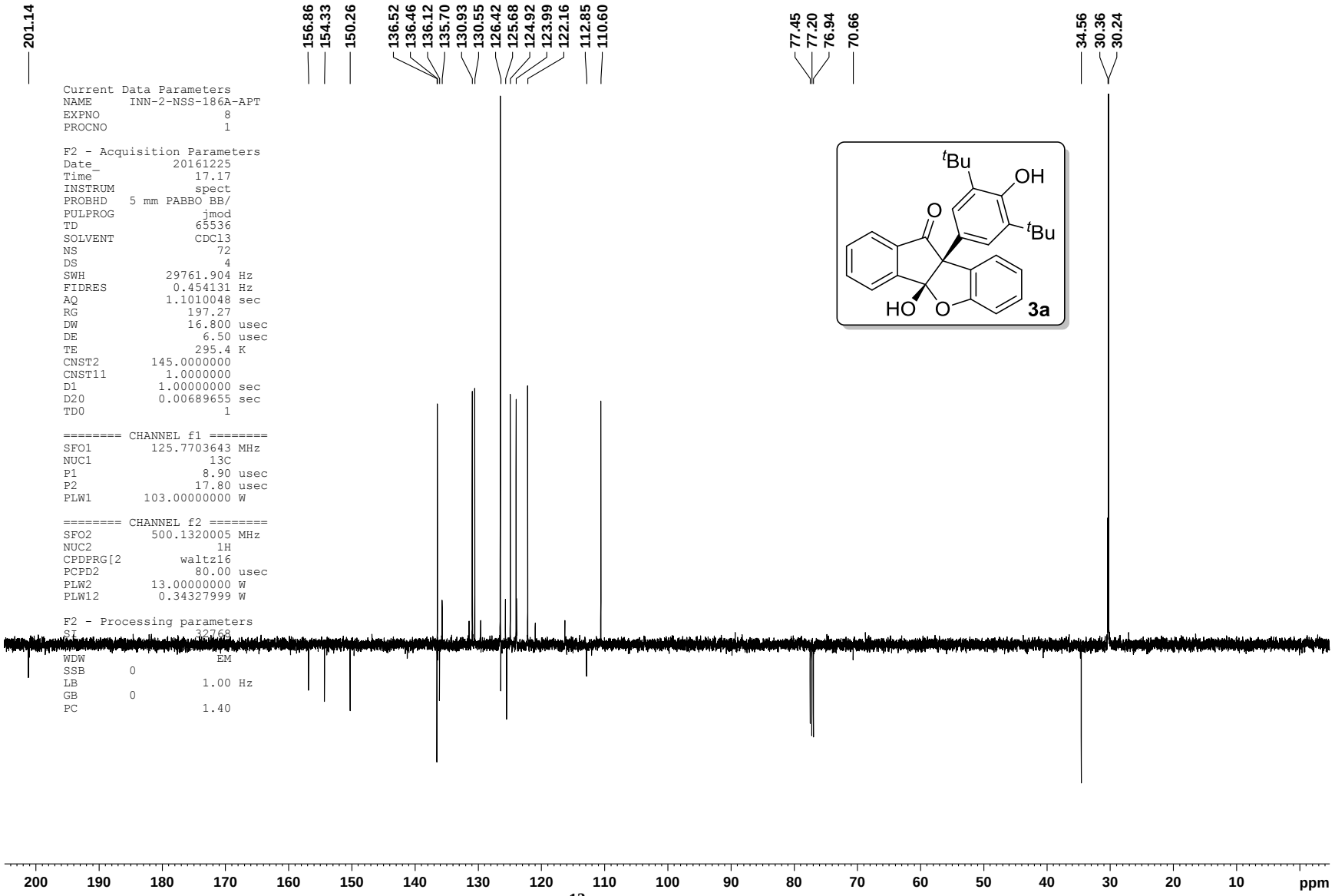


Figure S03. ^{13}C-APT NMR Spectrum of 3a

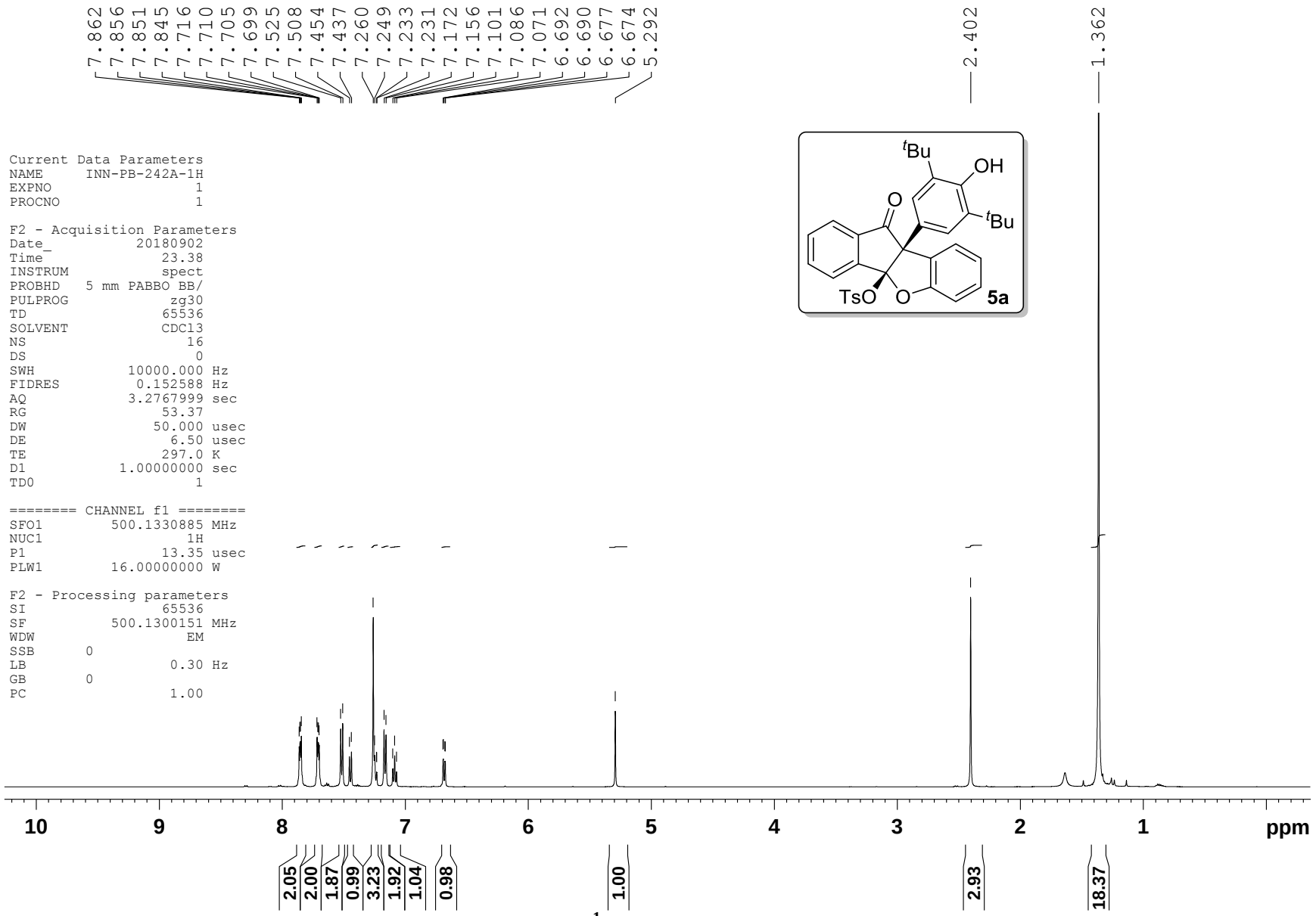


Figure S04. ^{1}H NMR Spectrum of 5a

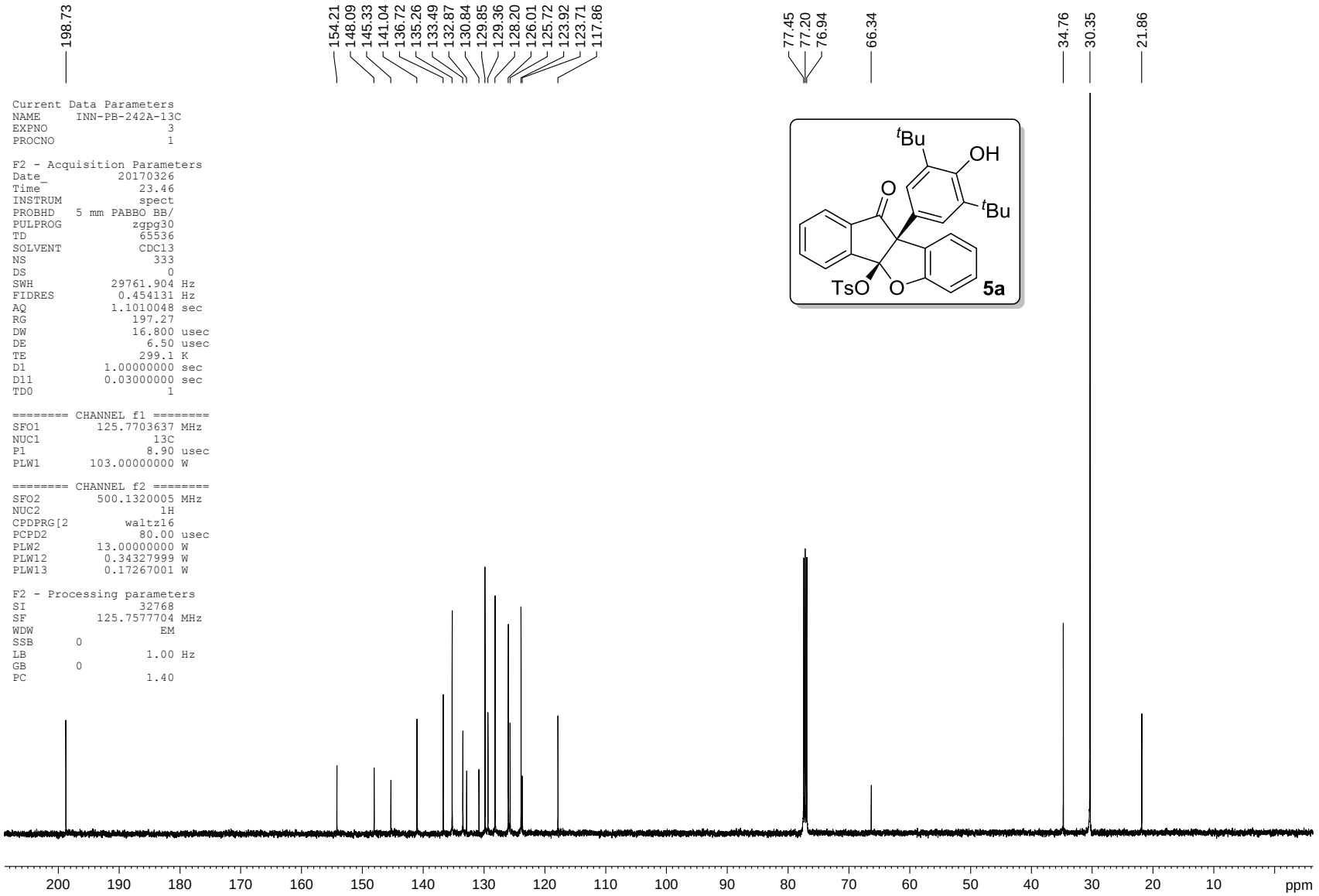


Figure S05. ^{13}C NMR Spectrum of 5a

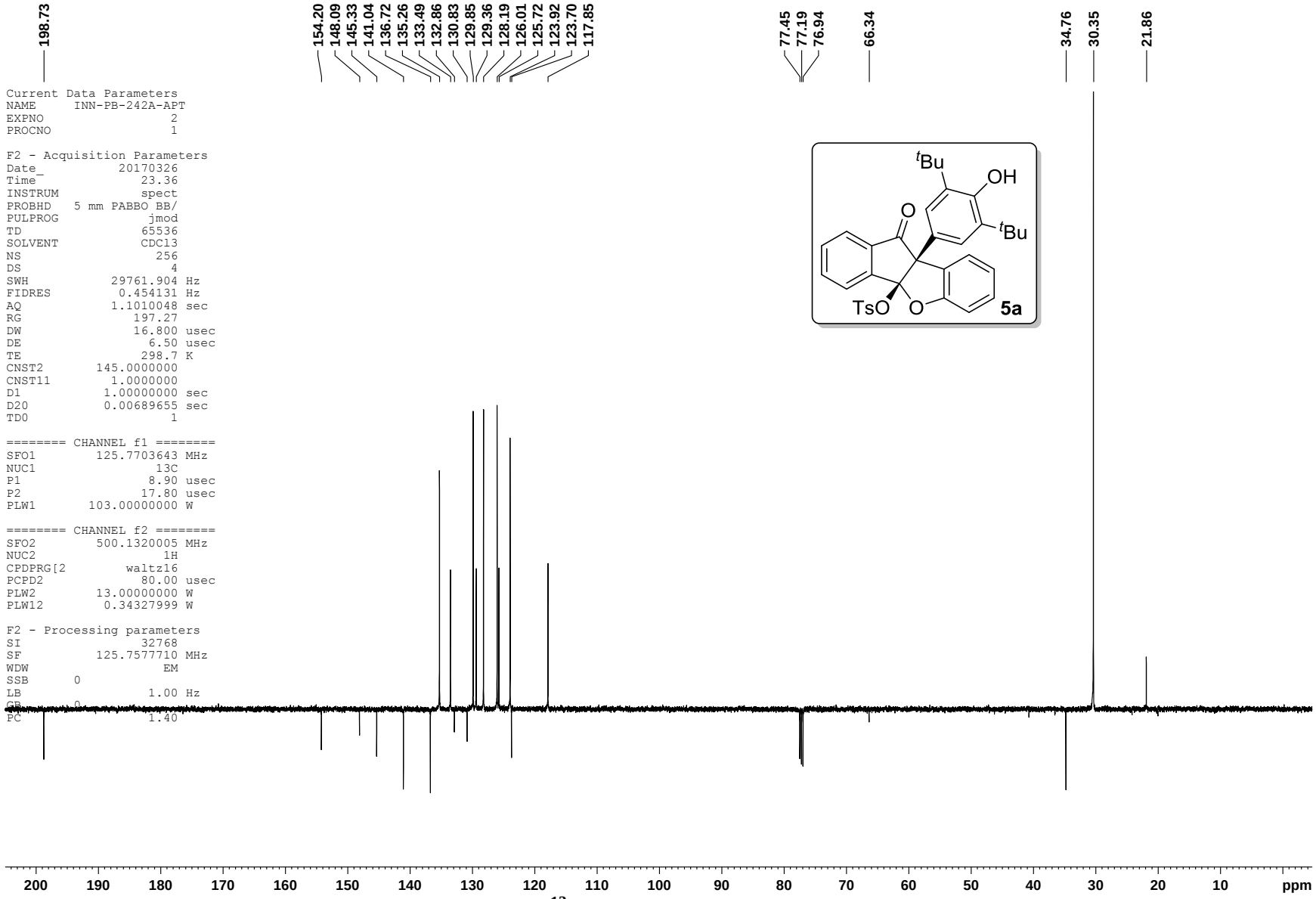


Figure S06. ^{13}C-APT NMR Spectrum of 5a

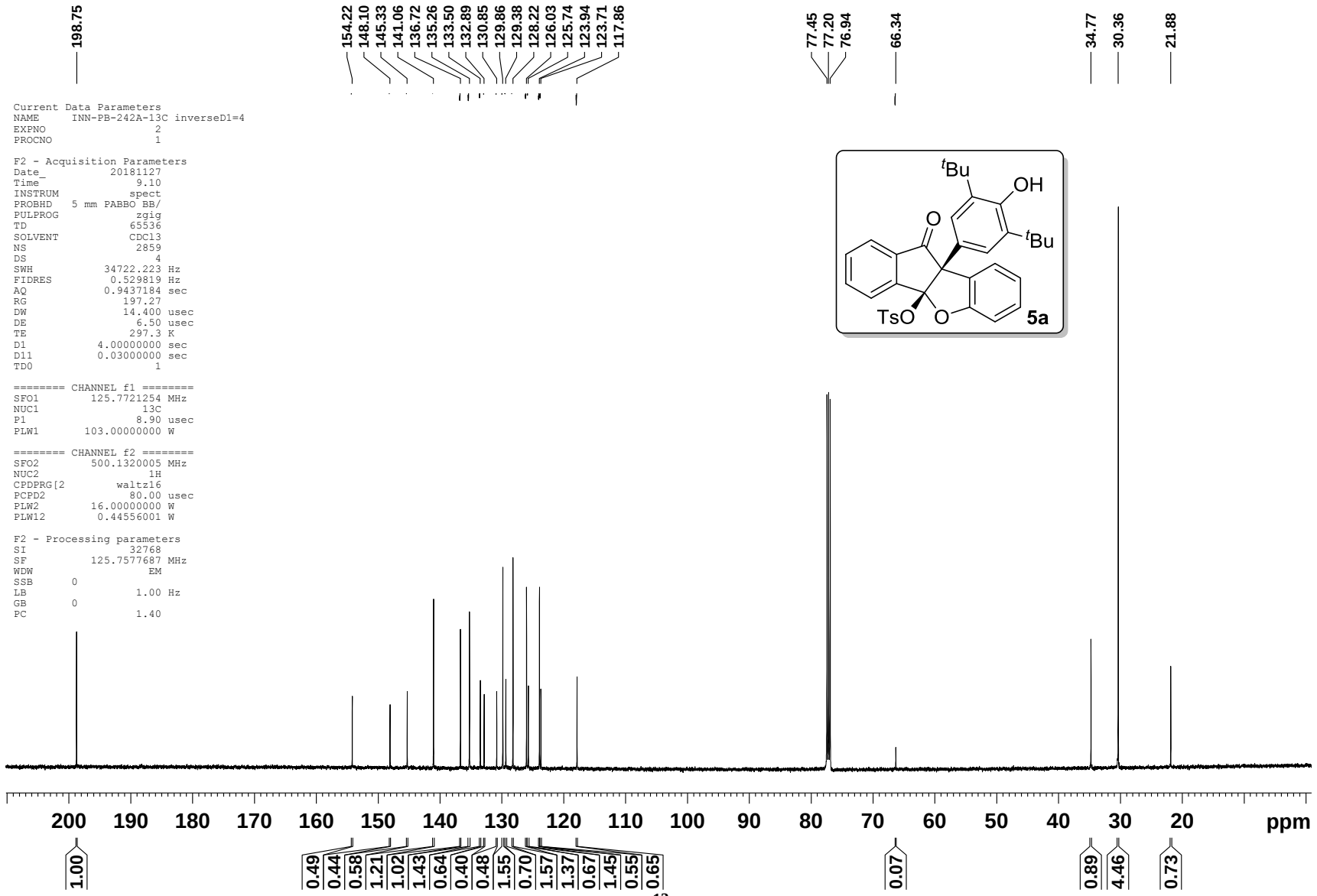


Figure S07. Inverse Gated ^{13}C NMR Spectrum of 5a

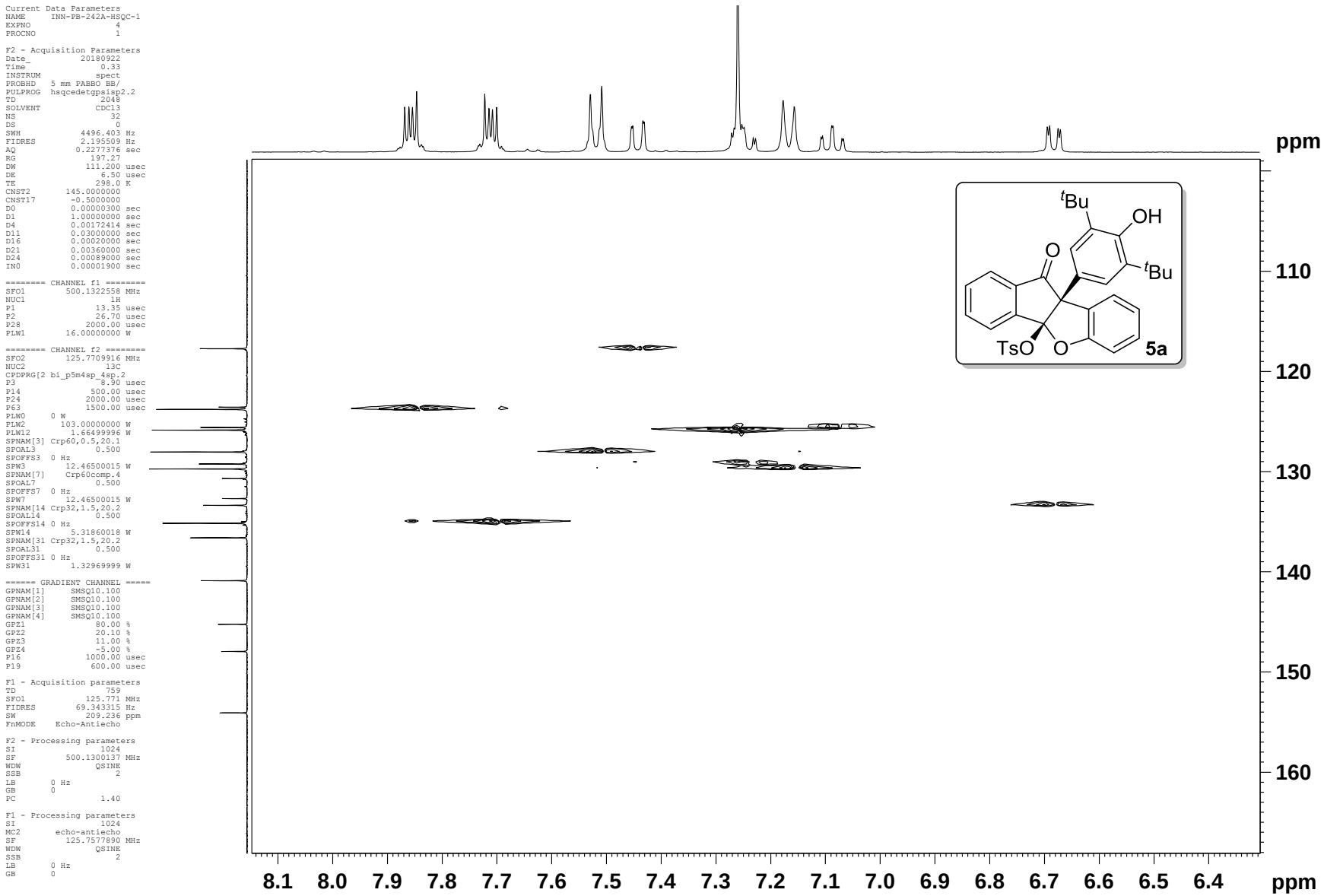


Figure S08. ^{1}H-^{13}C HSQC NMR Spectrum of 5a

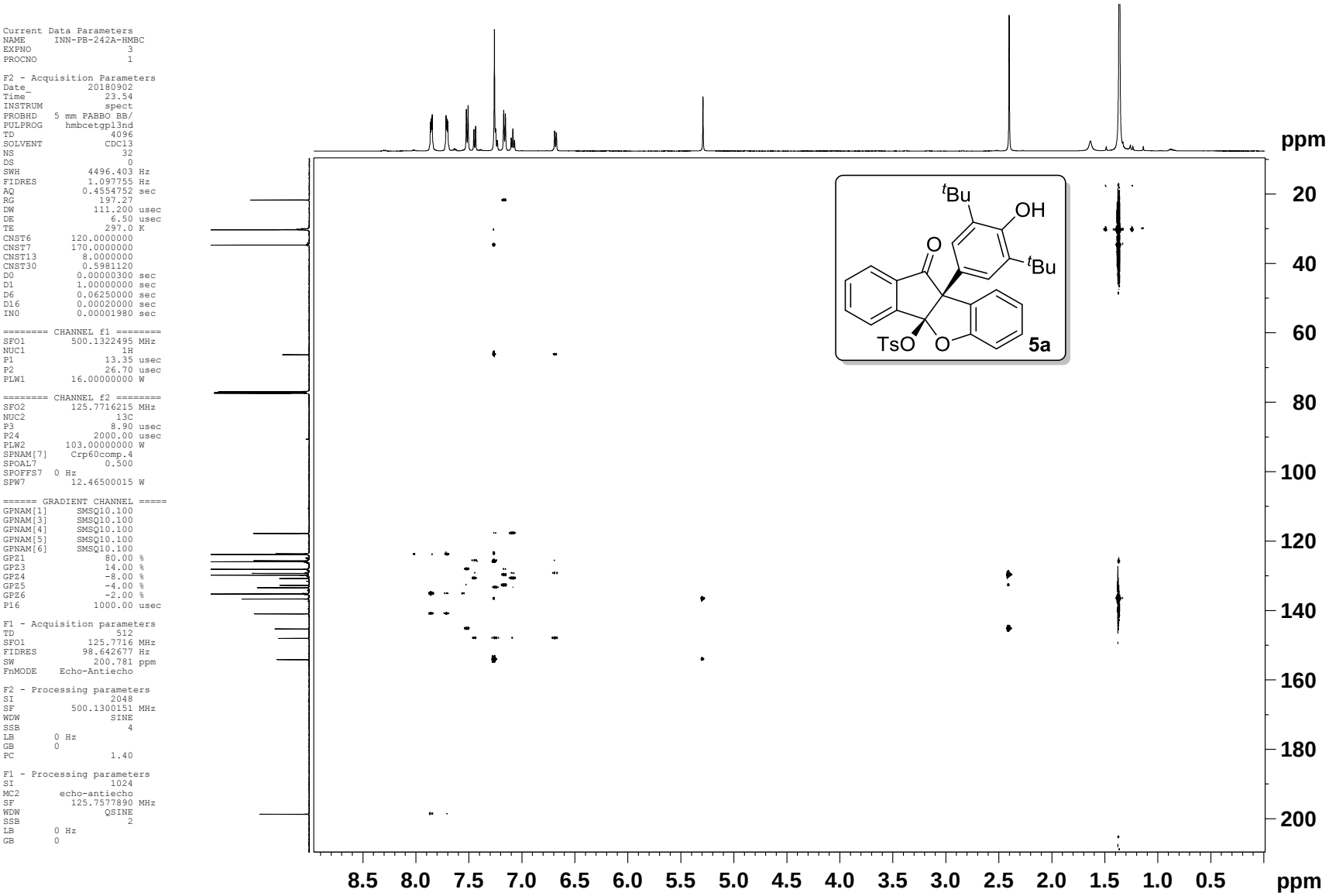


Figure S09. ^{1}H-^{13}C HMBC NMR Spectrum of 5a

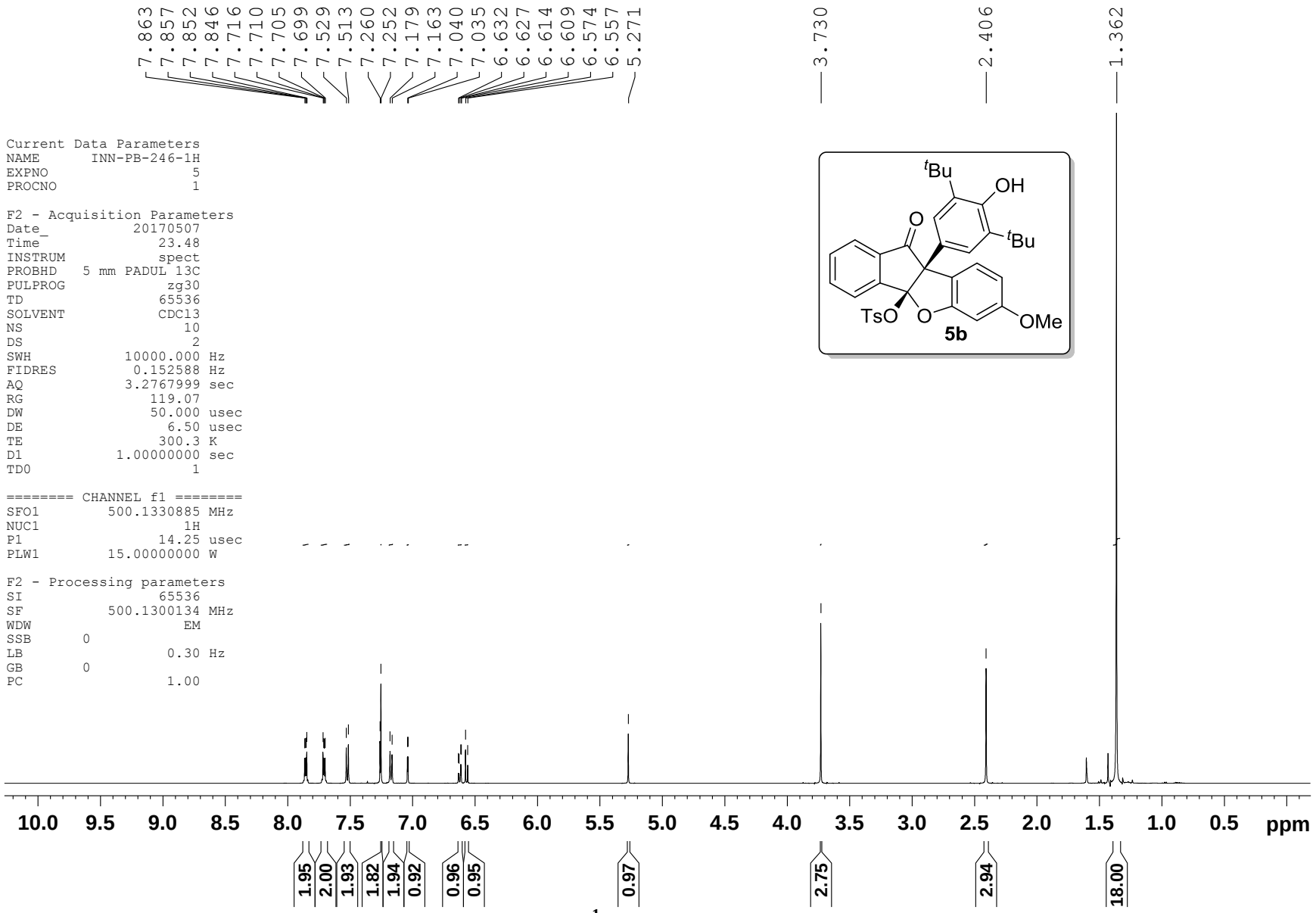


Figure S10. ^{1}H NMR Spectrum of 5b

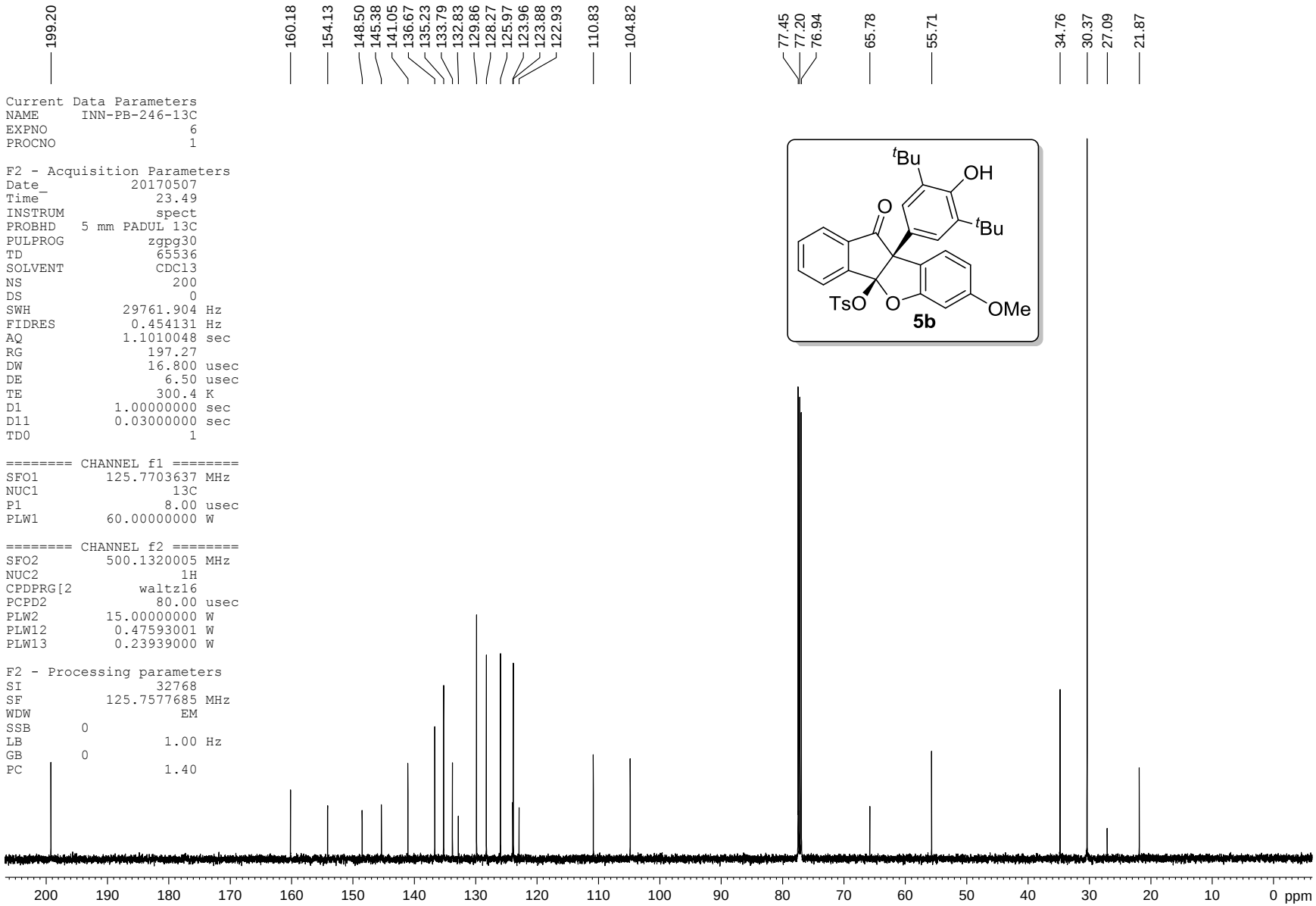


Figure S11. ^{13}C NMR Spectrum of 5b

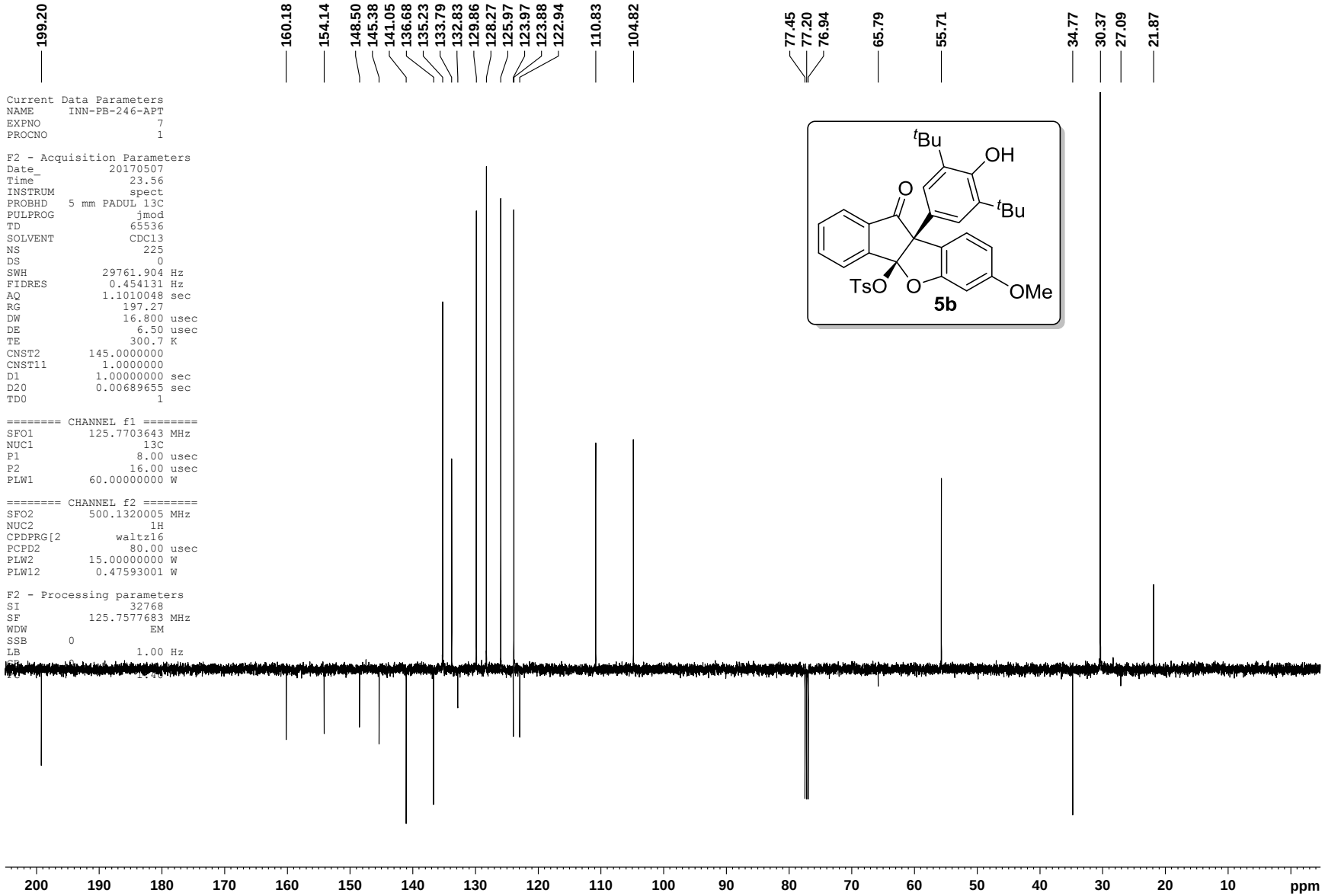


Figure S12. ^{13}C-APT NMR Spectrum of 5b

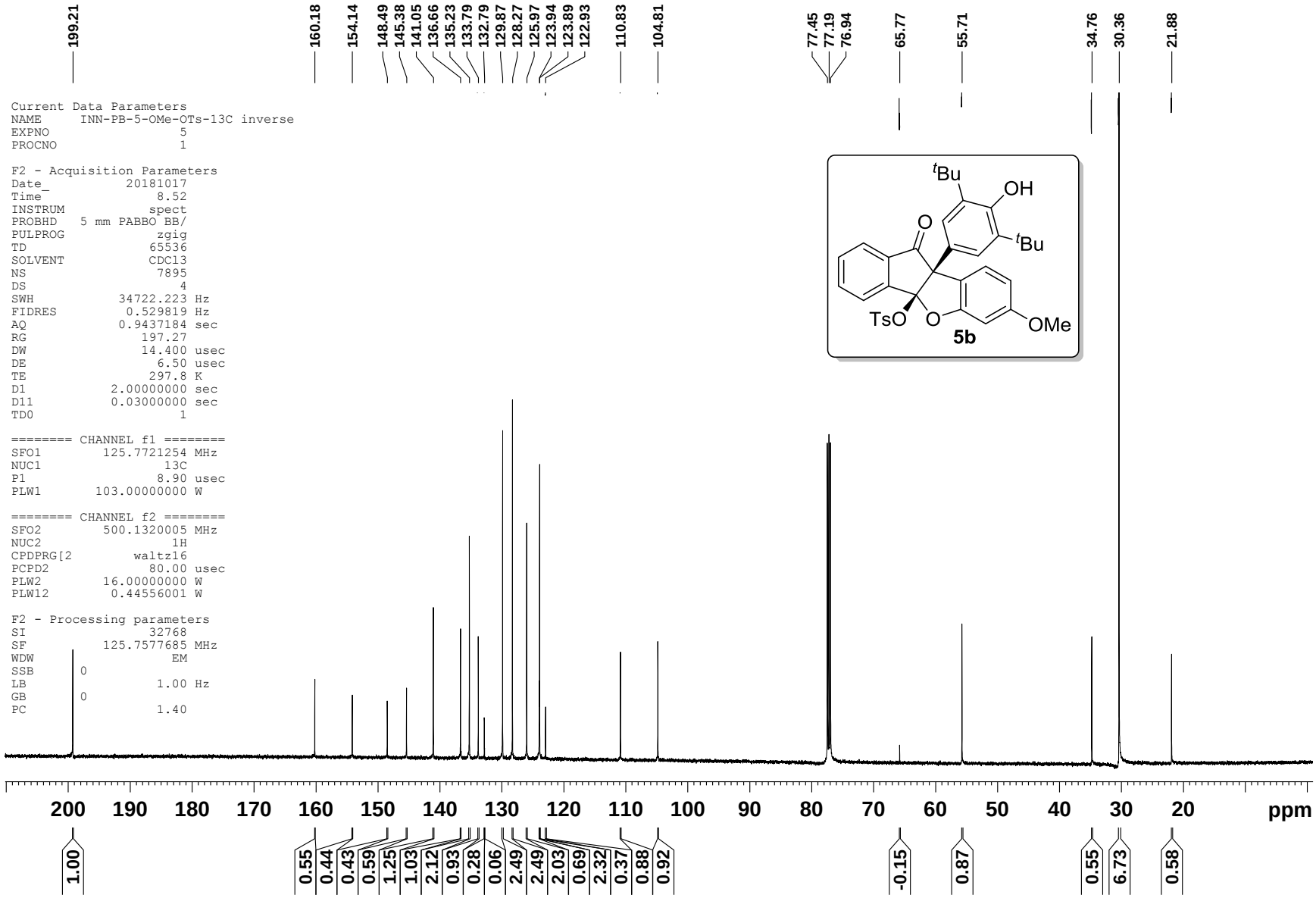


Figure S13. Inverse-Gated ^{13}C NMR Spectrum of 5b

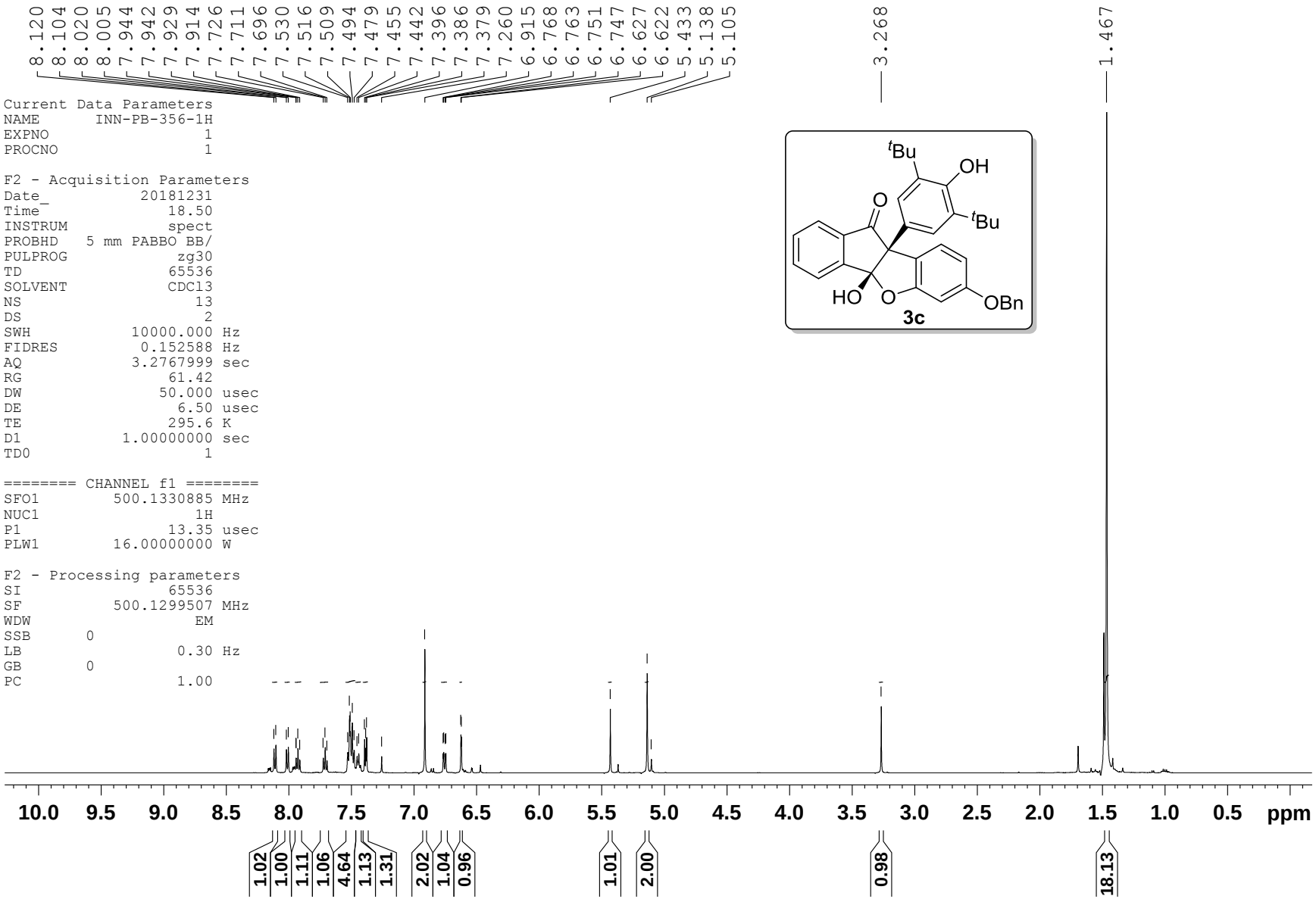


Figure S14. ^{1}H NMR Spectrum of 3c

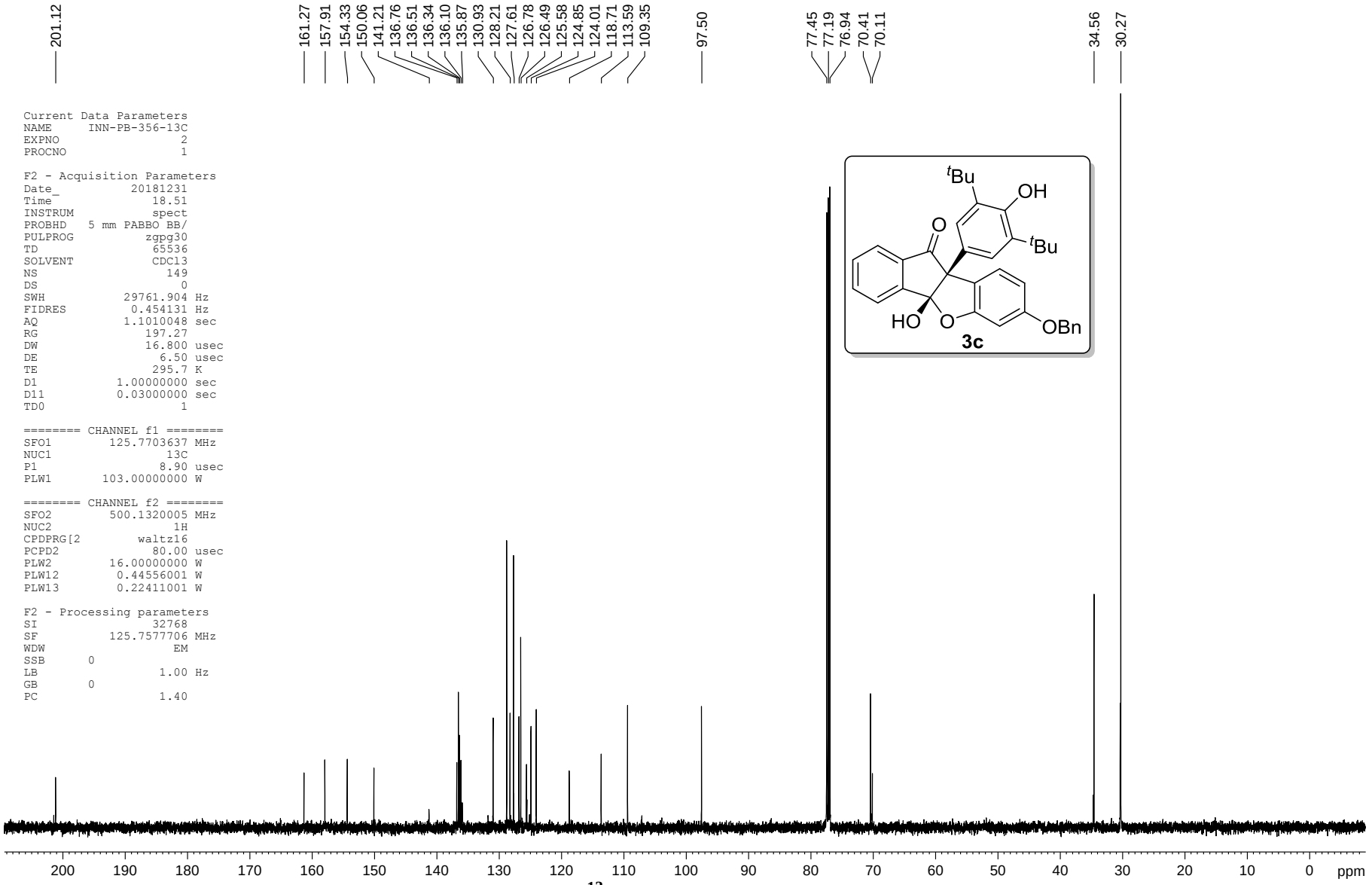


Figure S15. ^{13}C NMR Spectrum of 3c

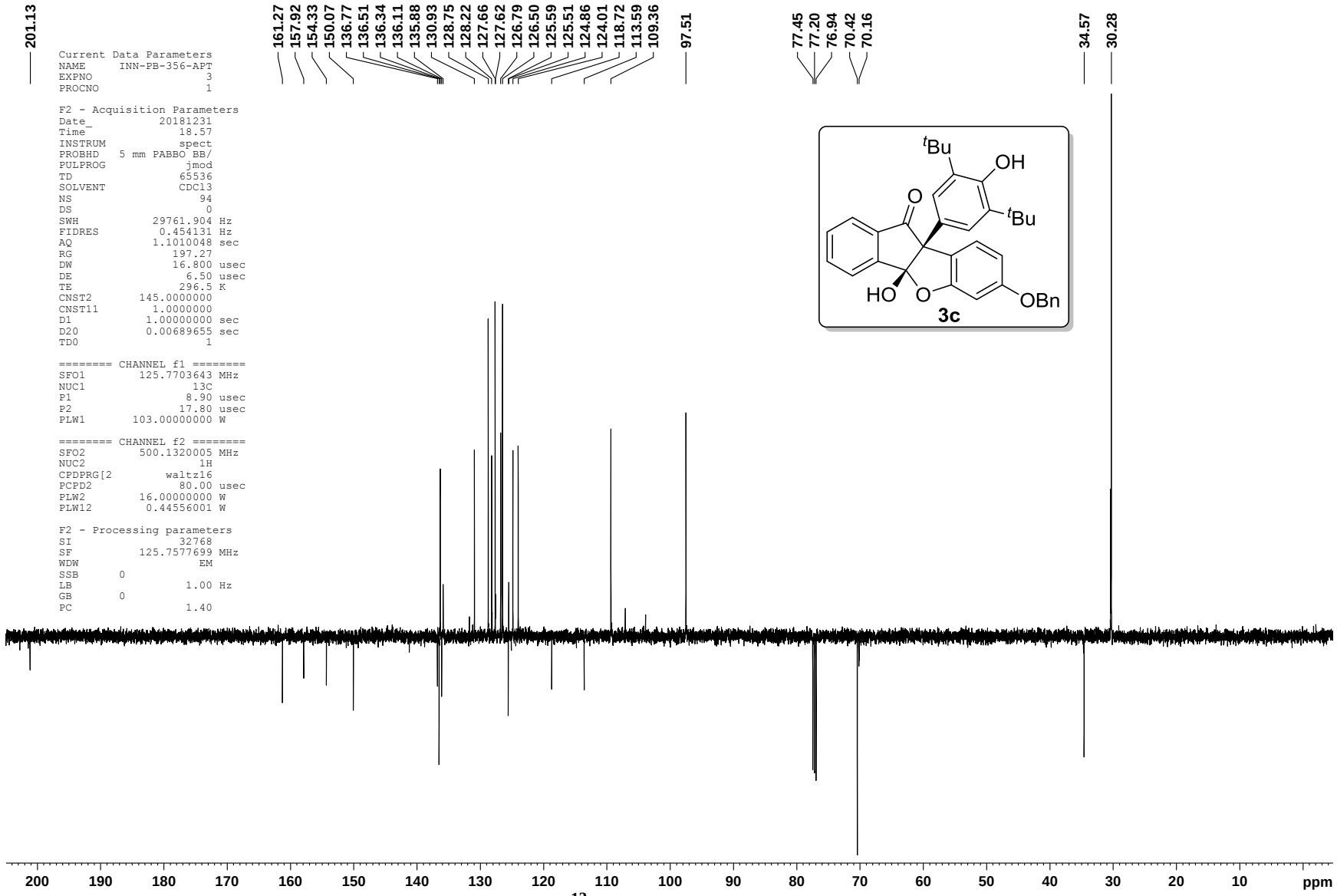


Figure S16. ^{13}C-APT NMR Spectrum of 3c

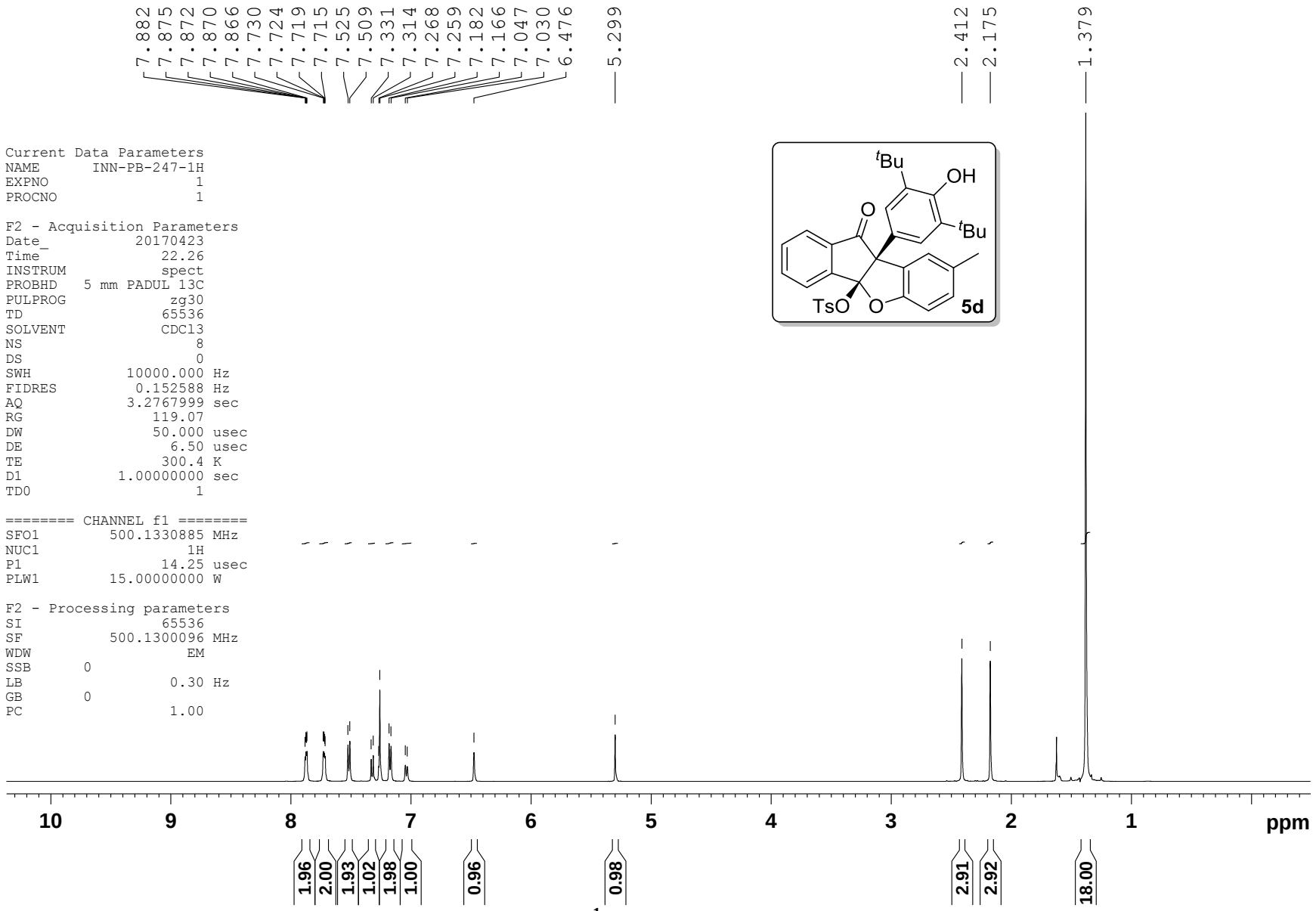


Figure S17. ^{1}H NMR Spectrum of 5d

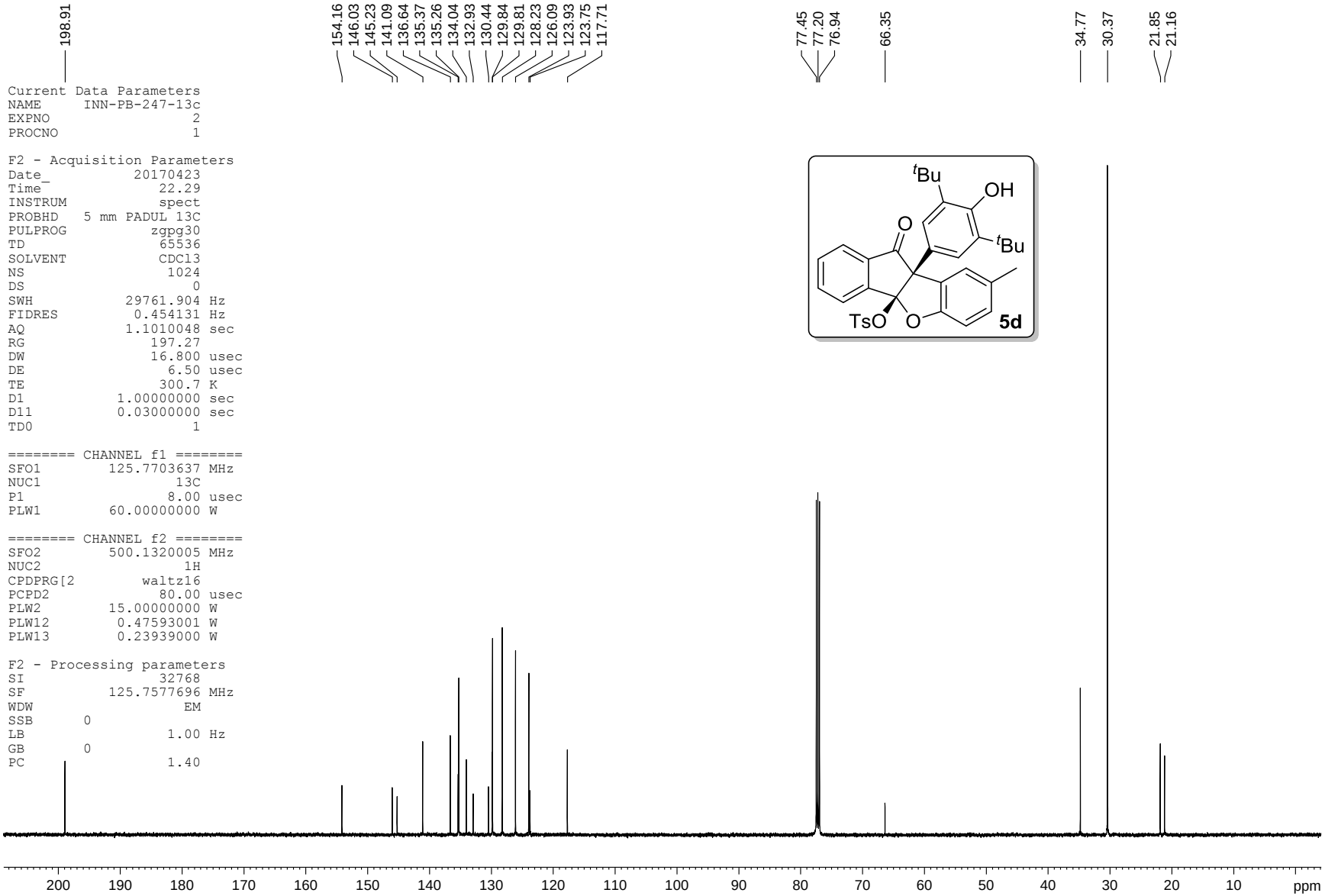


Figure S18. ^{13}C NMR Spectrum of 5d

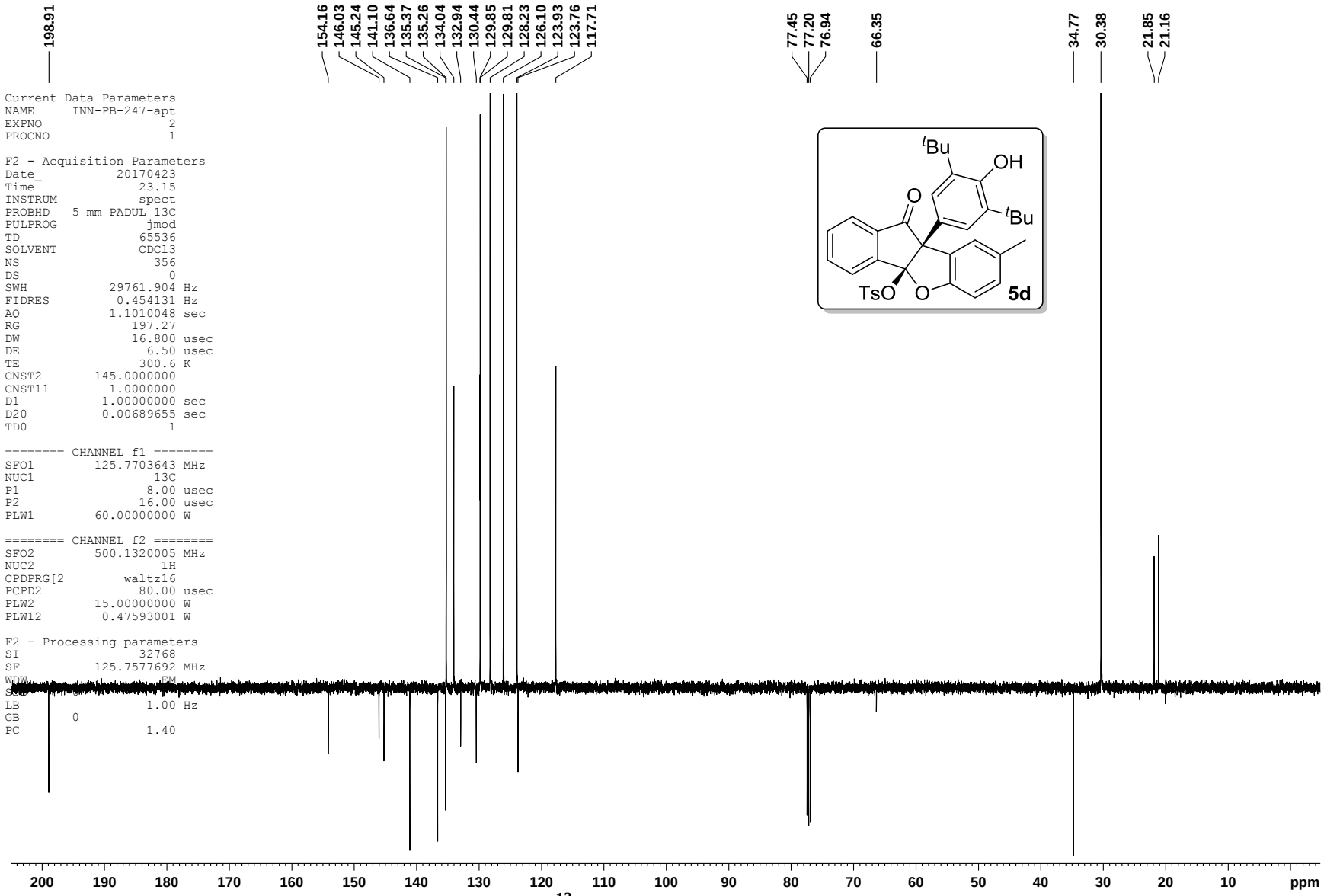


Figure S19. ^{13}C-APT NMR Spectrum of 5d

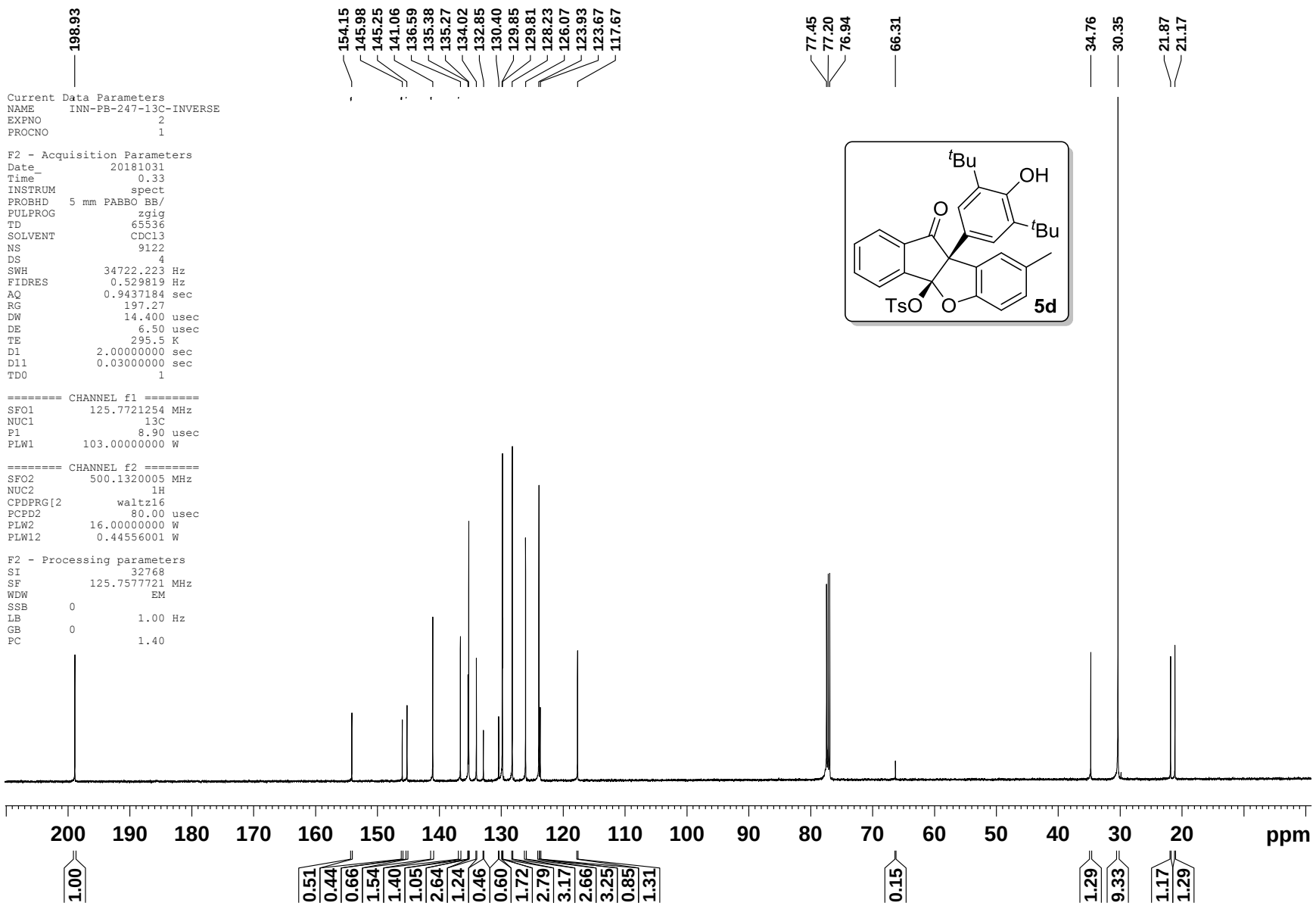


Figure S20. Inverse Gated ^{13}C NMR Spectrum of 5d

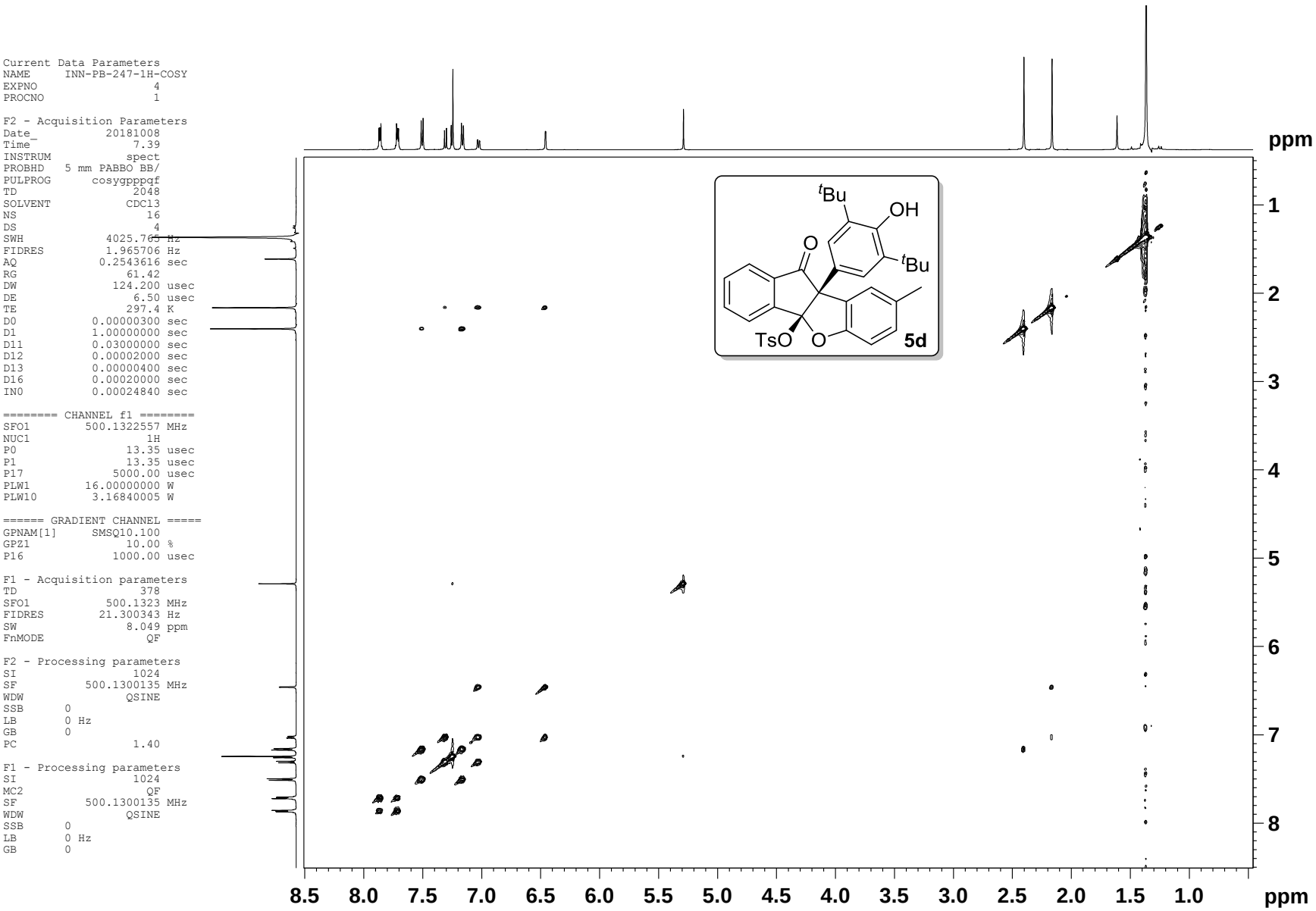


Figure S21. ^{1}H-^{1}H COSY NMR Spectrum of 5d

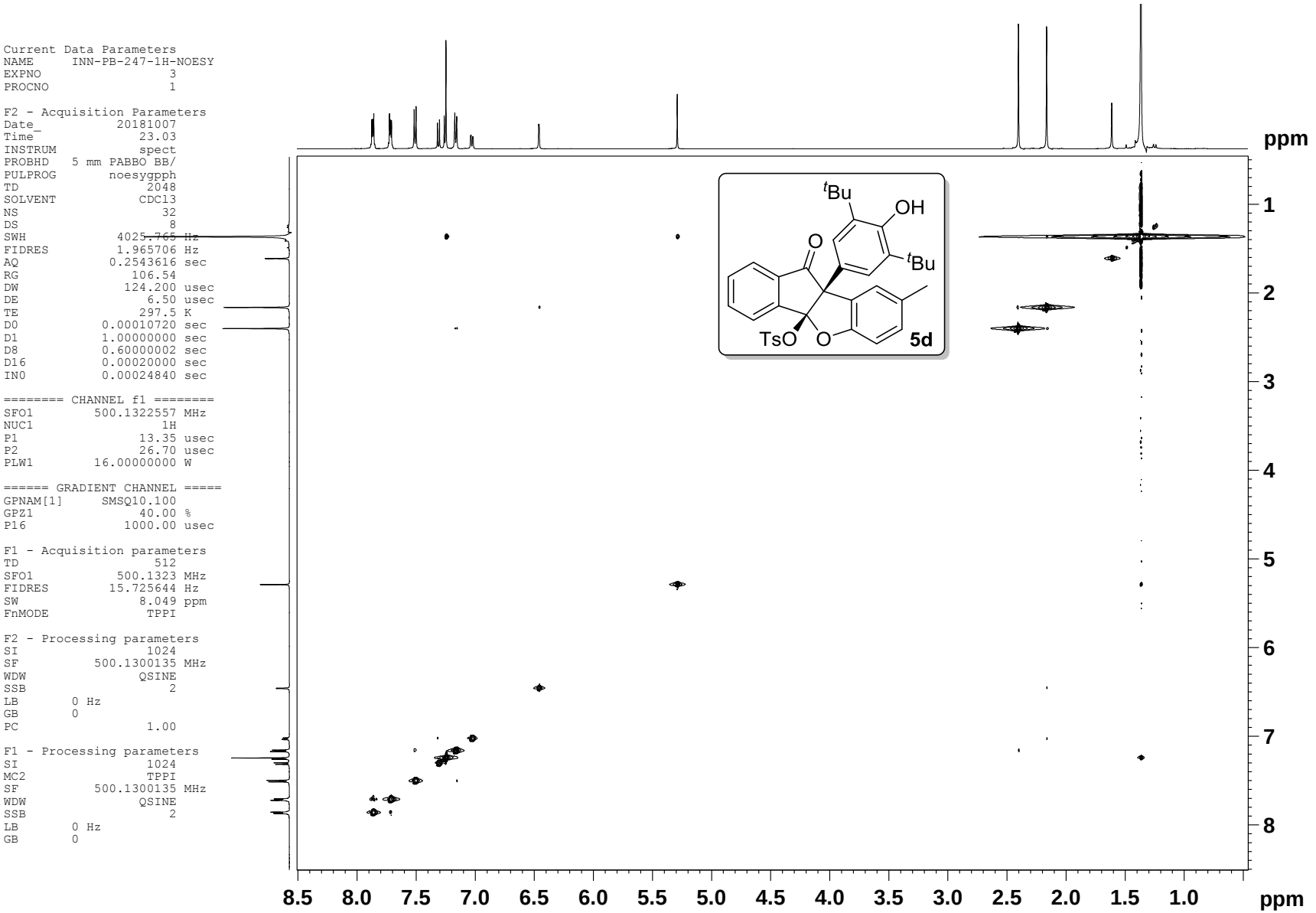


Figure S22. ^{1}H-^{1}H NOESY NMR Spectrum of 5d

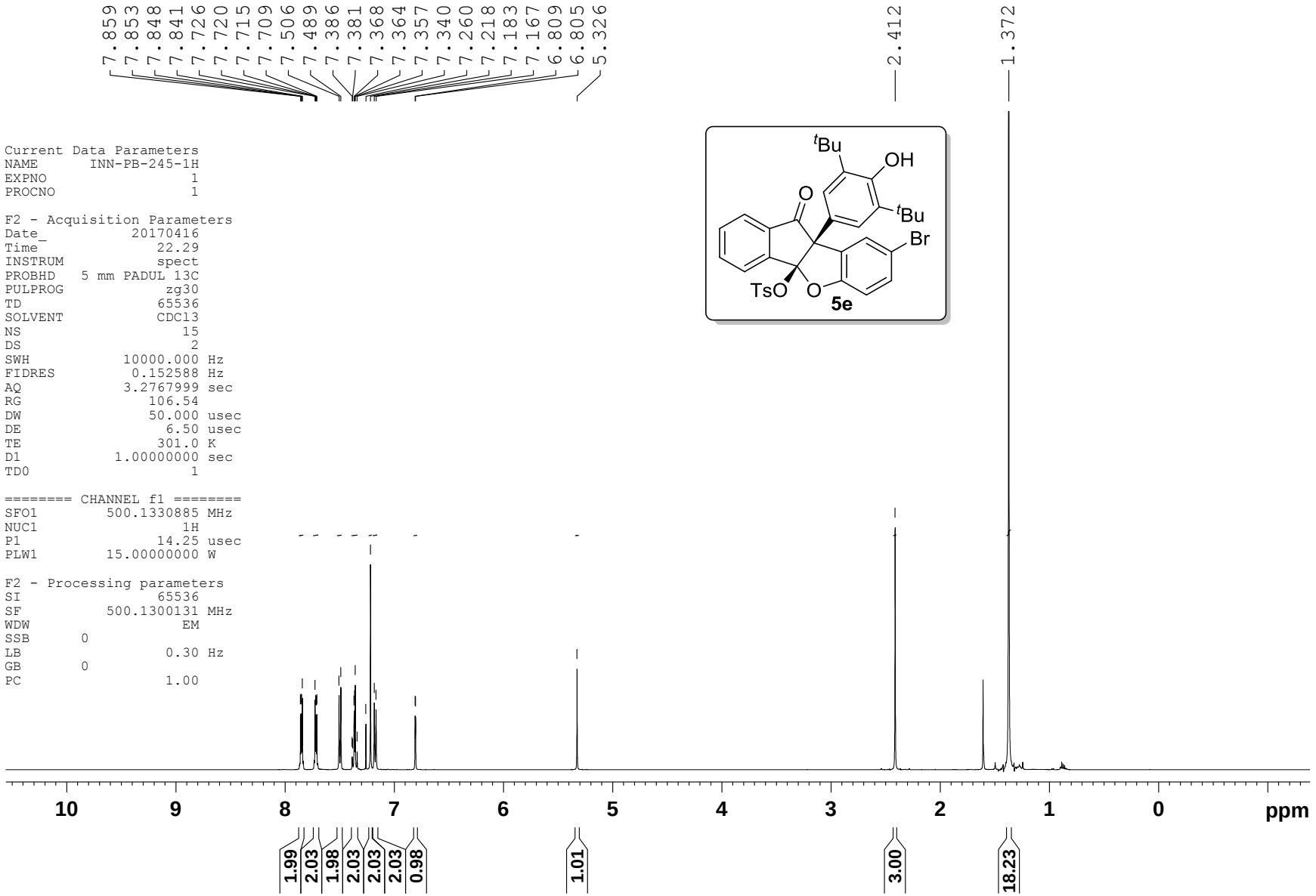


Figure S23. ^{1}H NMR Spectrum of 5e

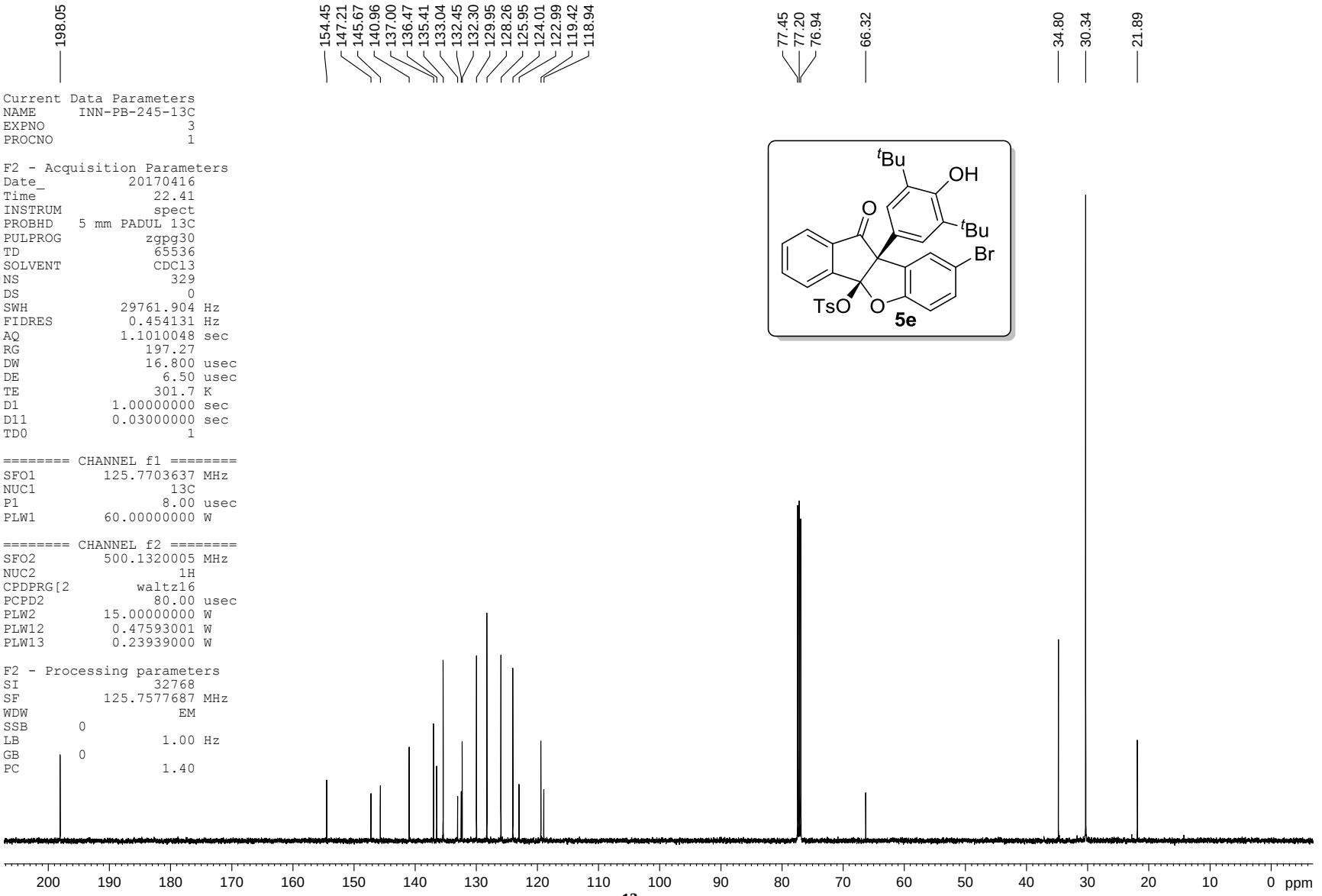


Figure S24. ^{13}CNMR Spectrum of 5e

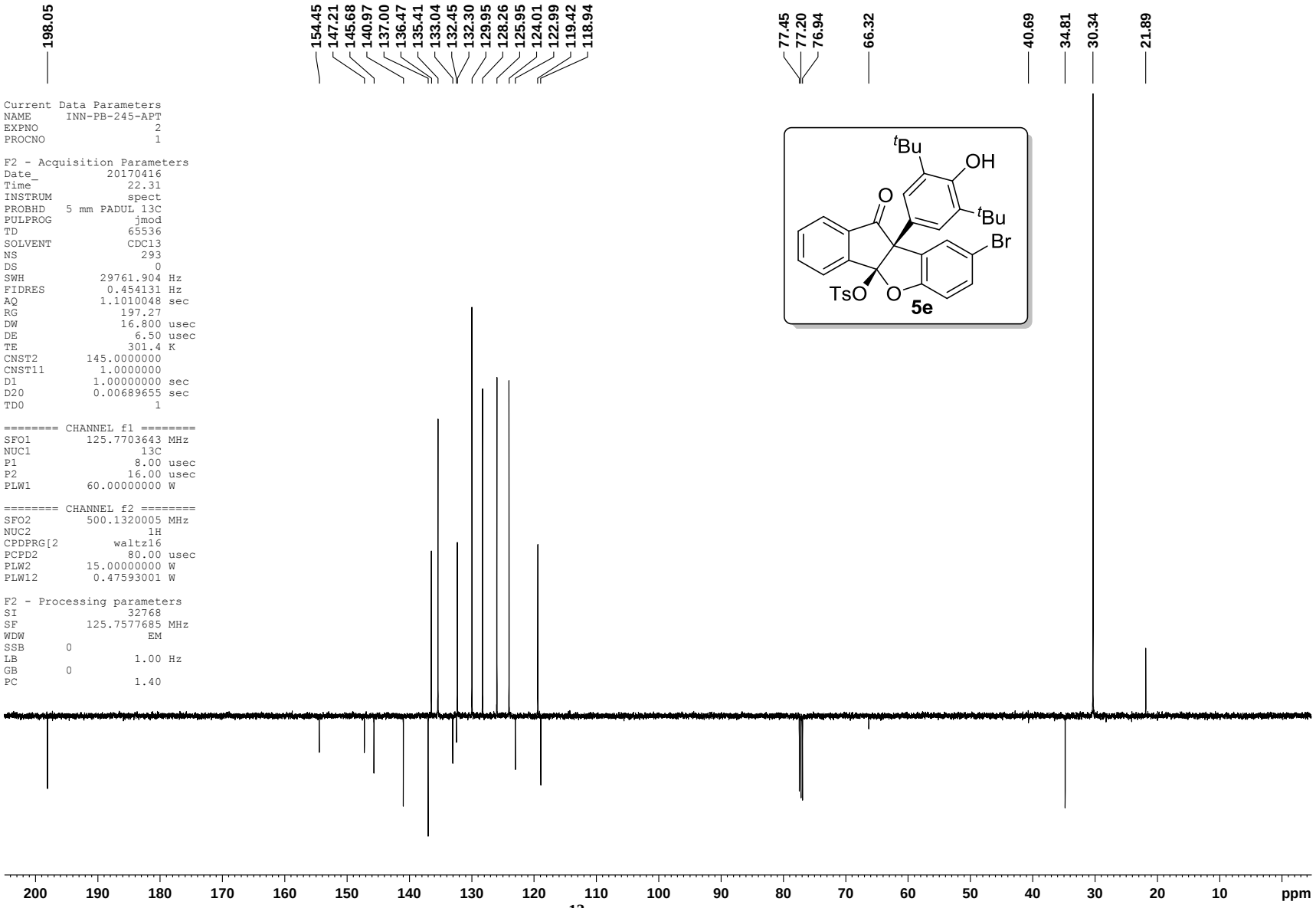


Figure S25. ^{13}C-APT NMR Spectrum of 5e

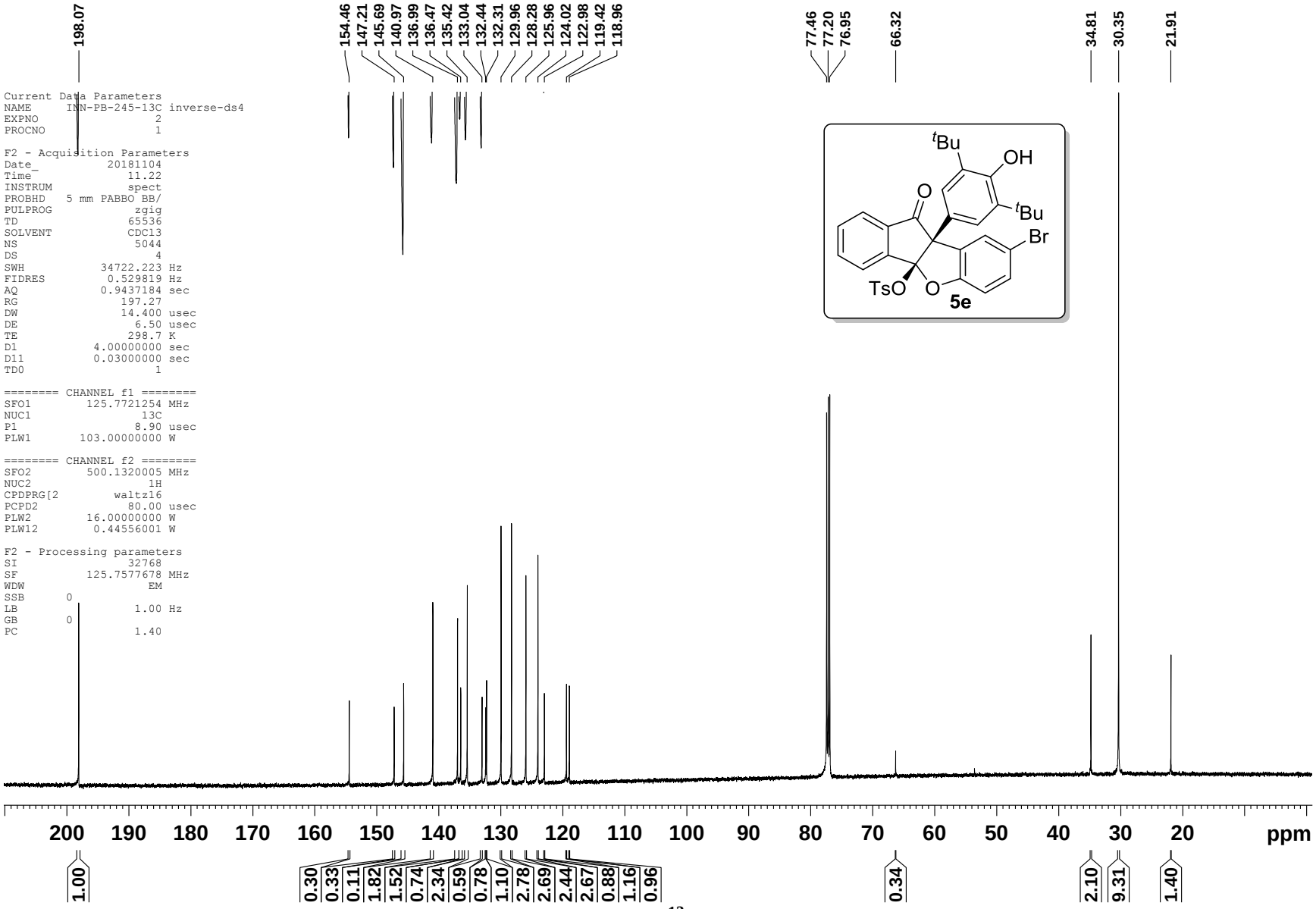


Figure S26. Inverse Gated ^{13}CNMR Spectrum of 5e

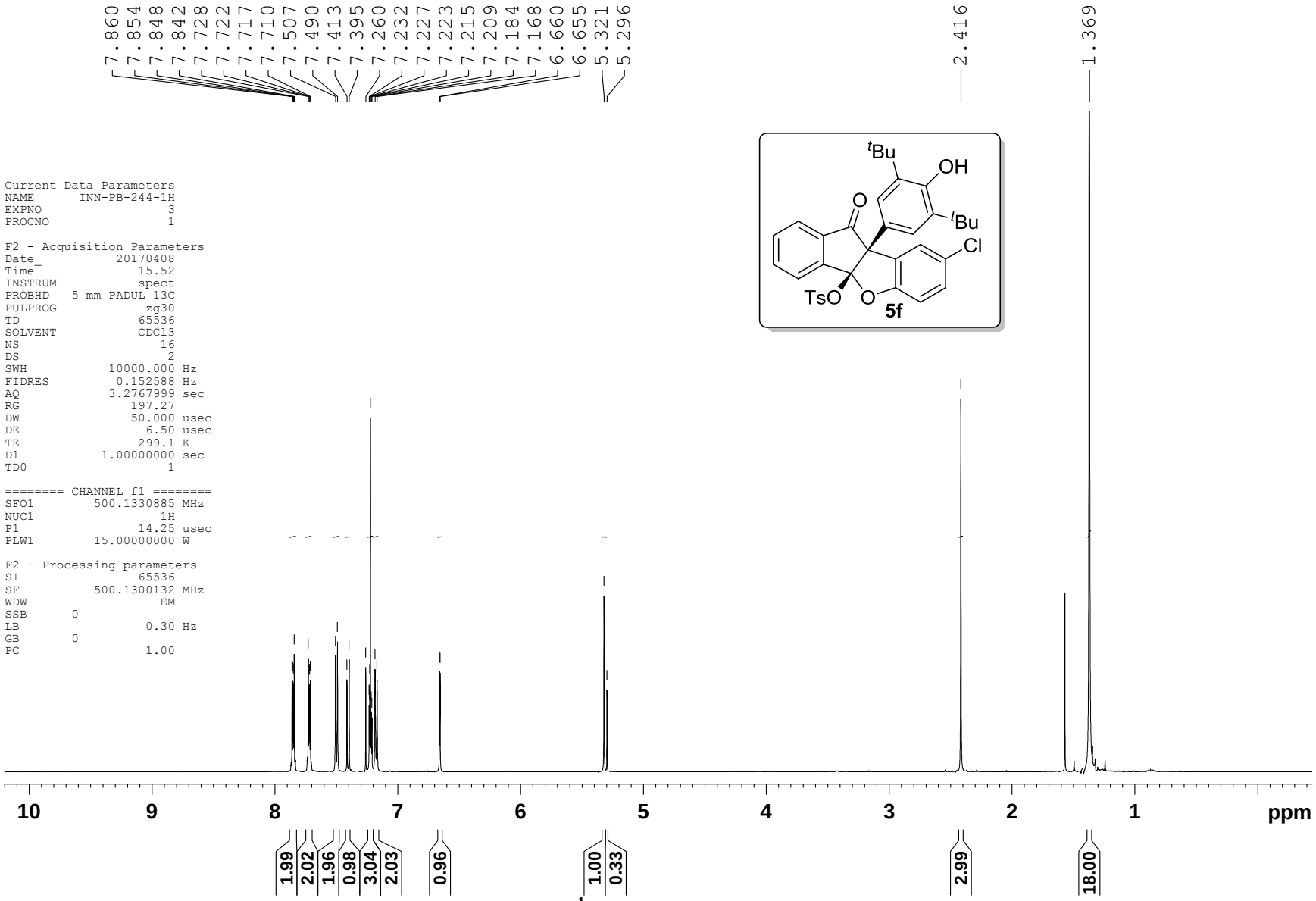


Figure S27. ^{1}H NMR Spectrum of 5f

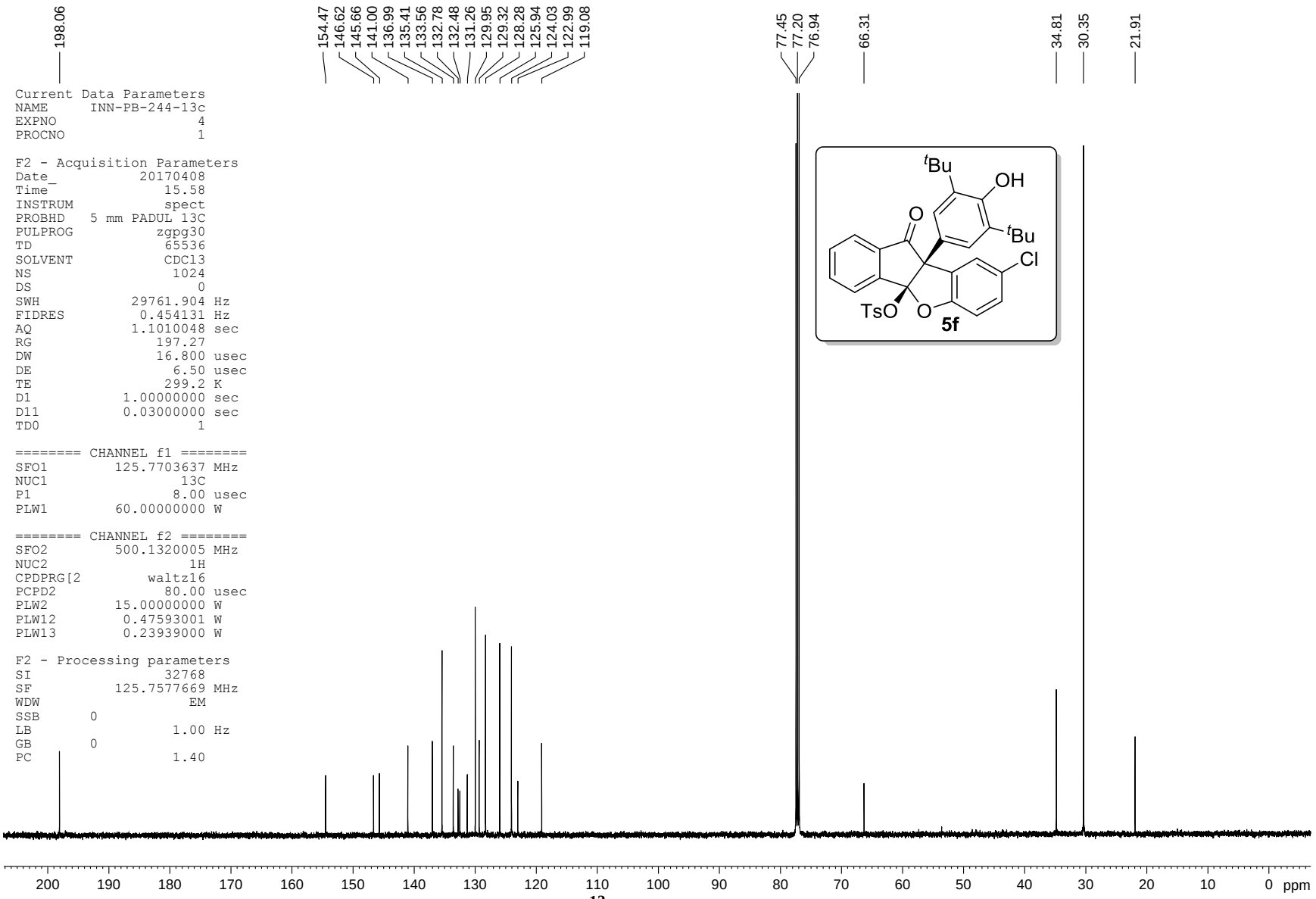


Figure S28. ^{13}C NMR Spectrum of 5f

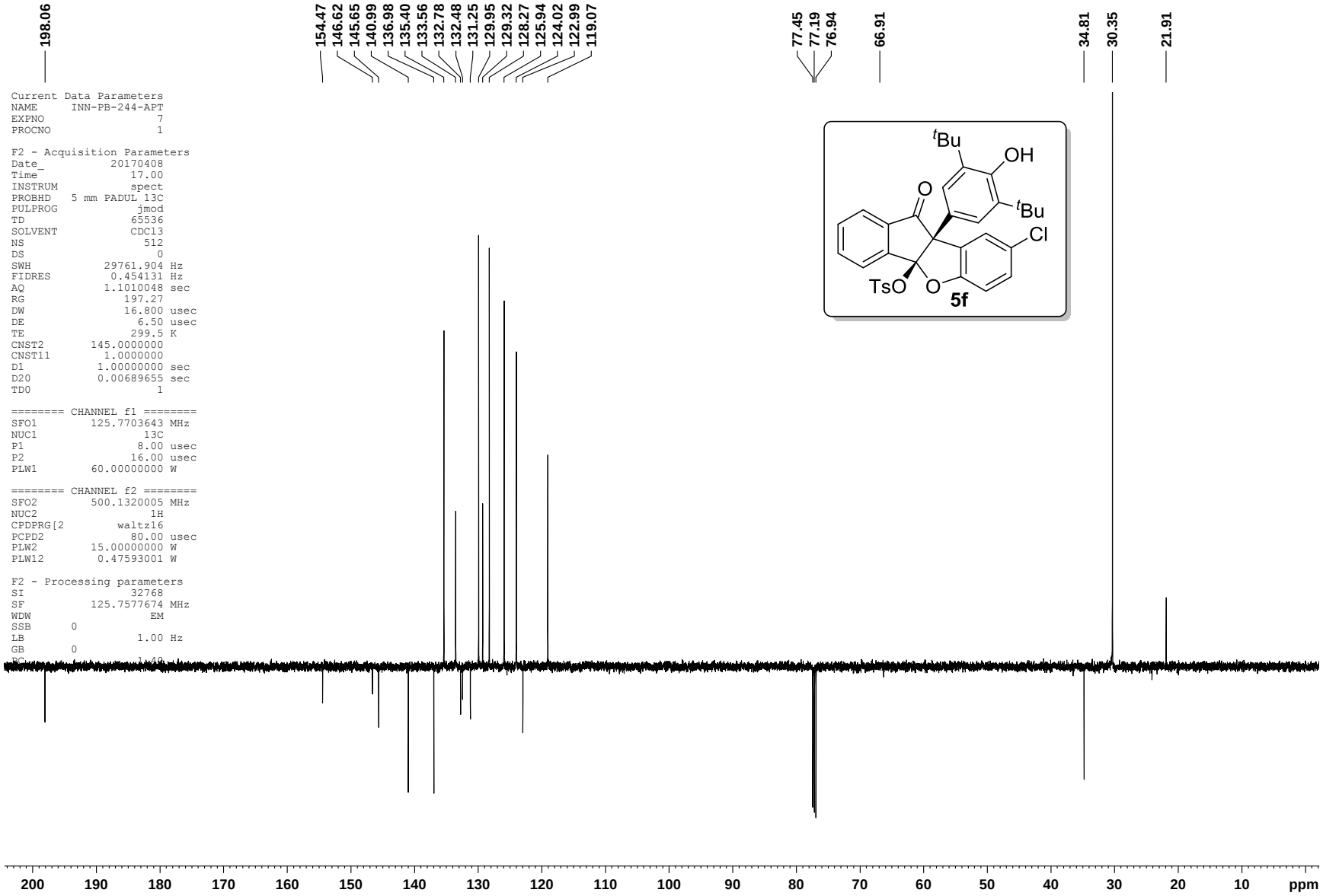


Figure S29. ^{13}C-APT NMR Spectrum of 5f

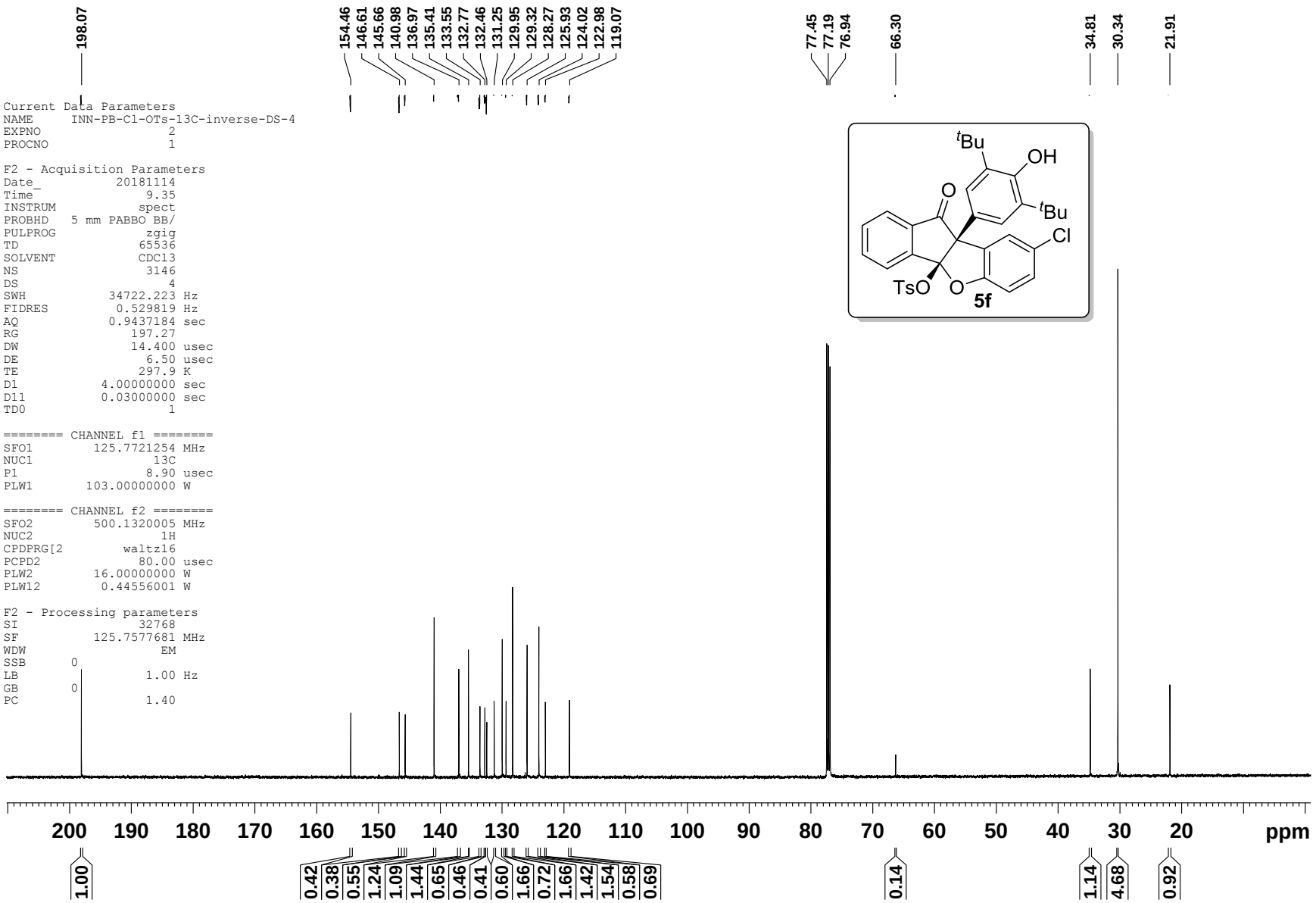


Figure S30. Inverse Gated ^{13}C NMR Spectrum of 5f

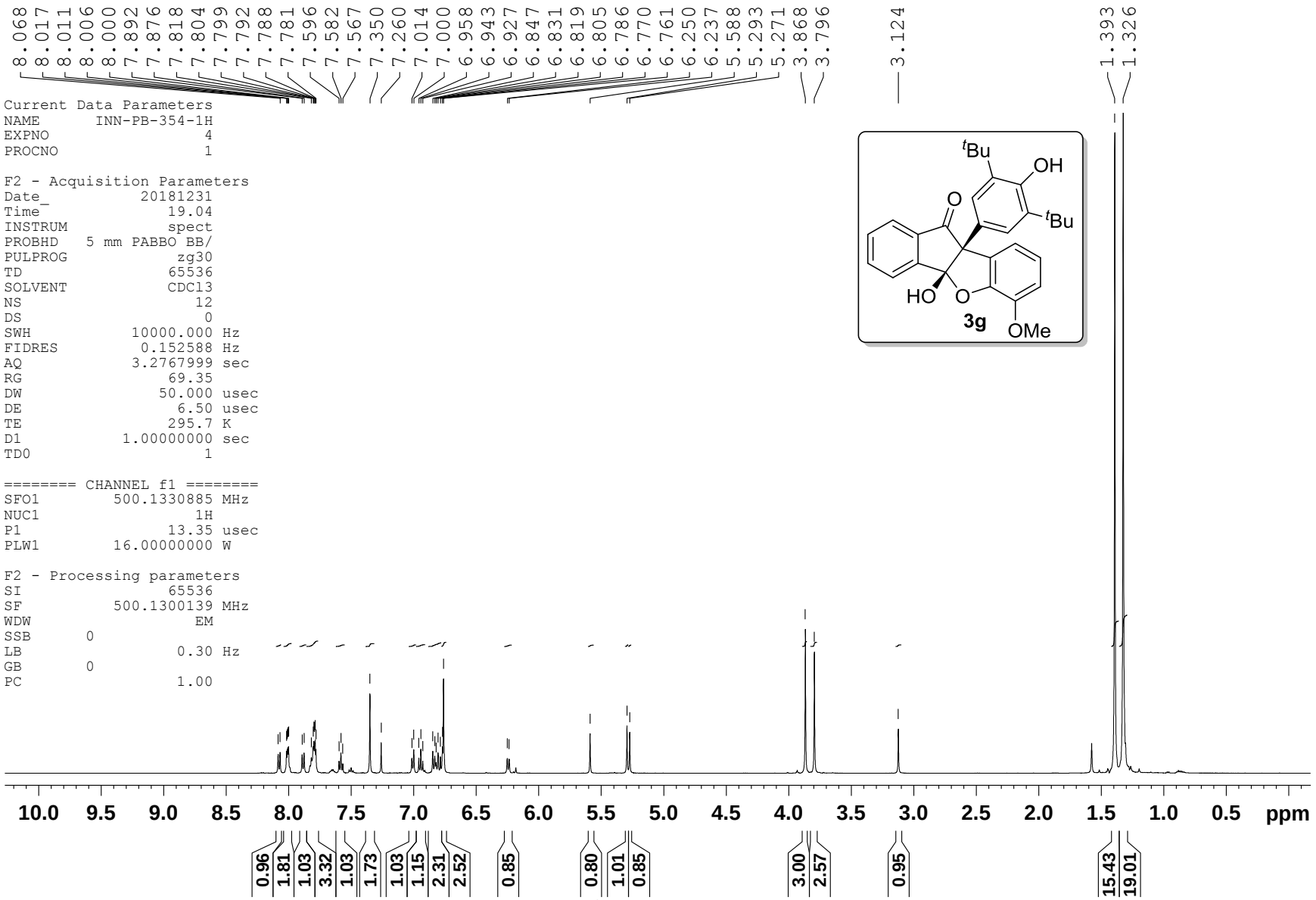


Figure S31. ^{1}H NMR Spectrum of 3g

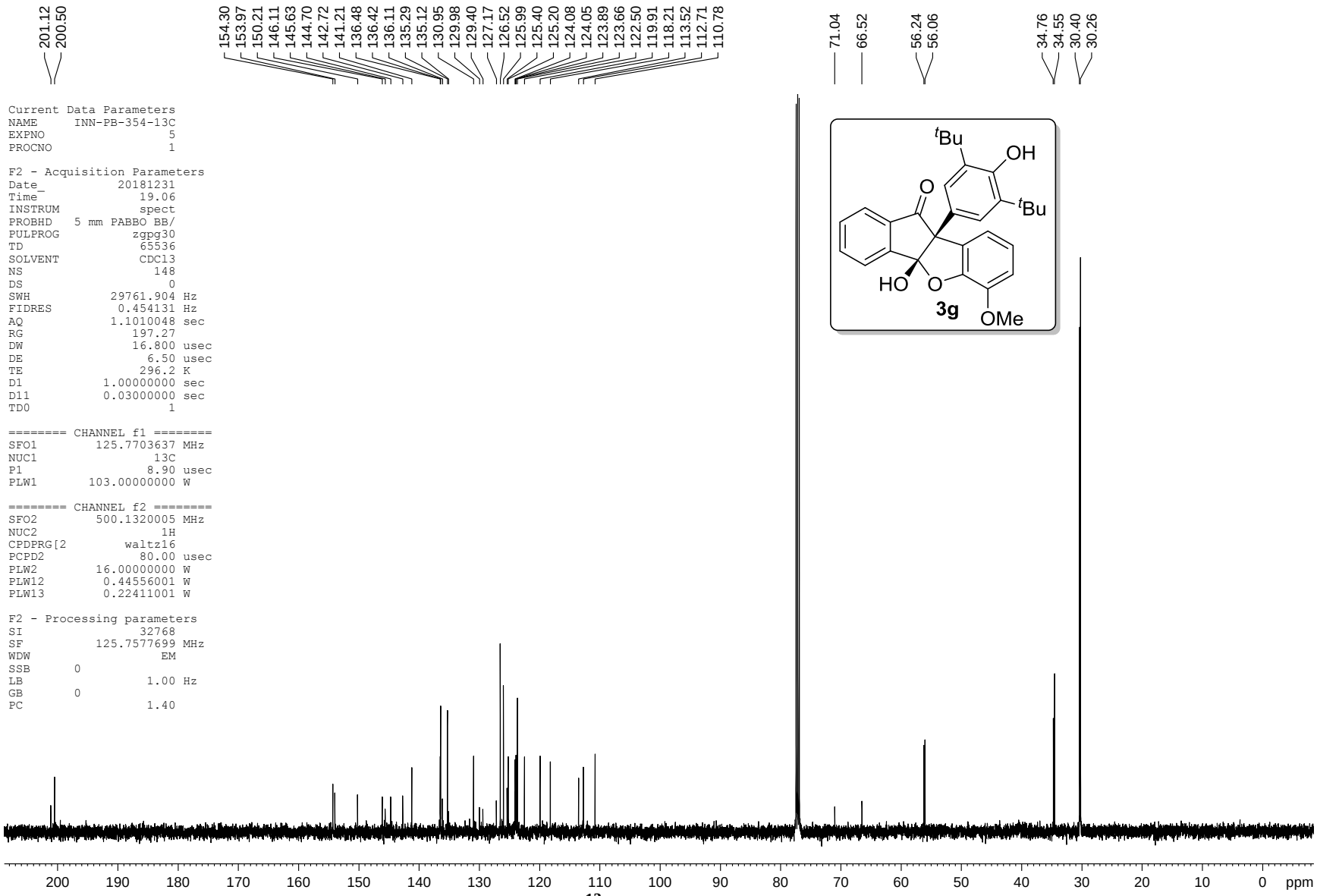


Figure S32. ^{13}C NMR Spectrum of 3g

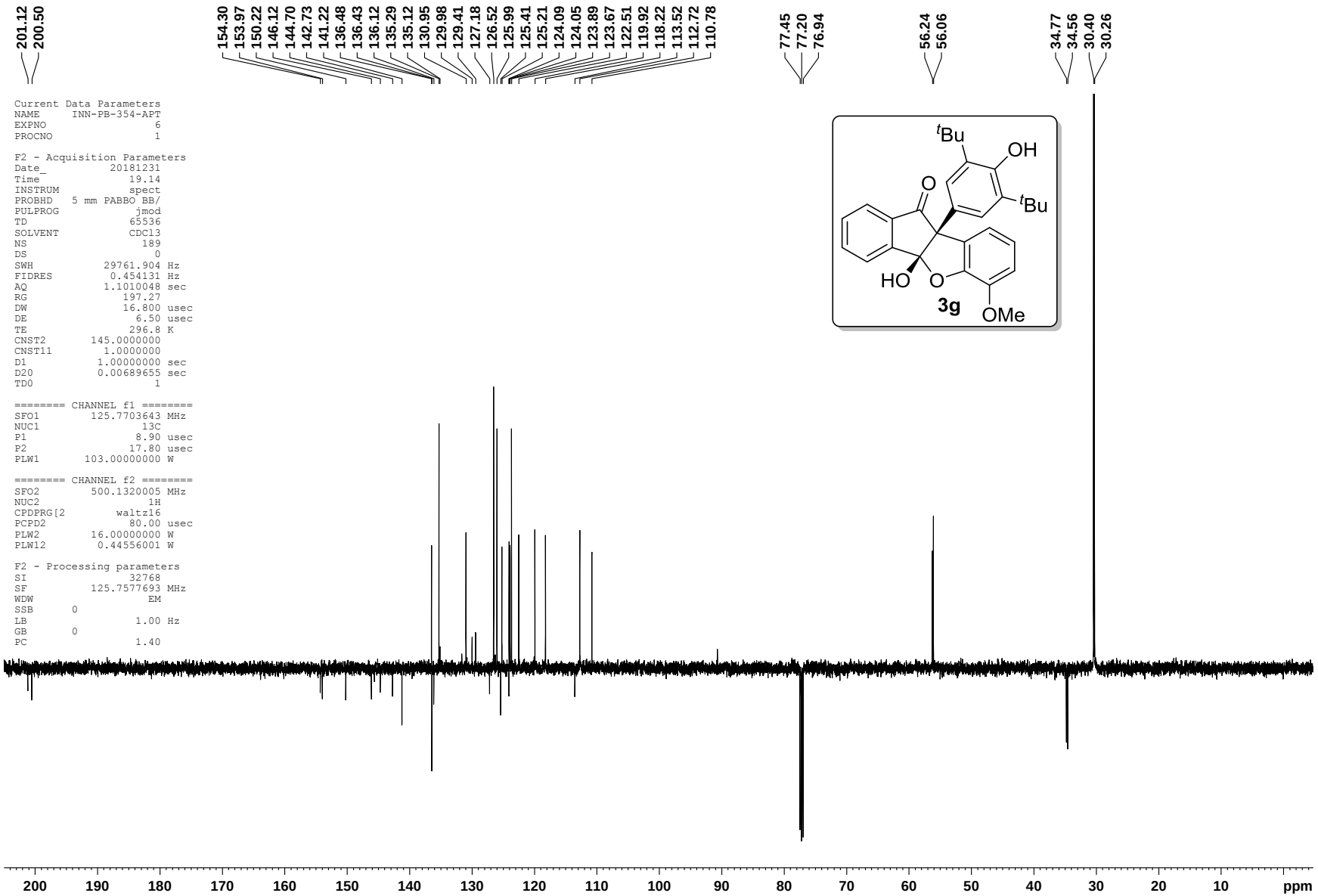


Figure S33. ^{13}C-APT NMR Spectrum of 3g

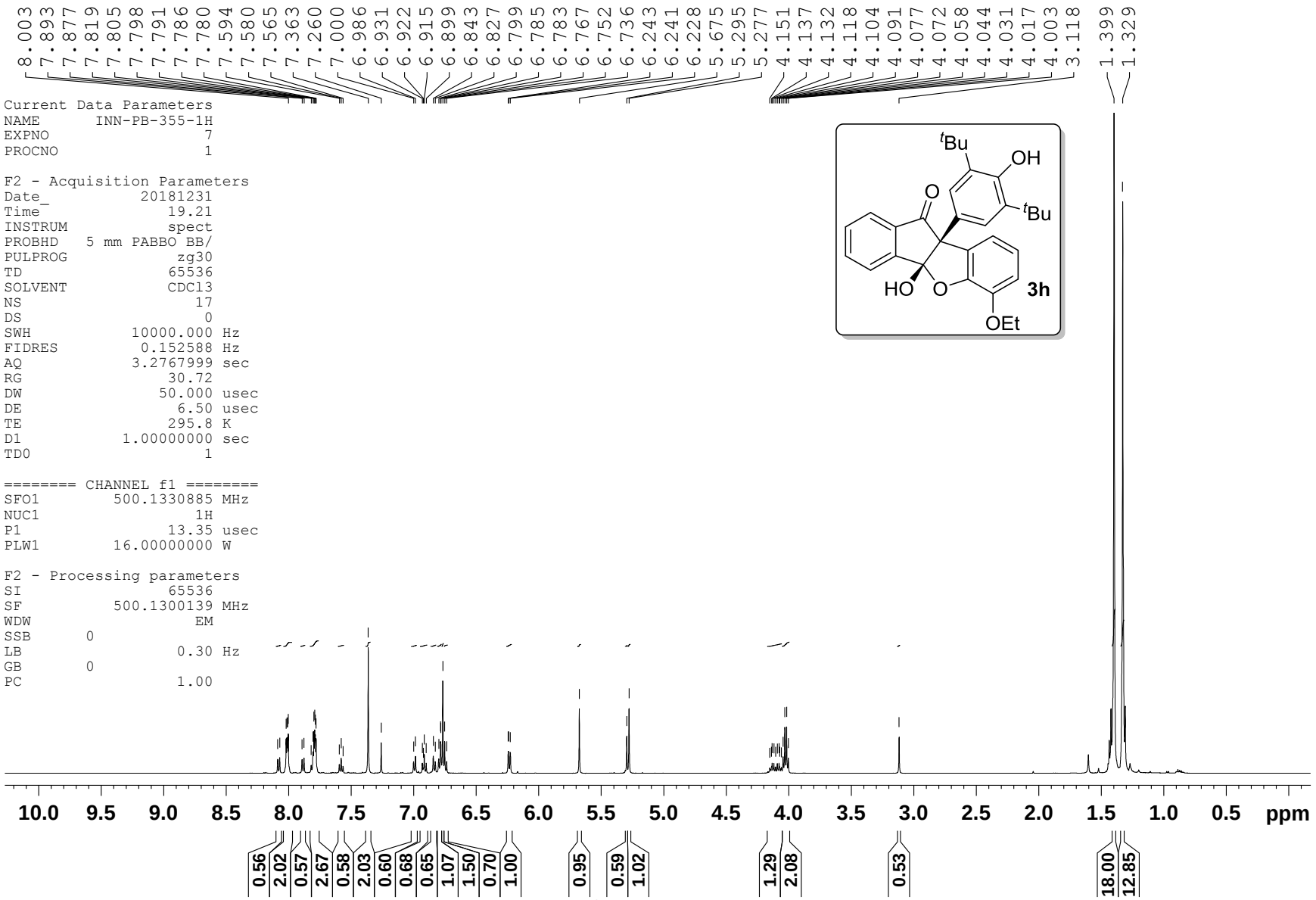


Figure S34. ^{1}H NMR Spectrum of 3h

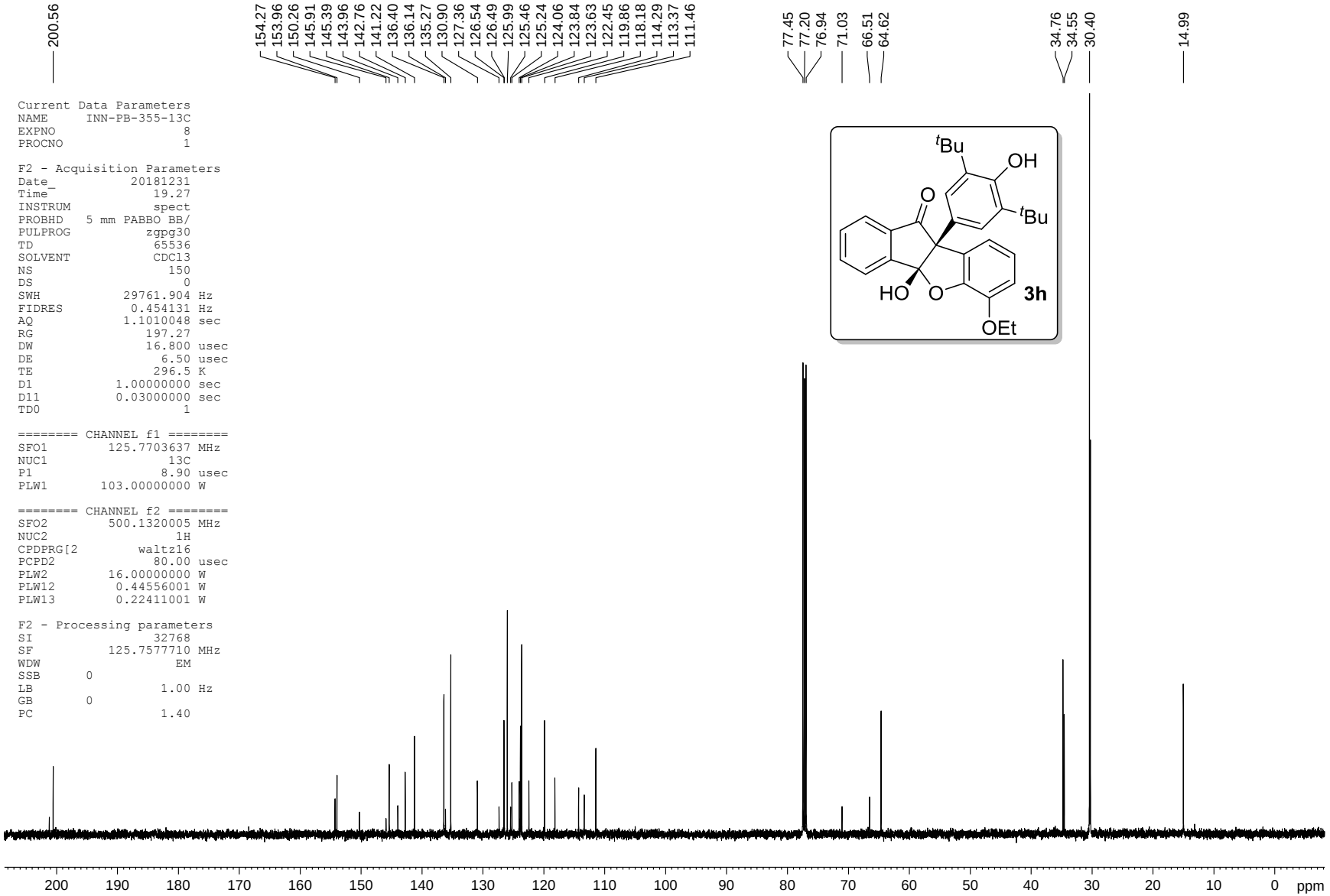


Figure S35. ^{13}C NMR Spectrum of 3h

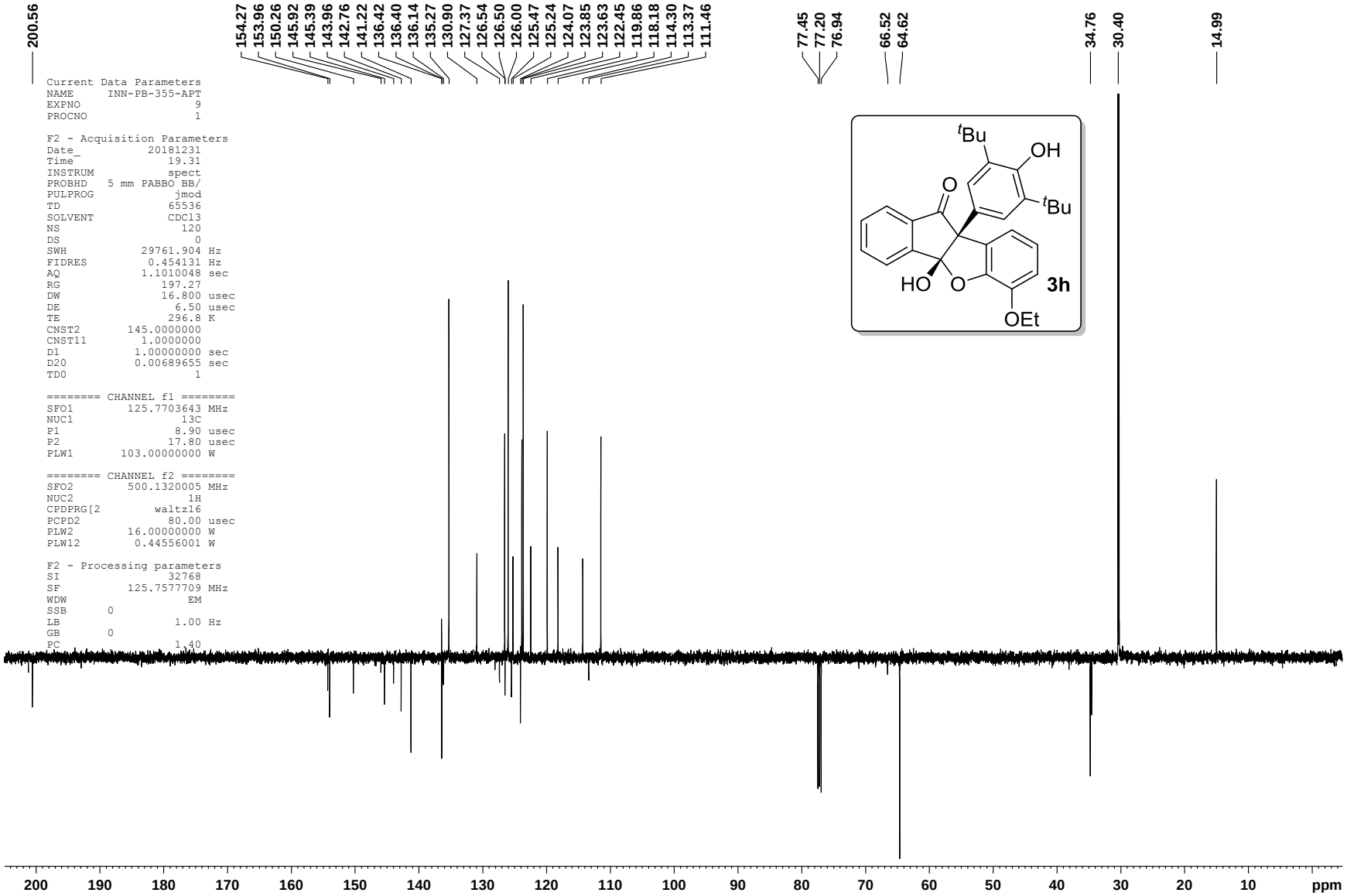


Figure S36. ^{13}C-APT NMR Spectrum of 3h

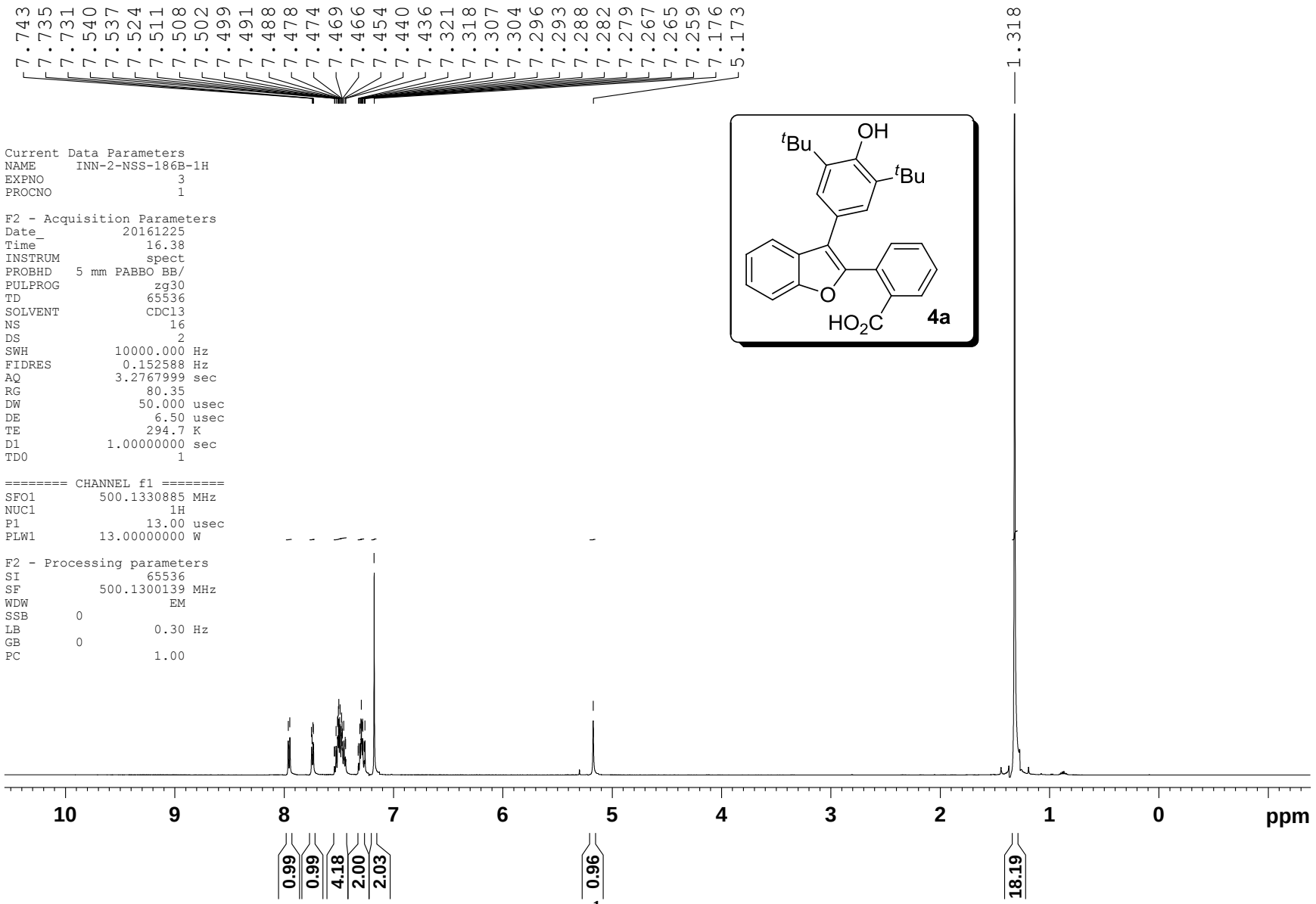


Figure S37. ^{1}H NMR Spectrum of 4a

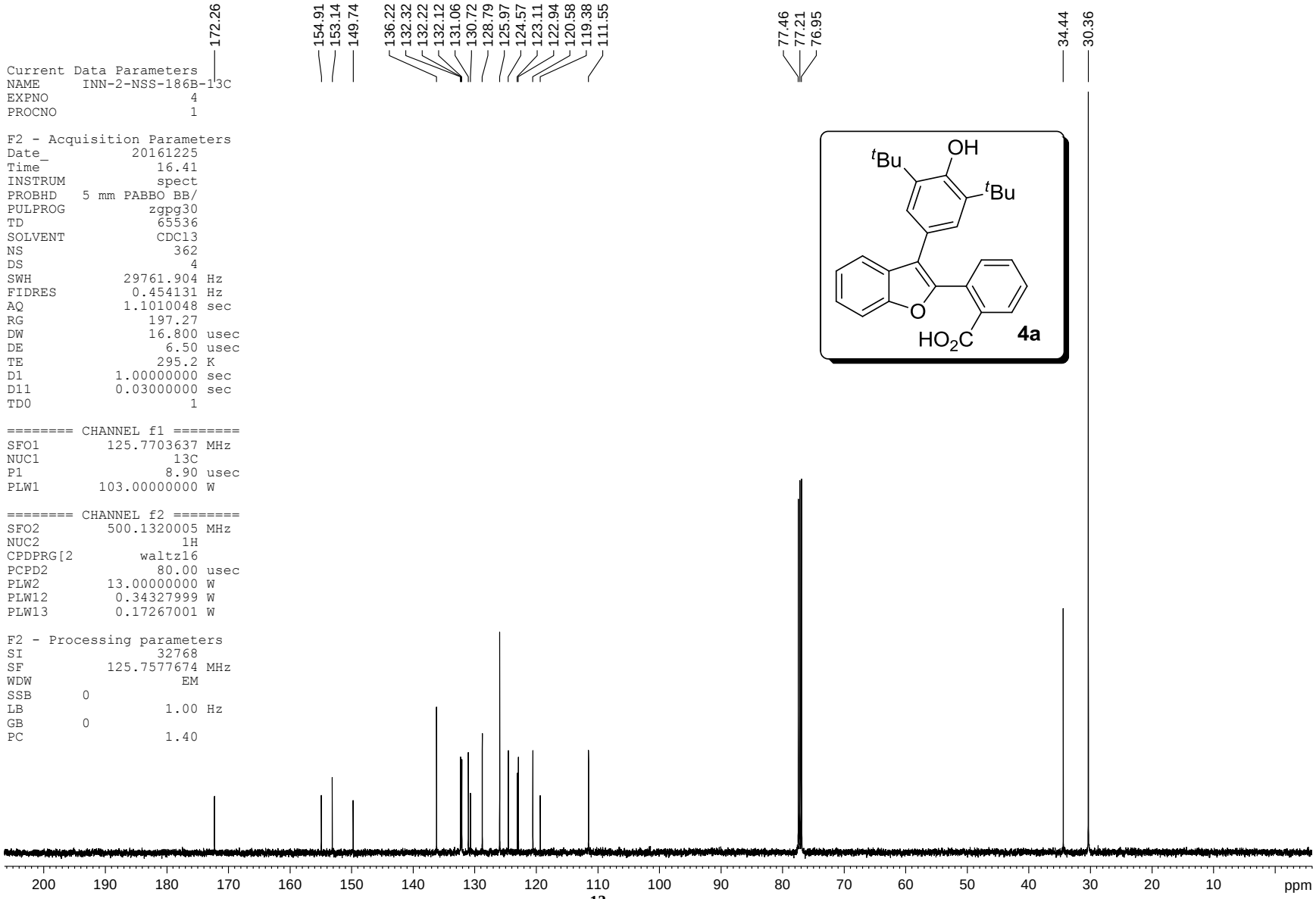


Figure S38. ^{13}C NMR Spectrum of 4a

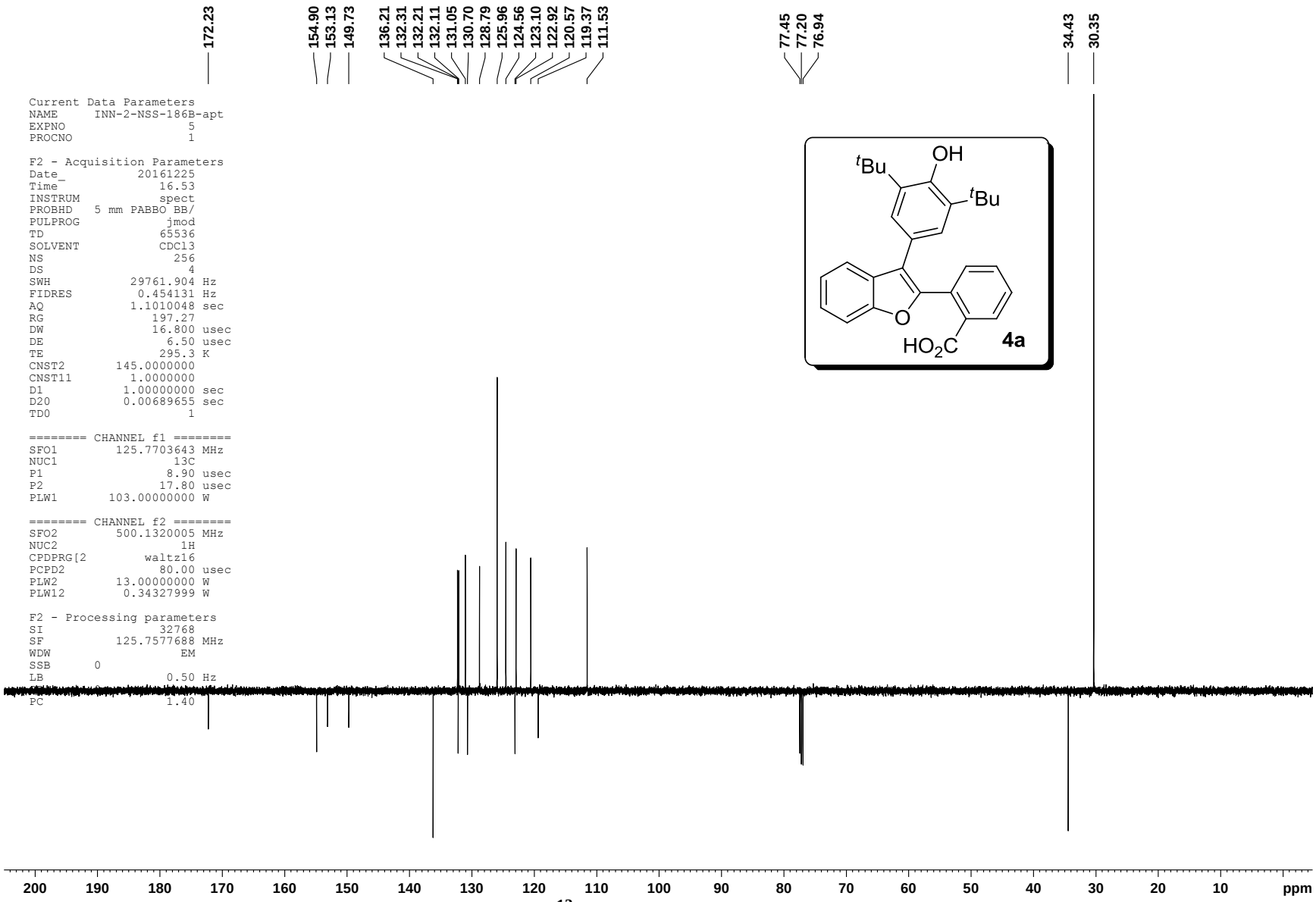


Figure S39. ^{13}C-APT NMR Spectrum of 4a

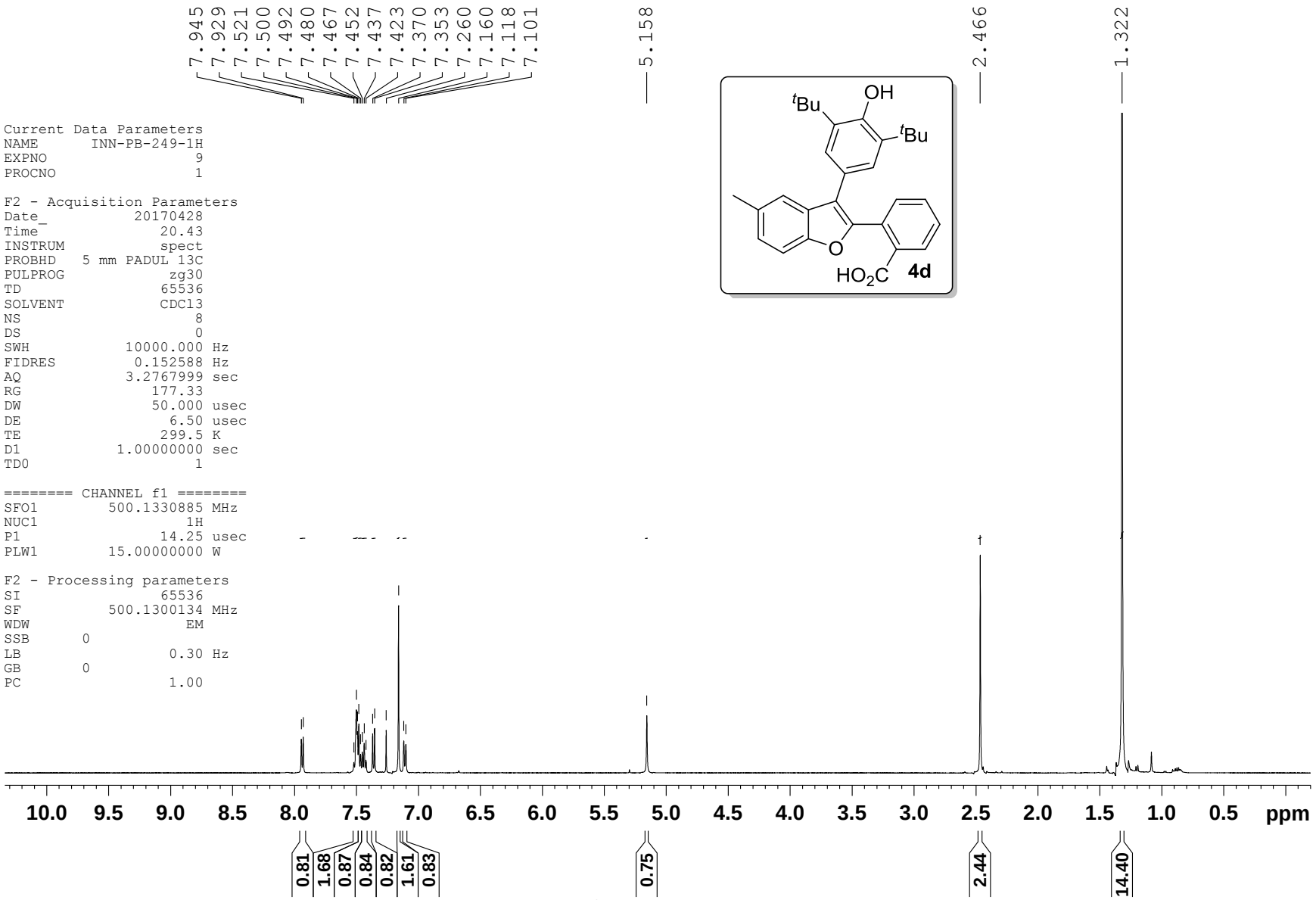


Figure S40. ^{1}H NMR Spectrum of 4d

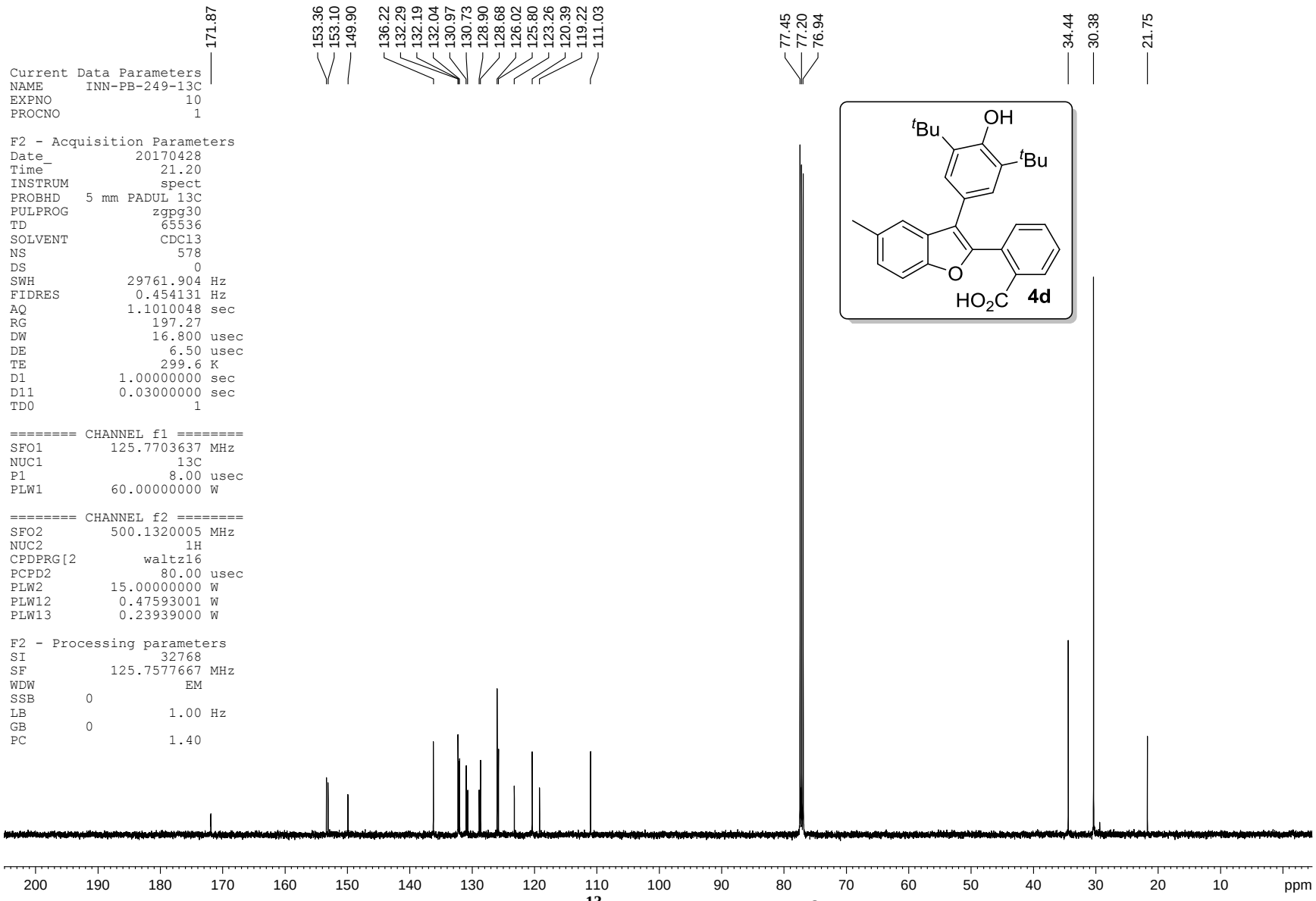


Figure S41. ^{13}C NMR Spectrum of 4d

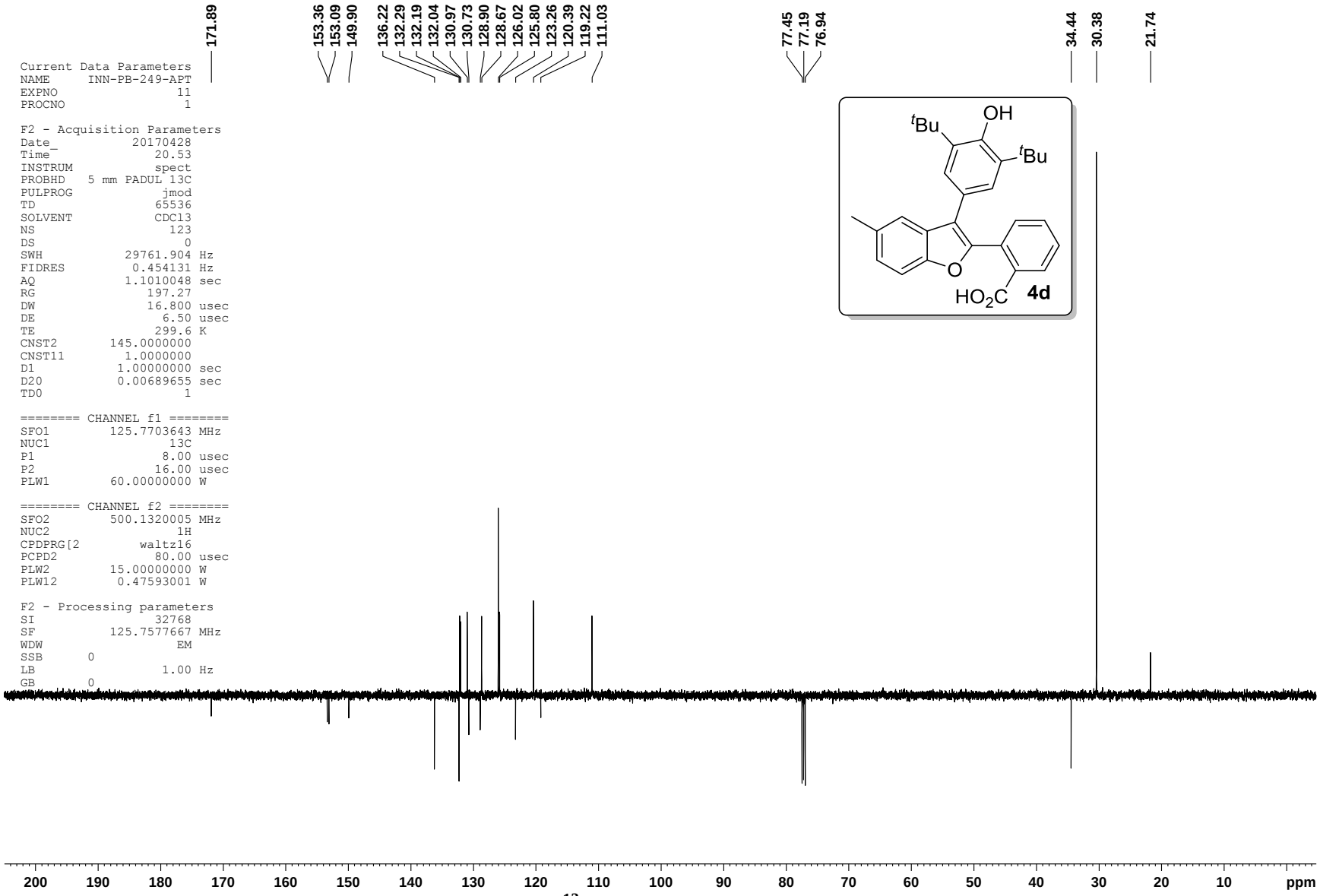


Figure S42. ^{13}C-APT NMR Spectrum of 4d

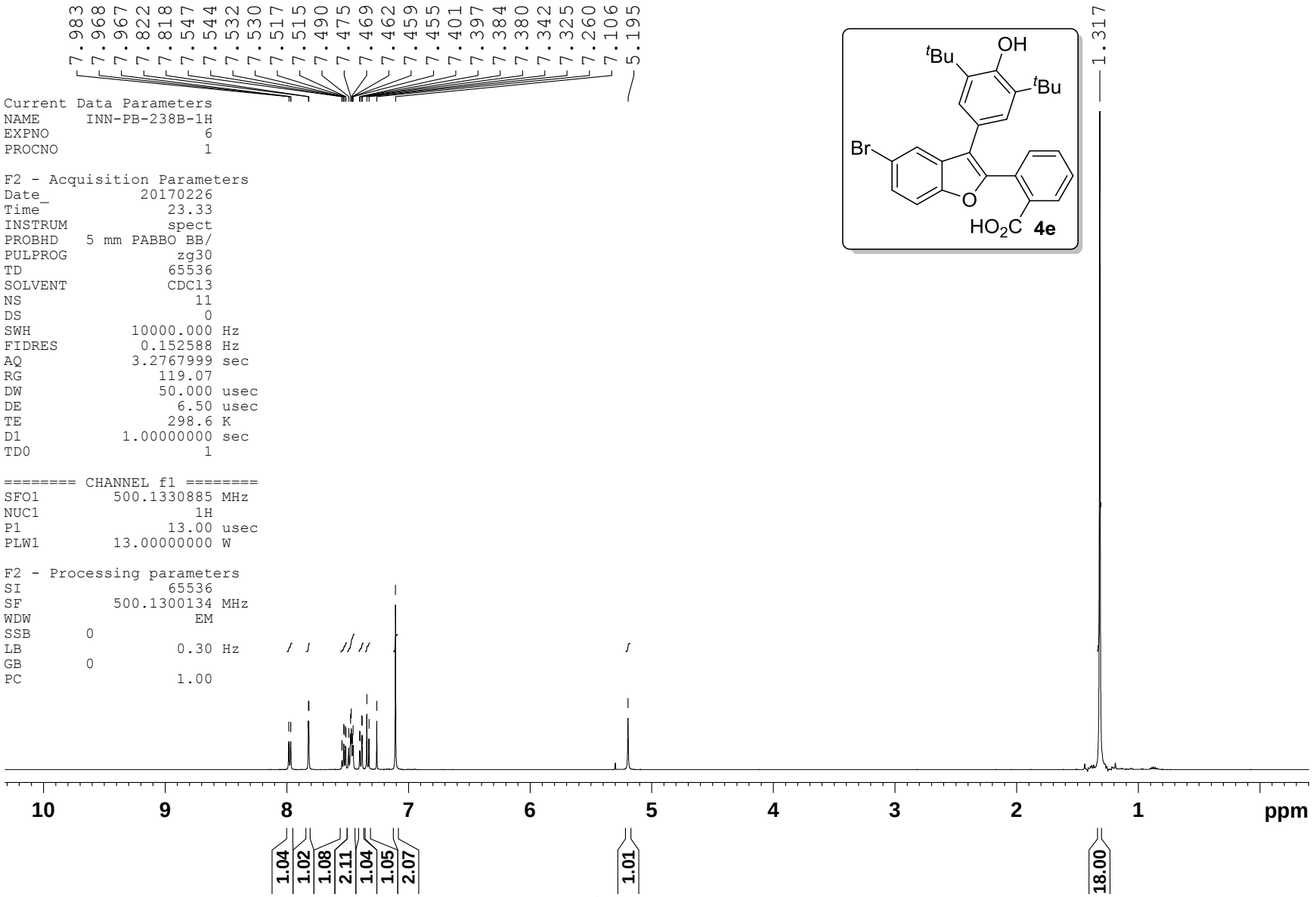


Figure S43. ^{1}H NMR Spectrum of 4e

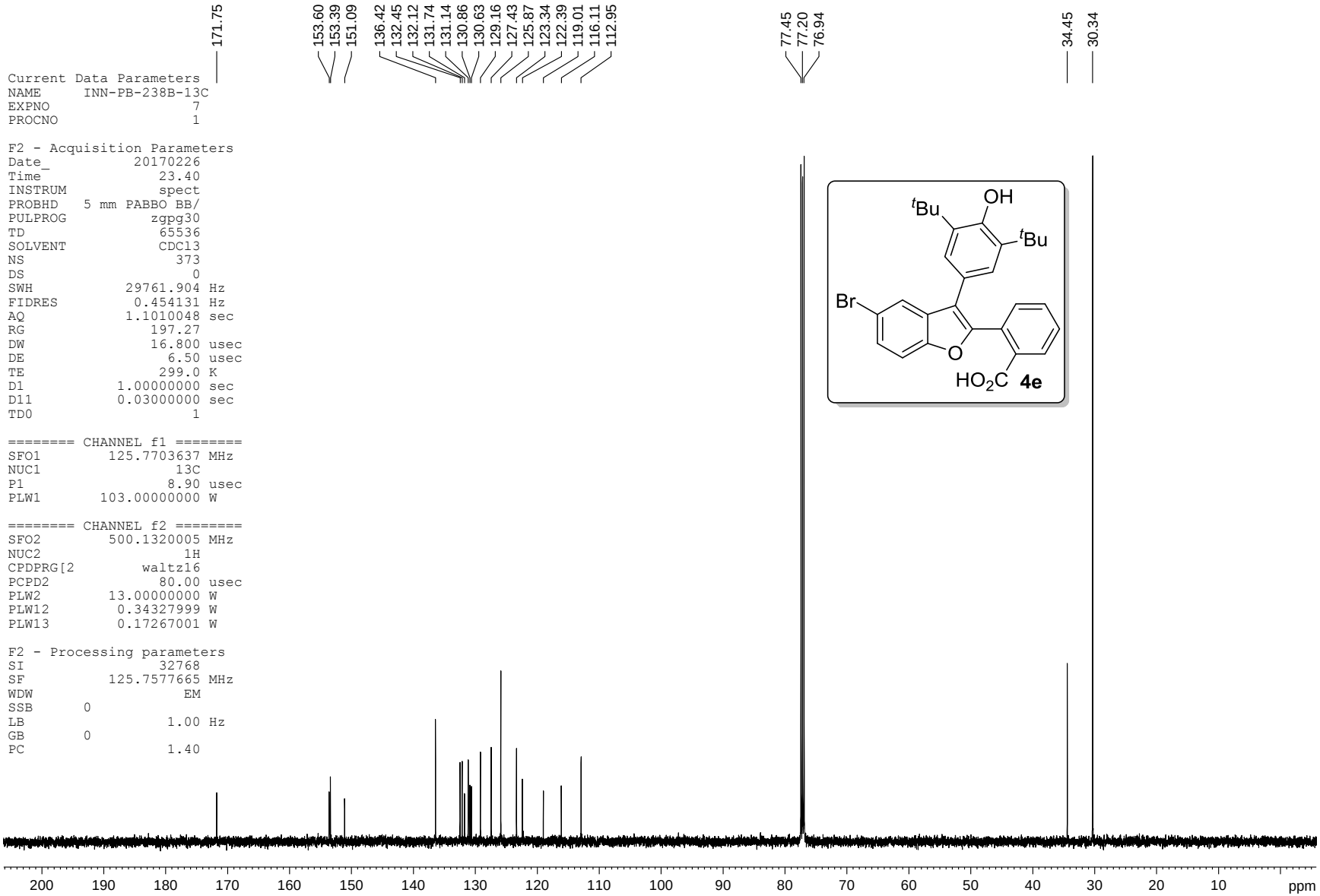


Figure S44. ^{13}C NMR Spectrum of 4e

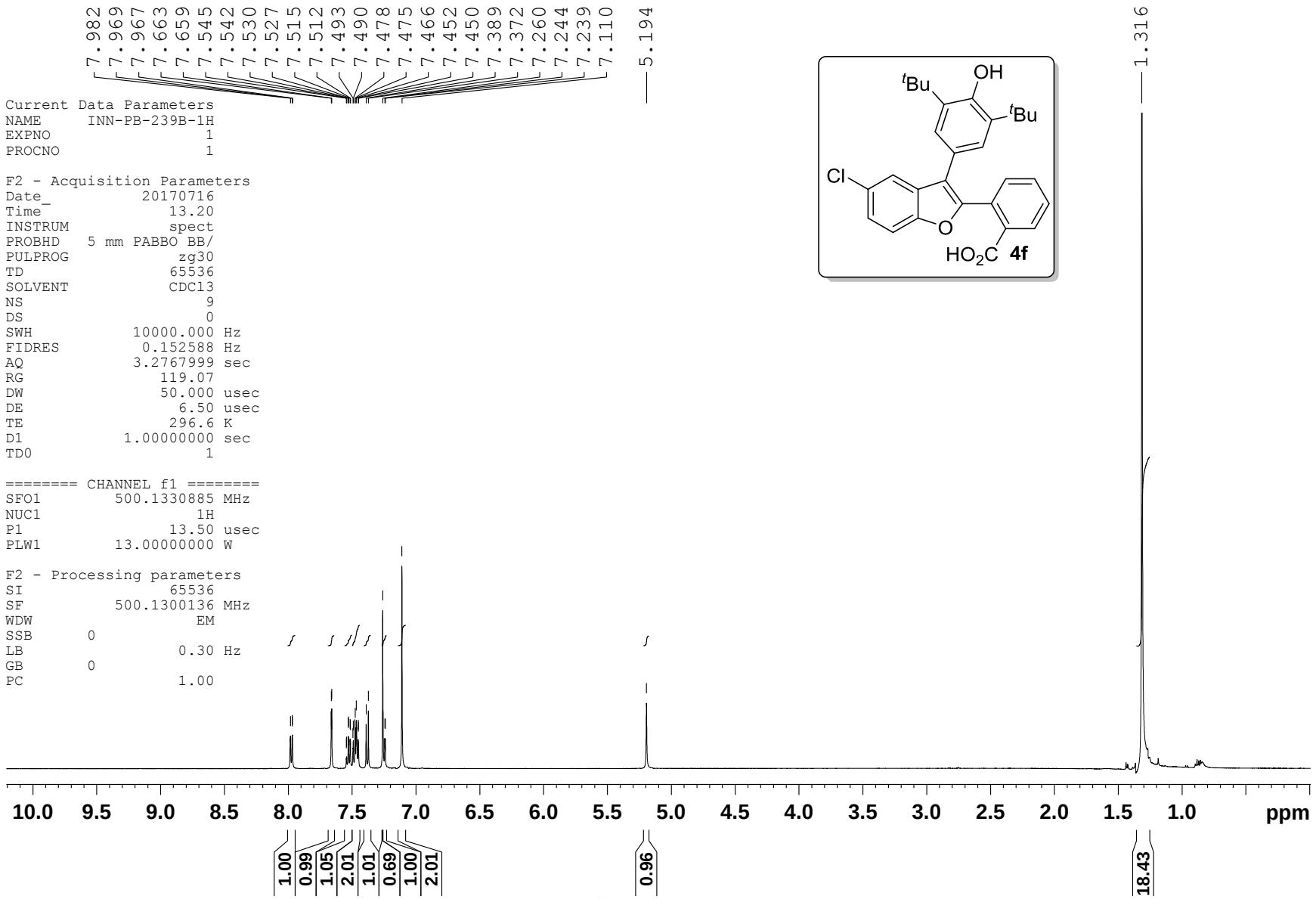


Figure S45. ^{1}H NMR Spectrum of 4f

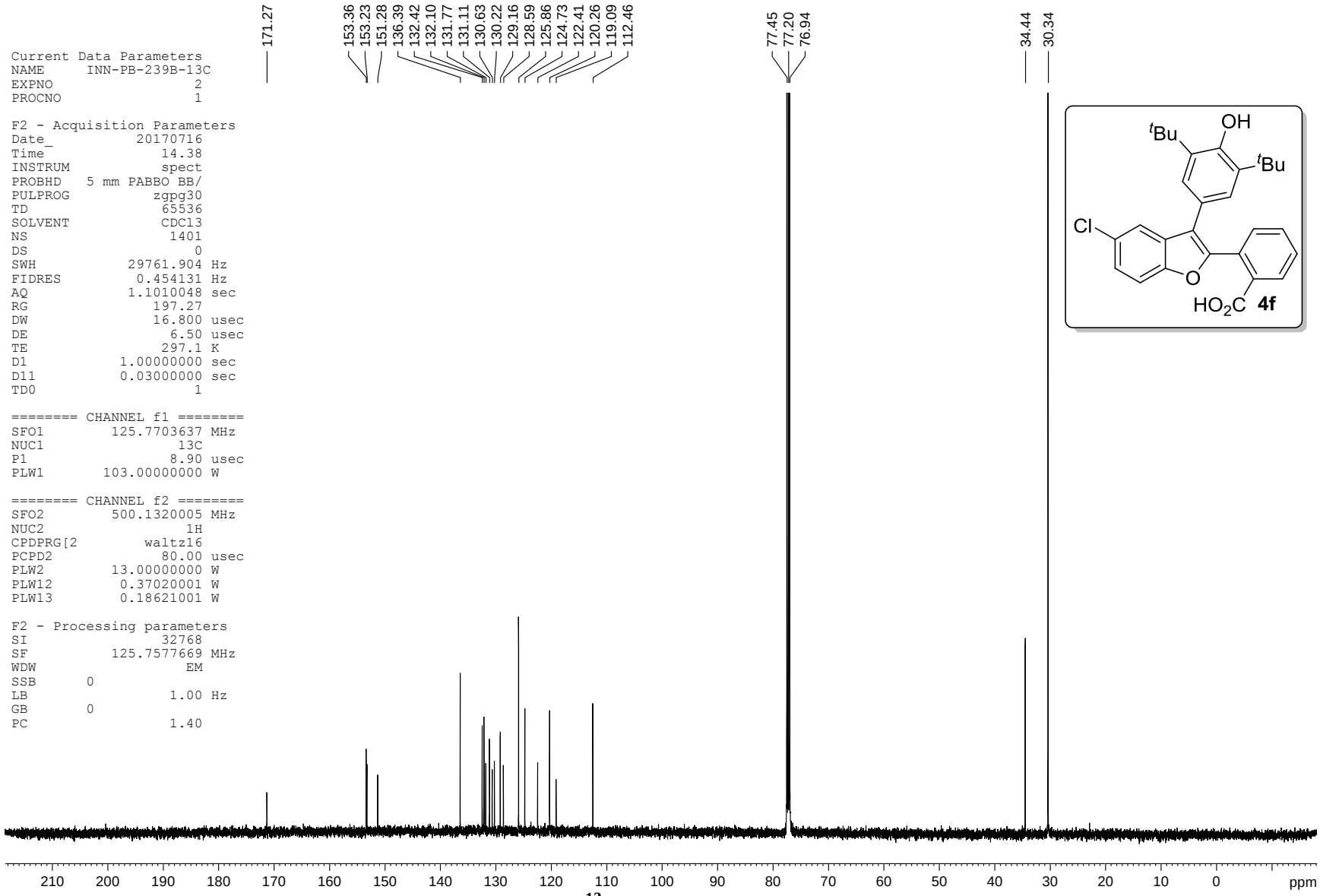


Figure S46. ^{13}C NMR Spectrum of 4f

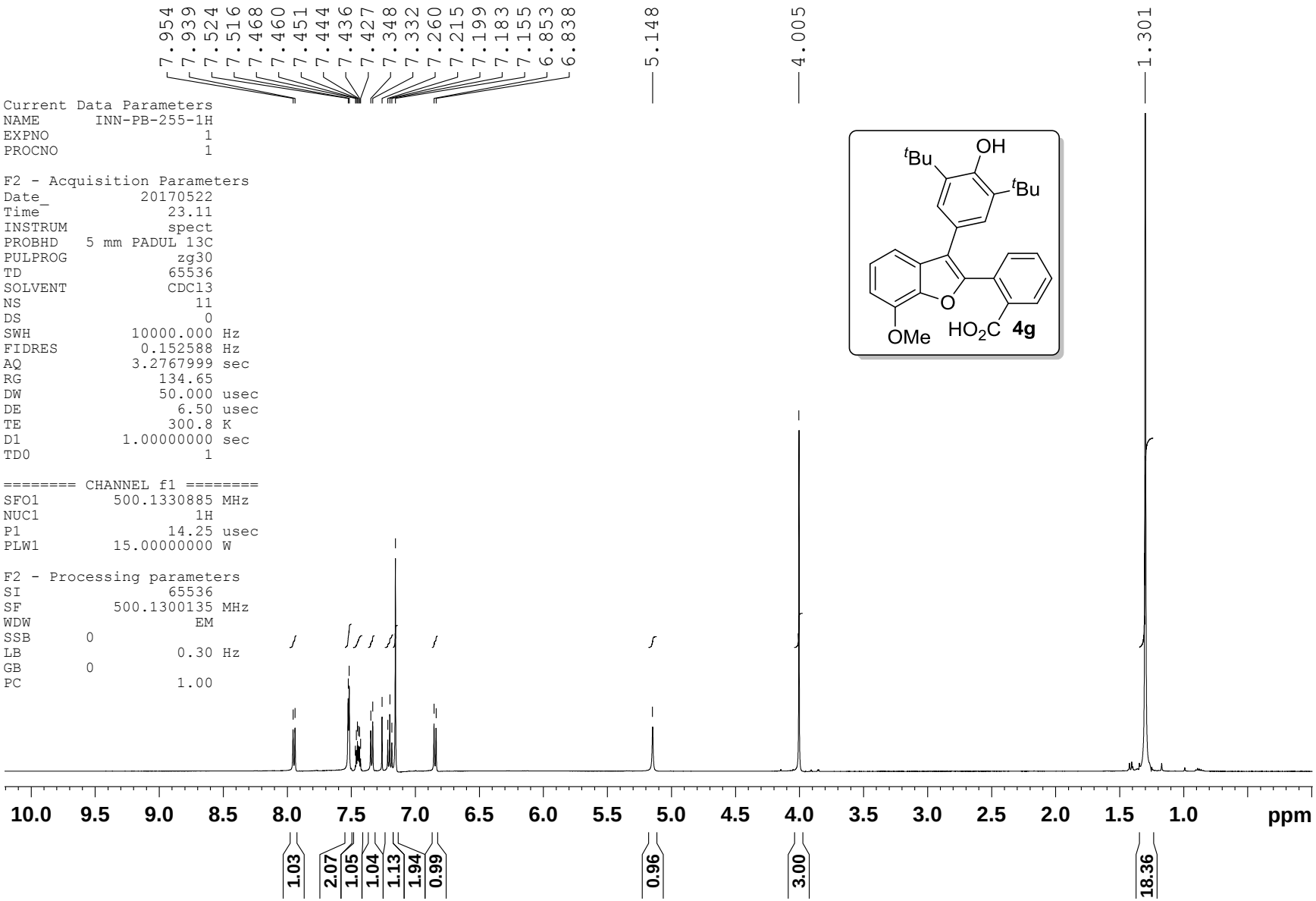


Figure S47. ^{1}H NMR Spectrum of 4g

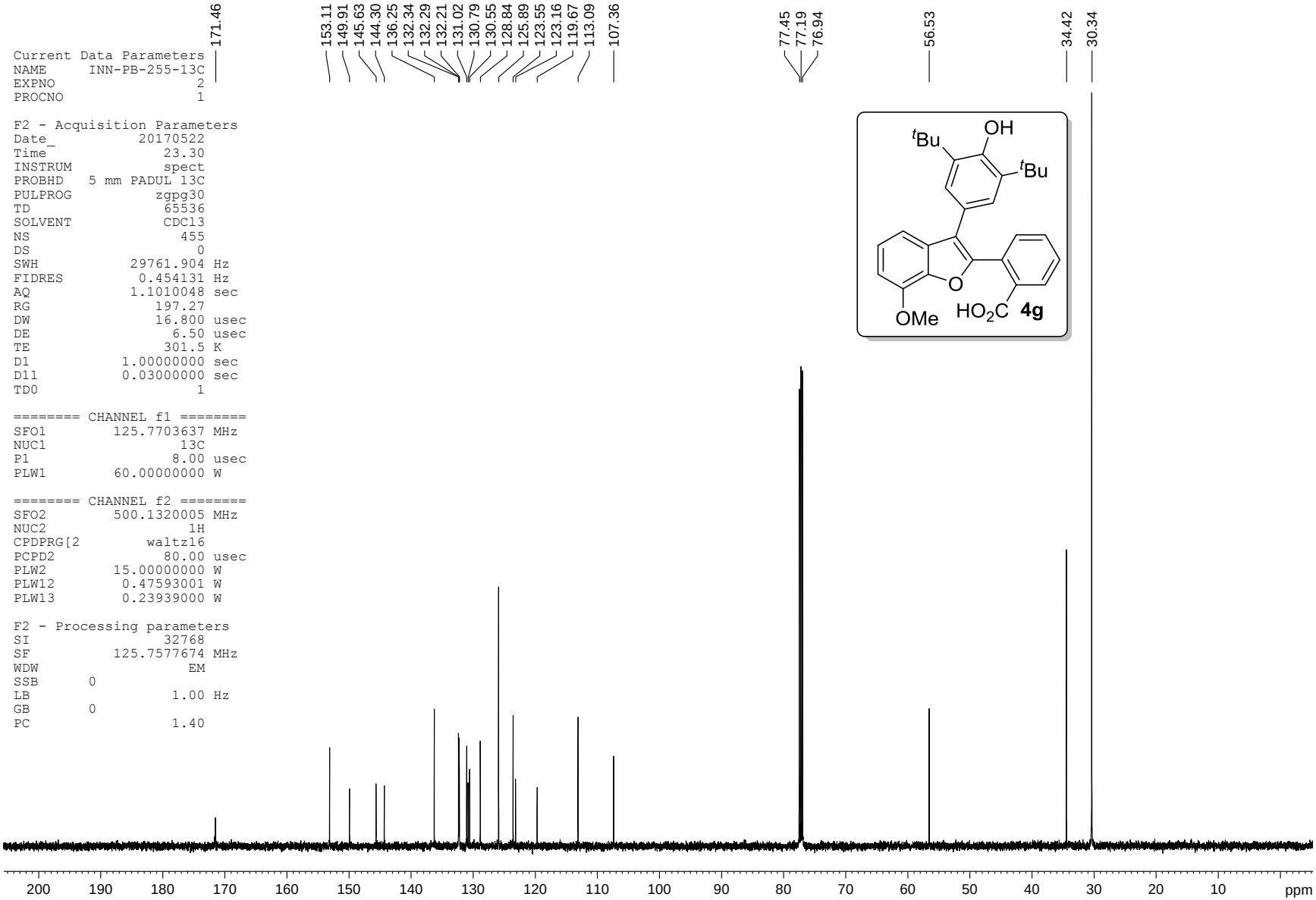


Figure S48. ^{13}C NMR Spectrum of 4g

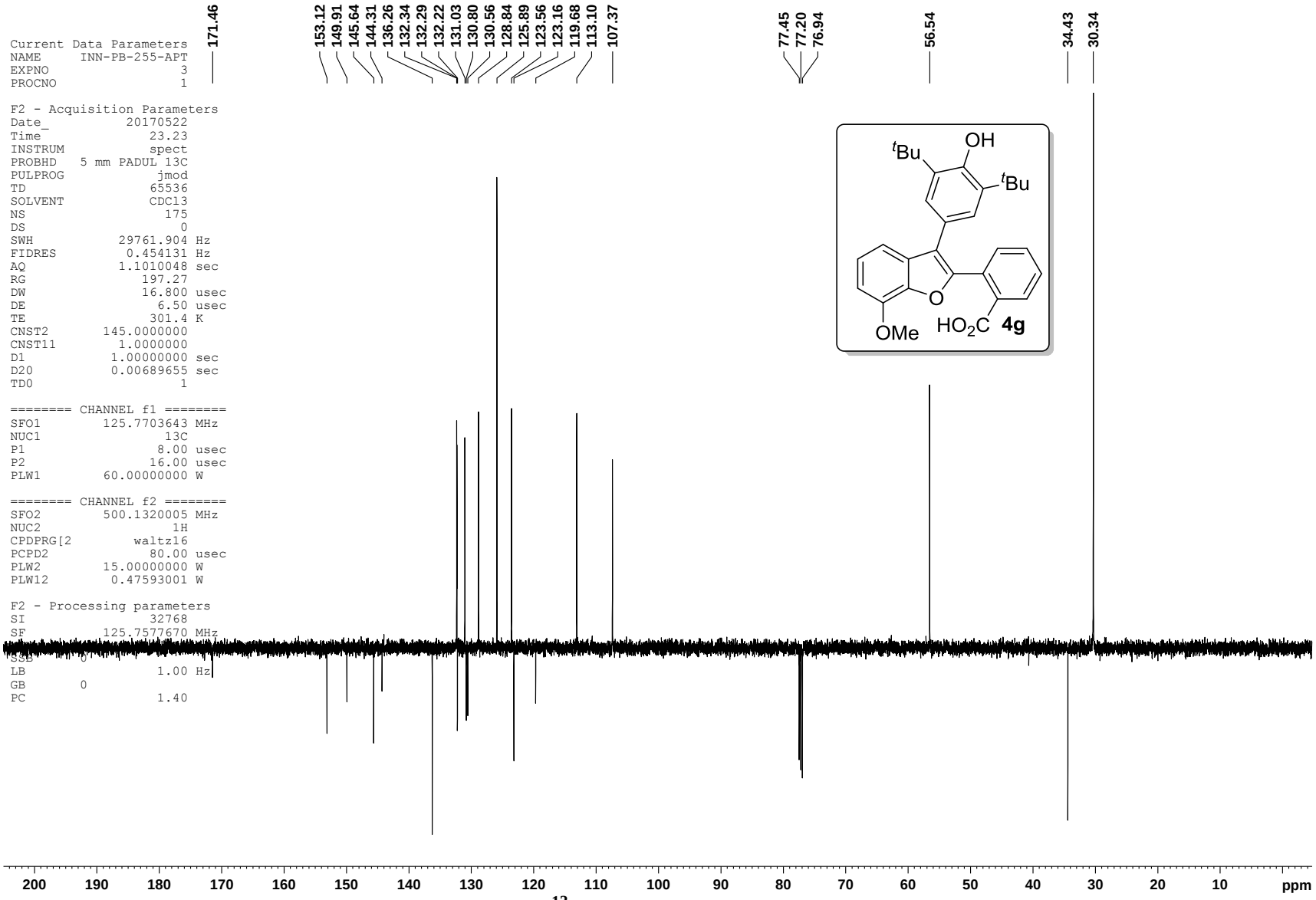


Figure S49. ^{13}C-APT NMR Spectrum of 4g

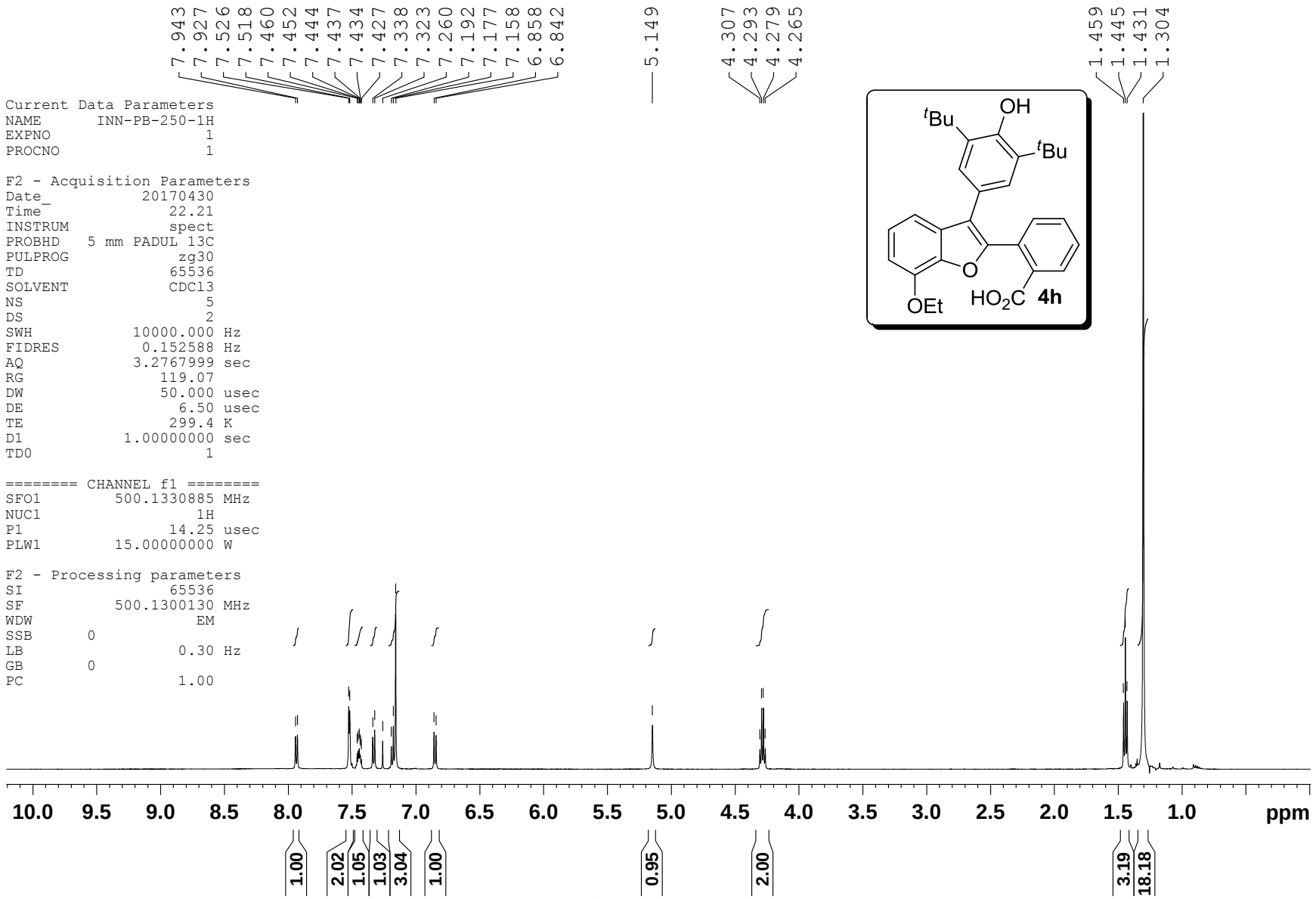


Figure S50. ^{1}H NMR Spectrum of 4h

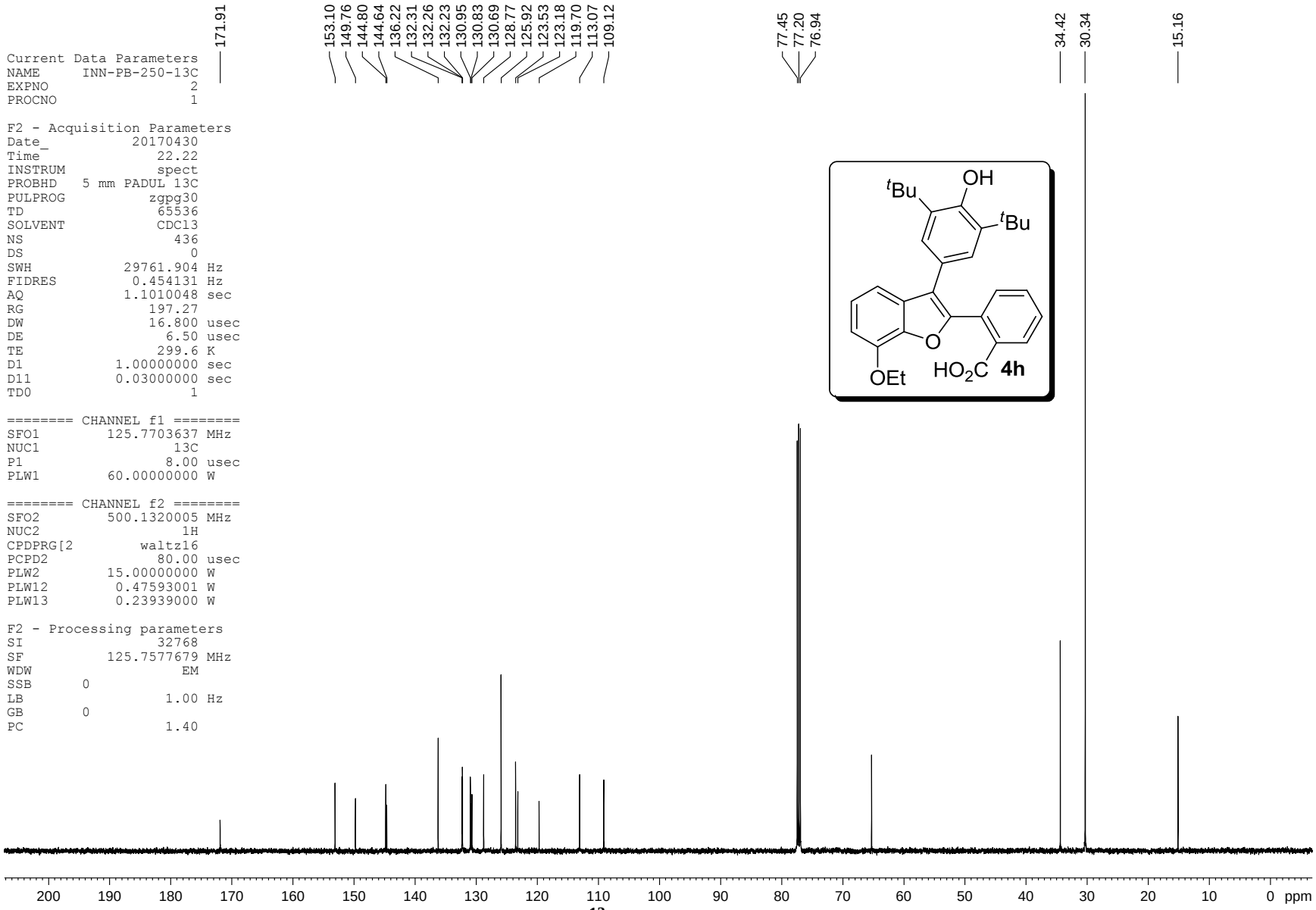


Figure S51. ^{13}C NMR Spectrum of 4h

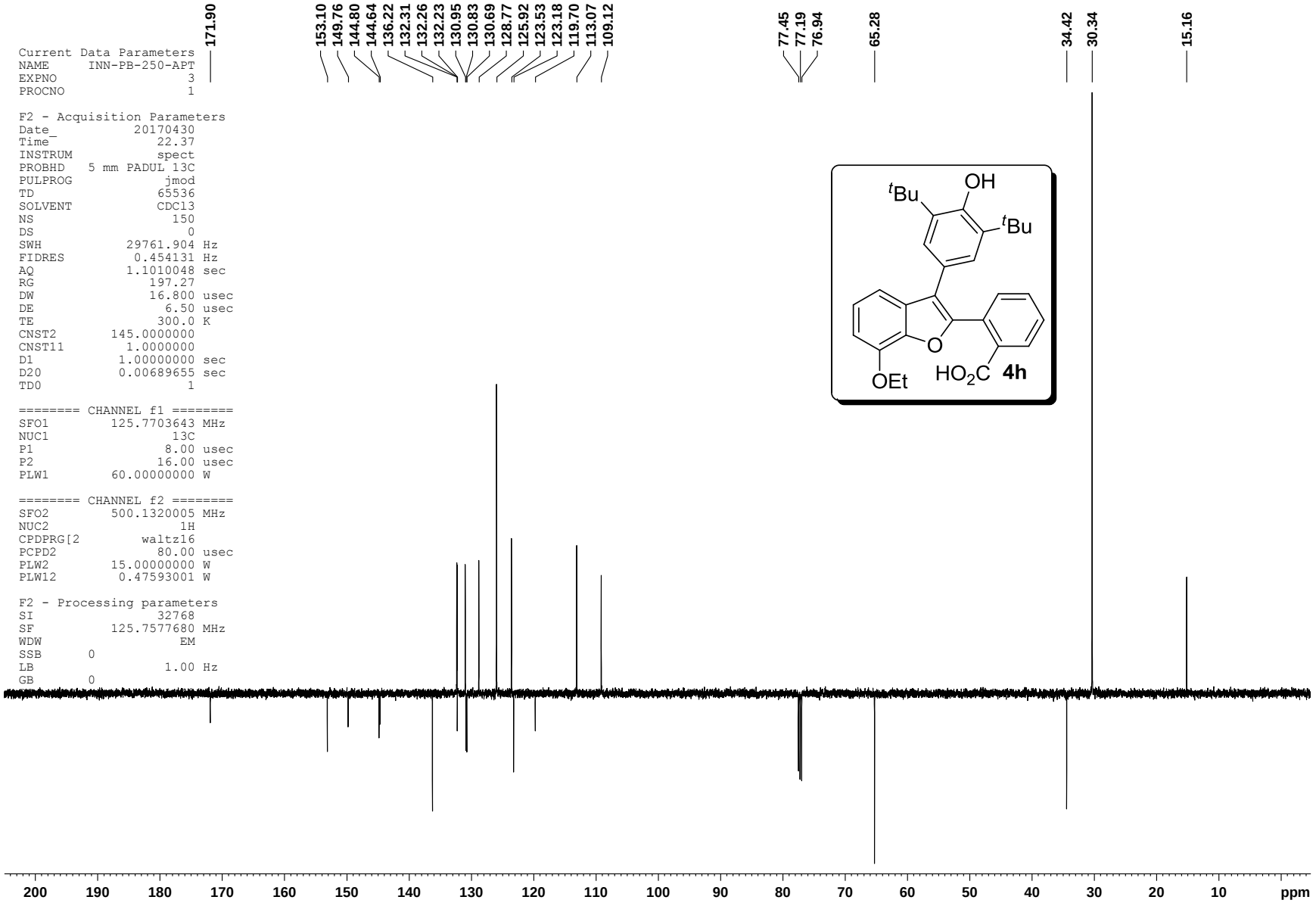


Figure S52. ^{13}C-APT NMR Spectrum of 4h

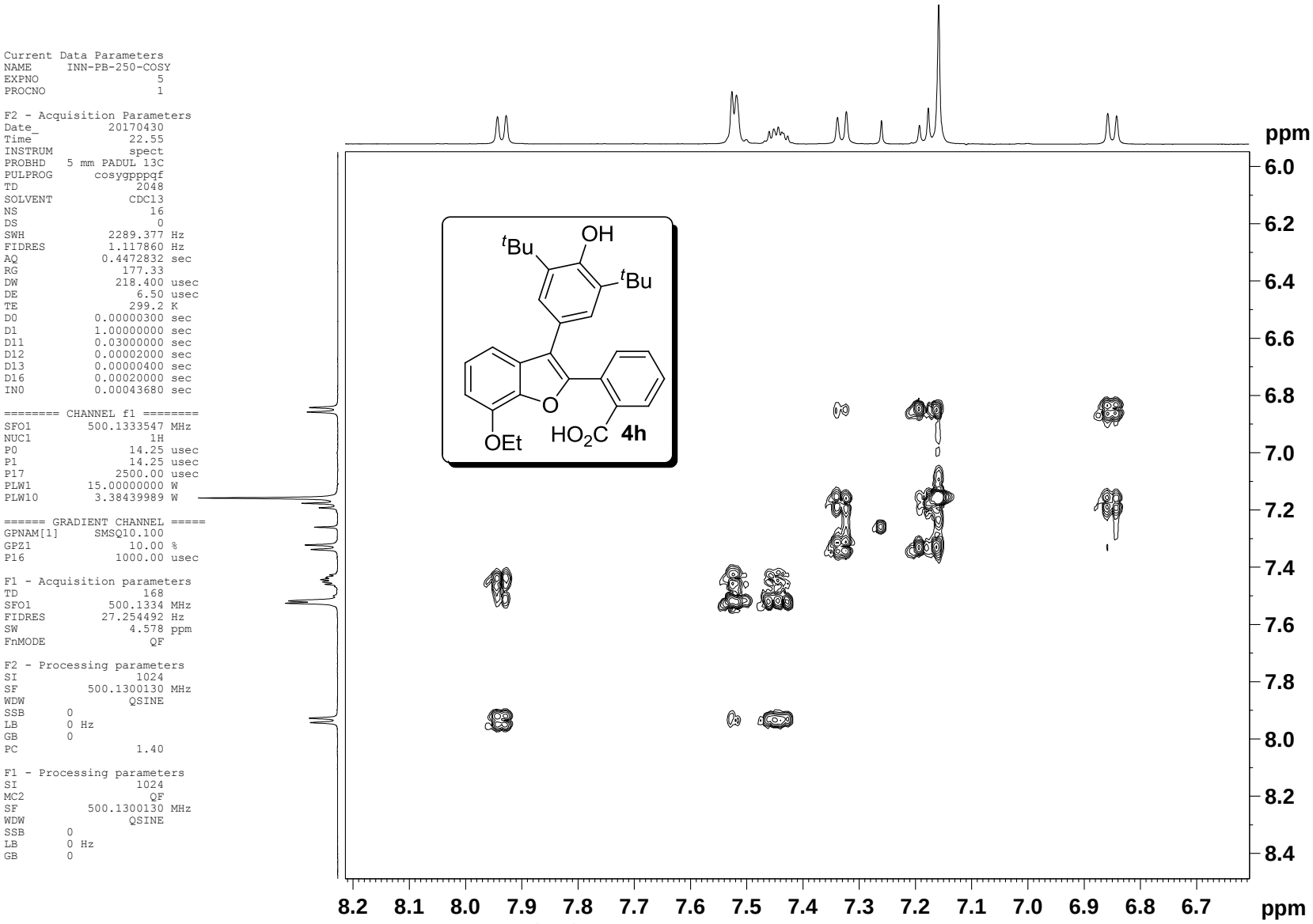


Figure S53. ^{1}H-^{1}H COSY NMR Spectrum of 4h

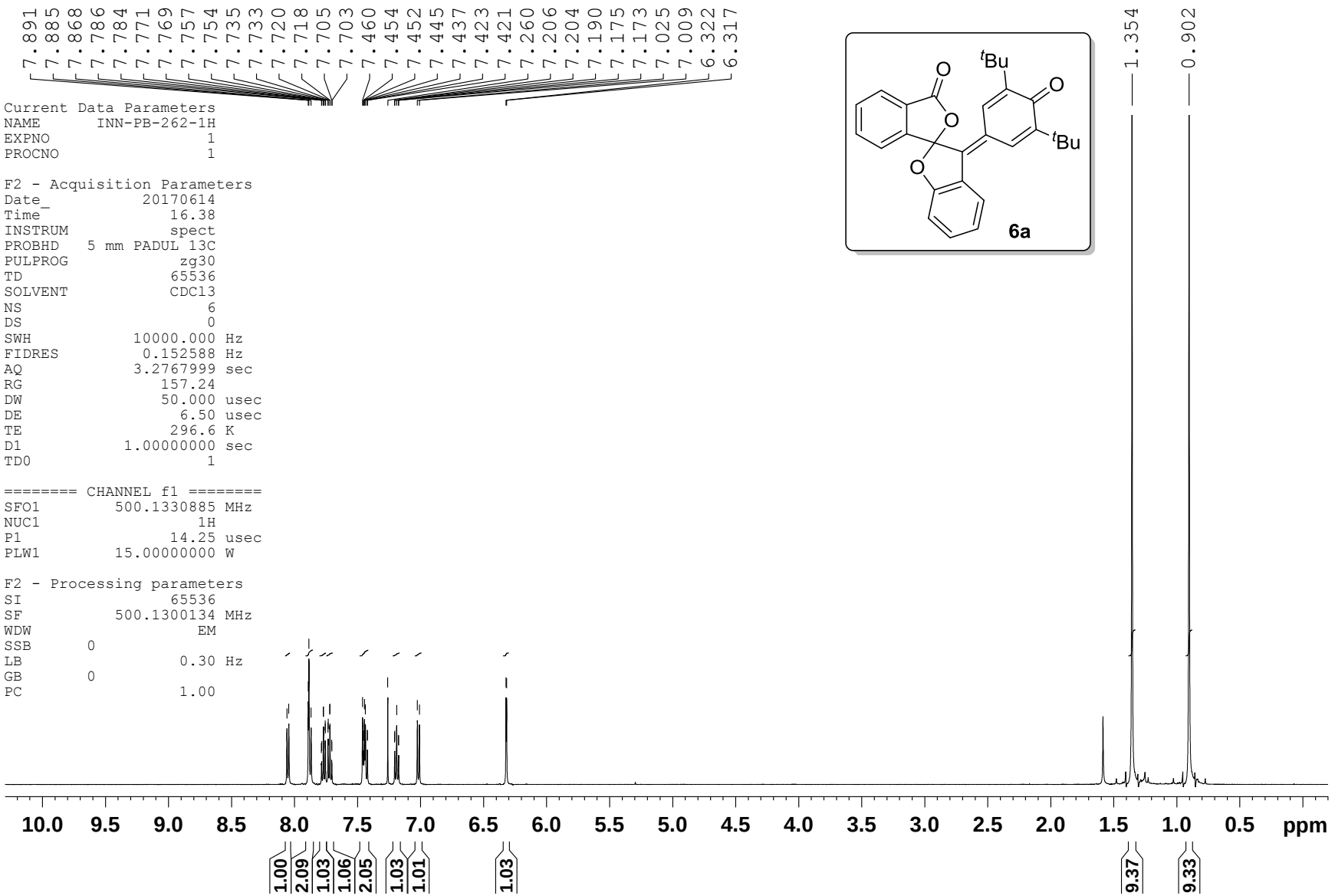


Figure S54. ^{1}H NMR Spectrum of 6a

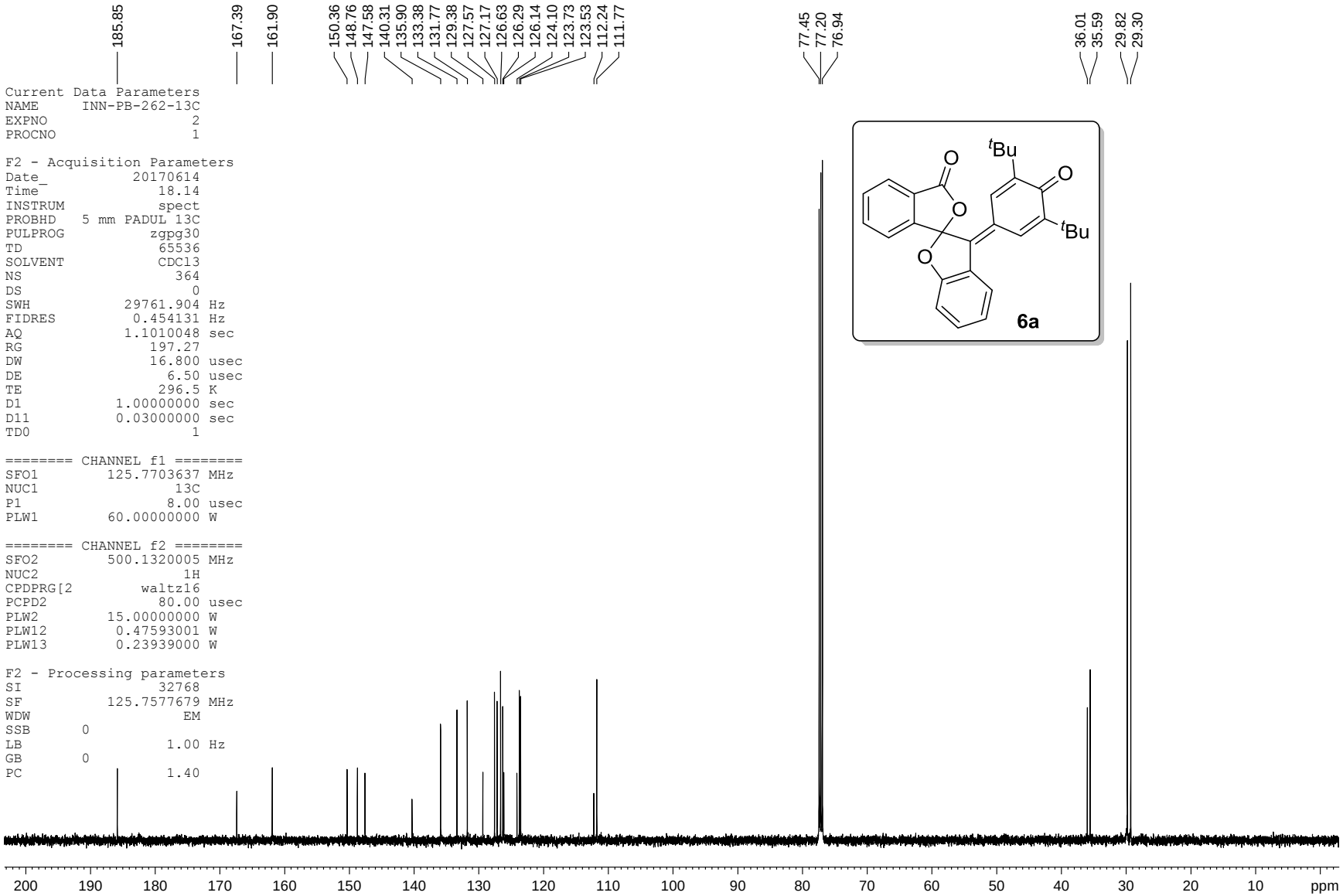


Figure S55. ^{13}C NMR Spectrum of 6a

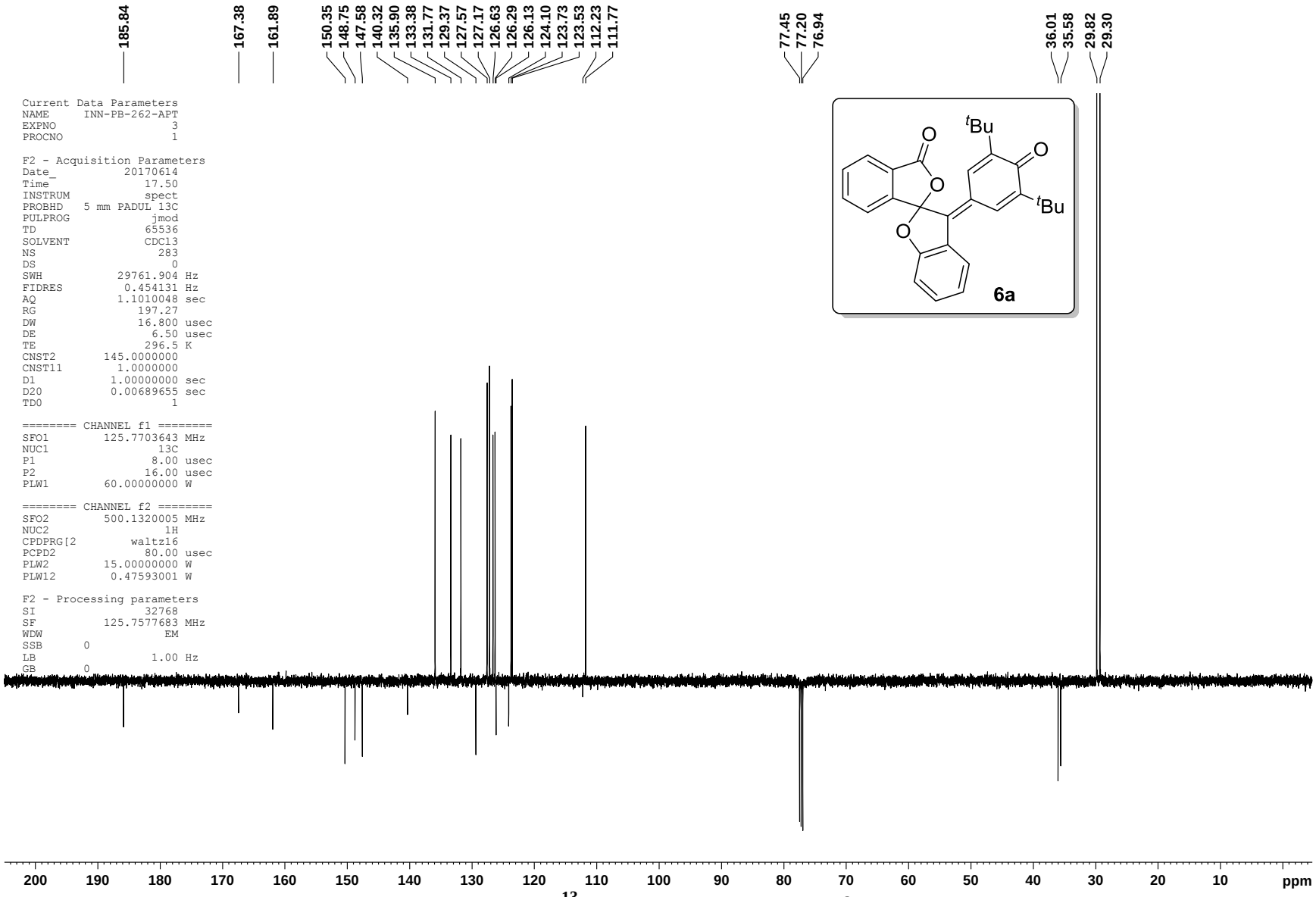


Figure S56. ^{13}C-APT NMR Spectrum of 6a

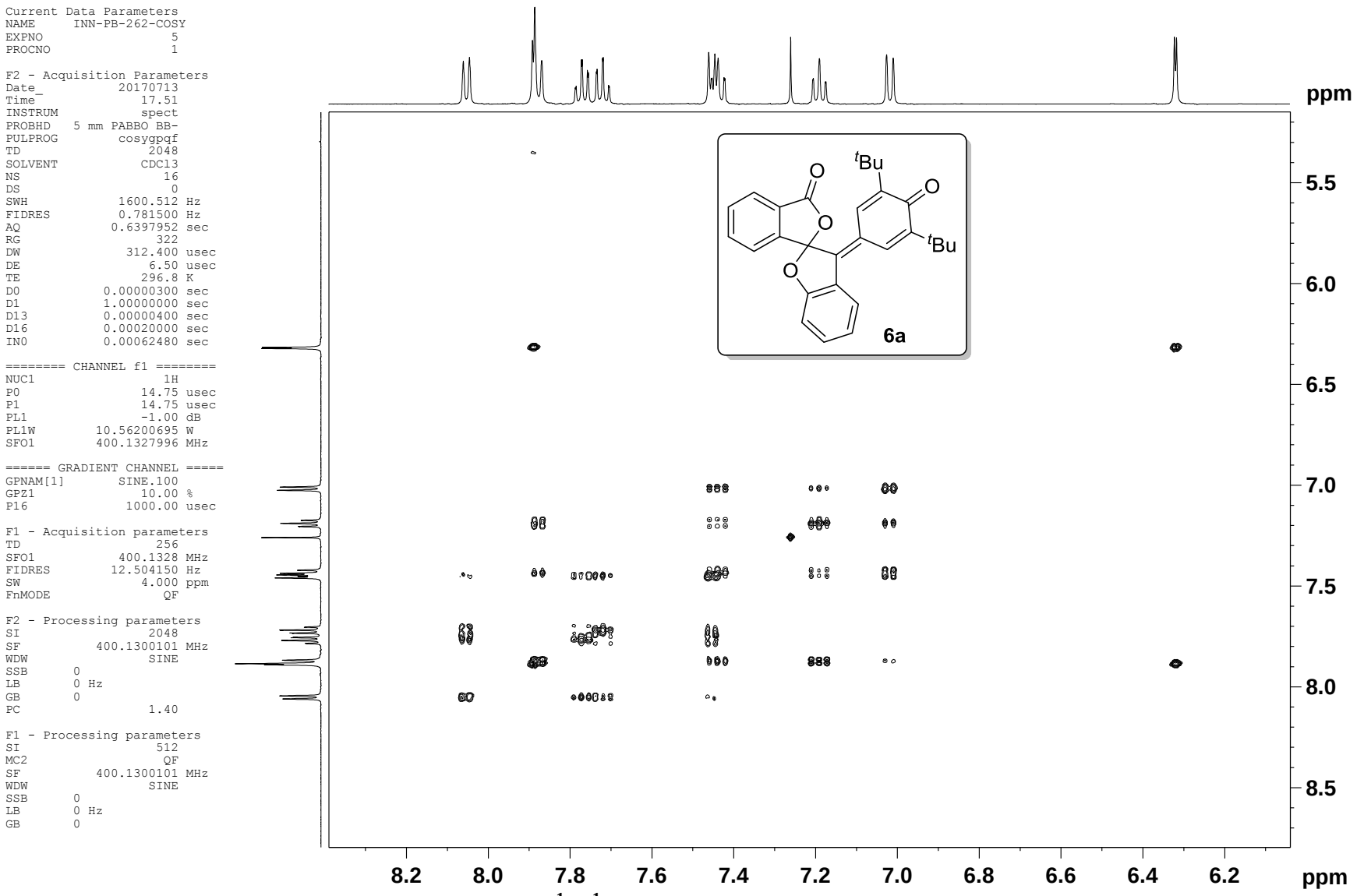


Figure S57. ^{1}H-^{1}H COSY NMR Spectrum of 6a

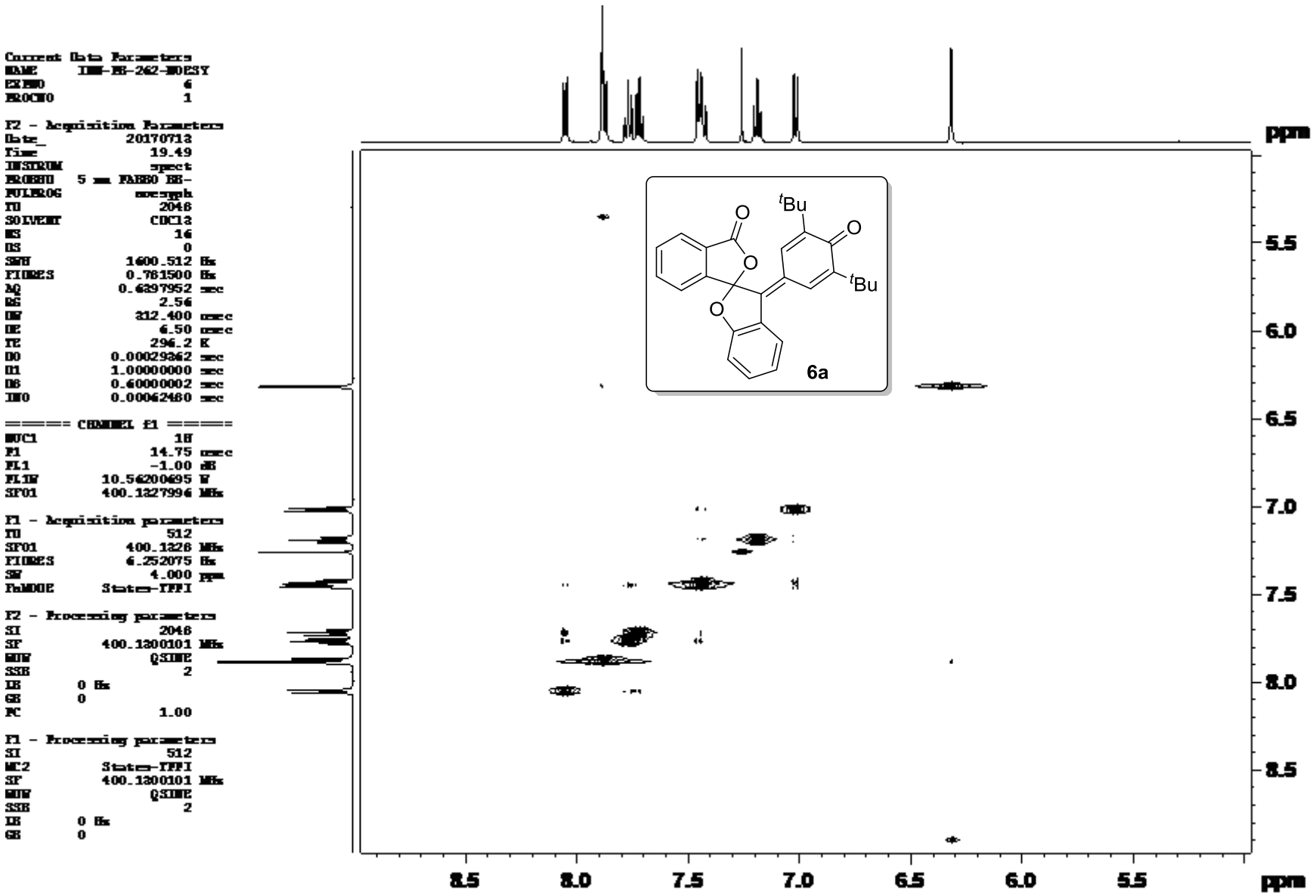


Figure S58. ^{1}H-^{1}H NOESY NMR Spectrum of 6a

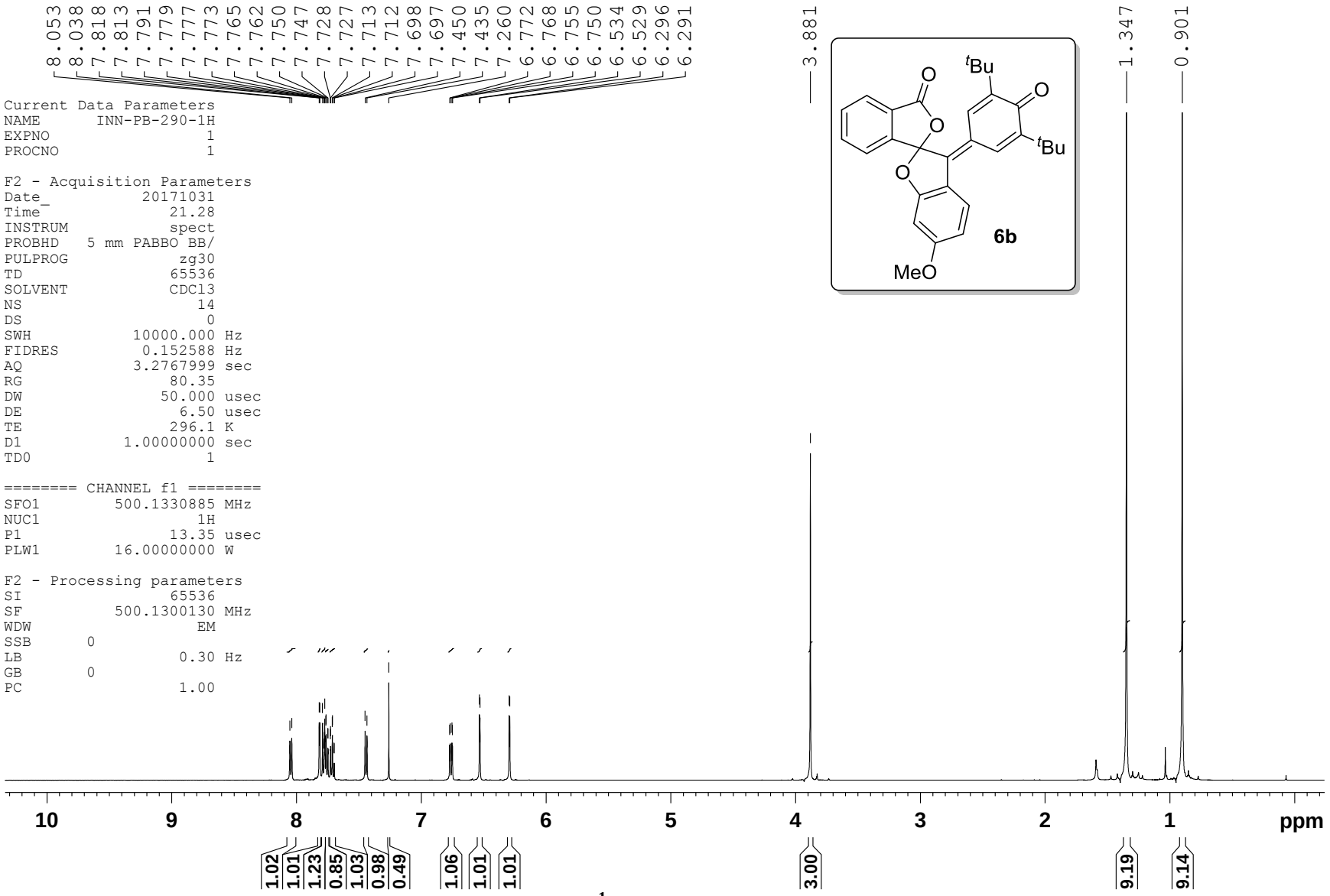


Figure S59. ^{1}H NMR Spectrum of 6b

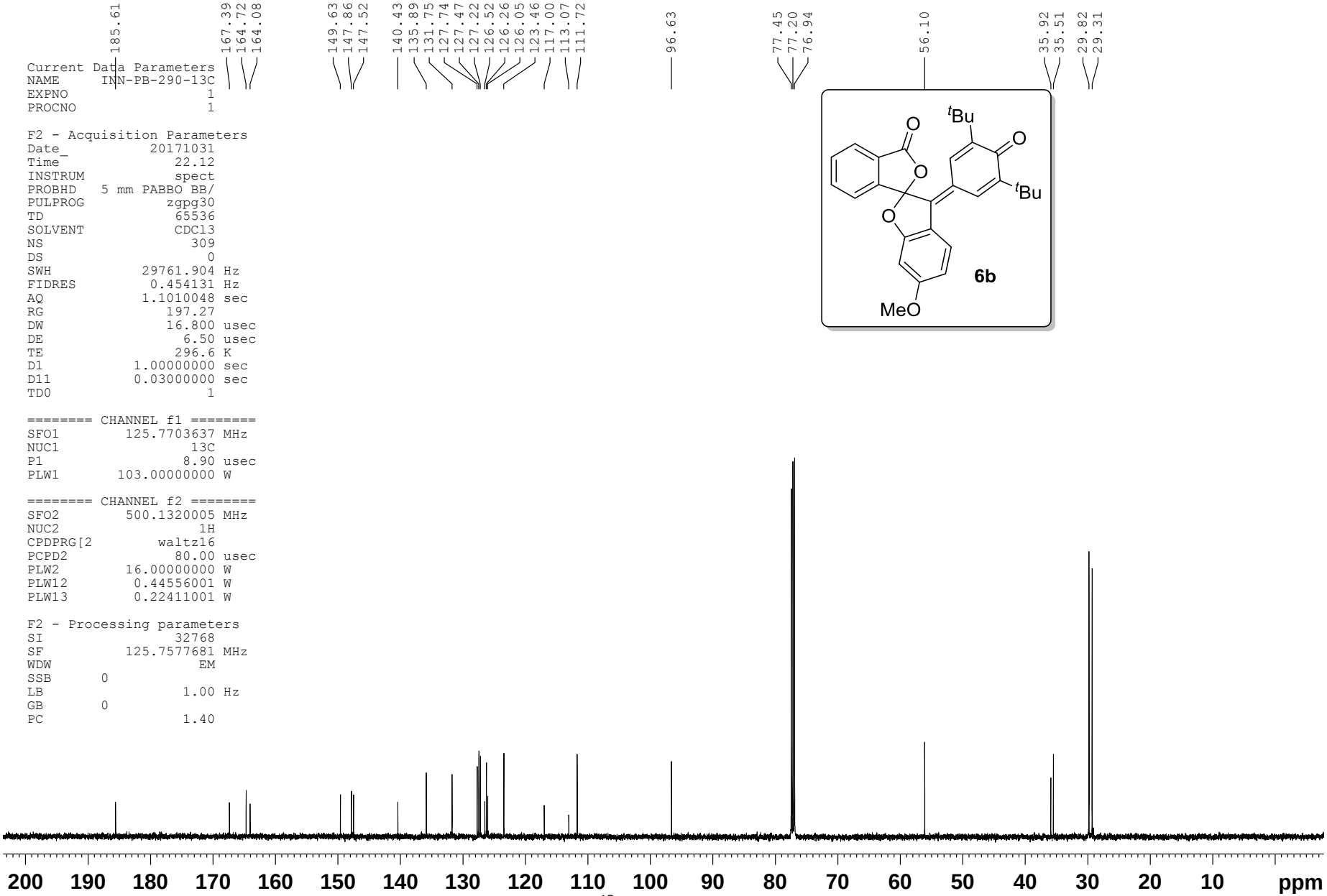


Figure S60. ^{13}C NMR Spectrum of 6b

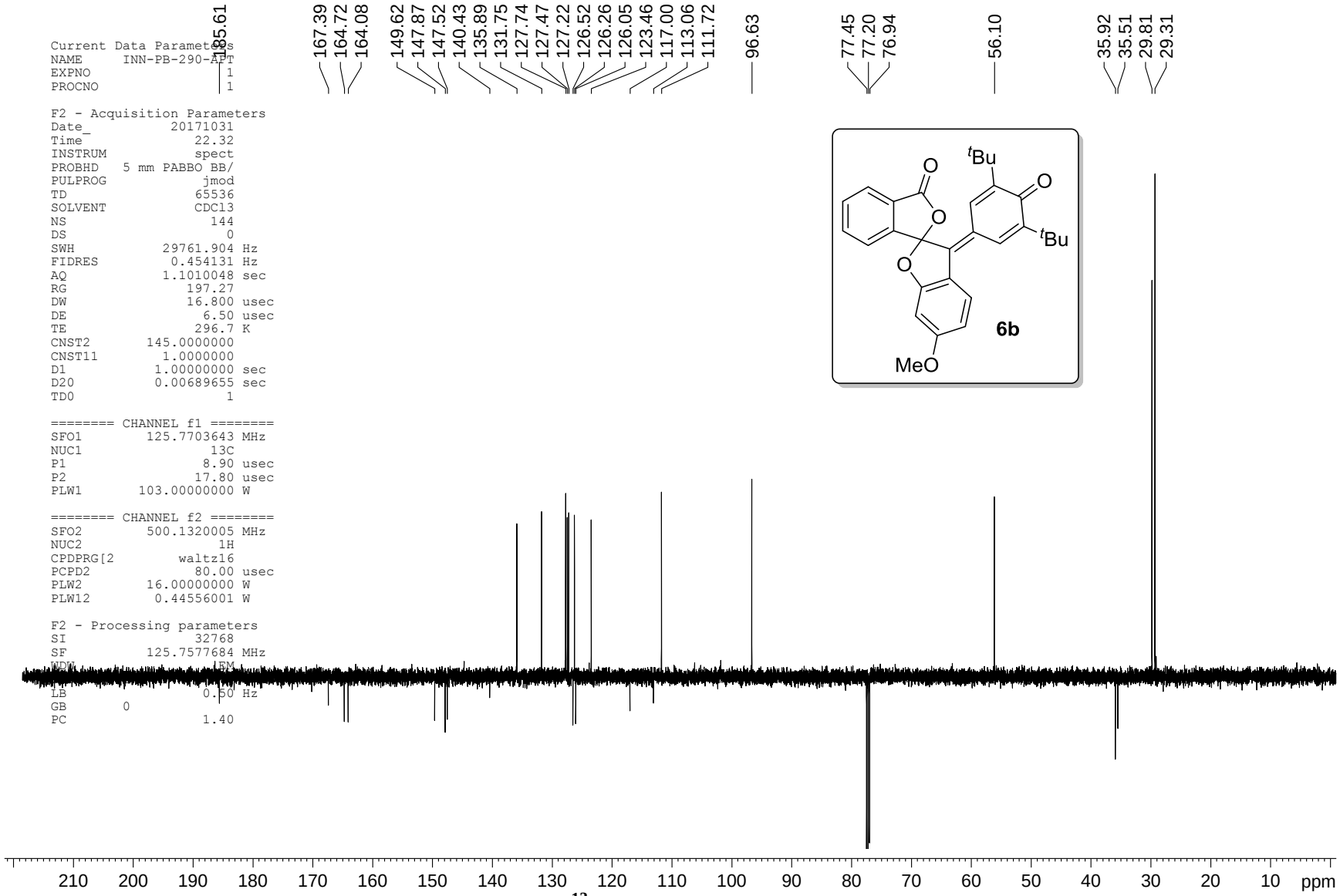


Figure S61. ^{13}C-APT NMR Spectrum of 6b

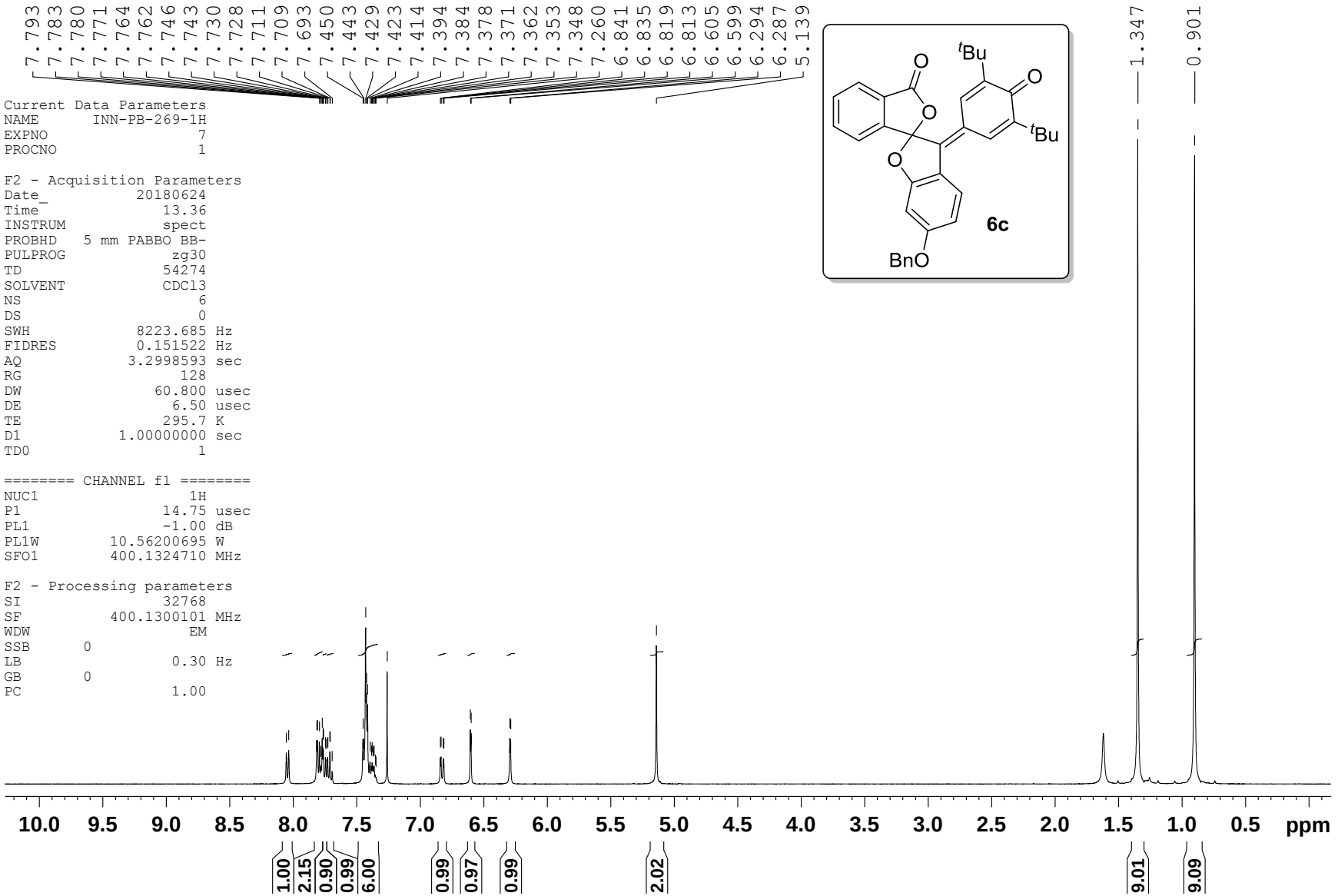


Figure S62. ^{1}H NMR Spectrum of 6c

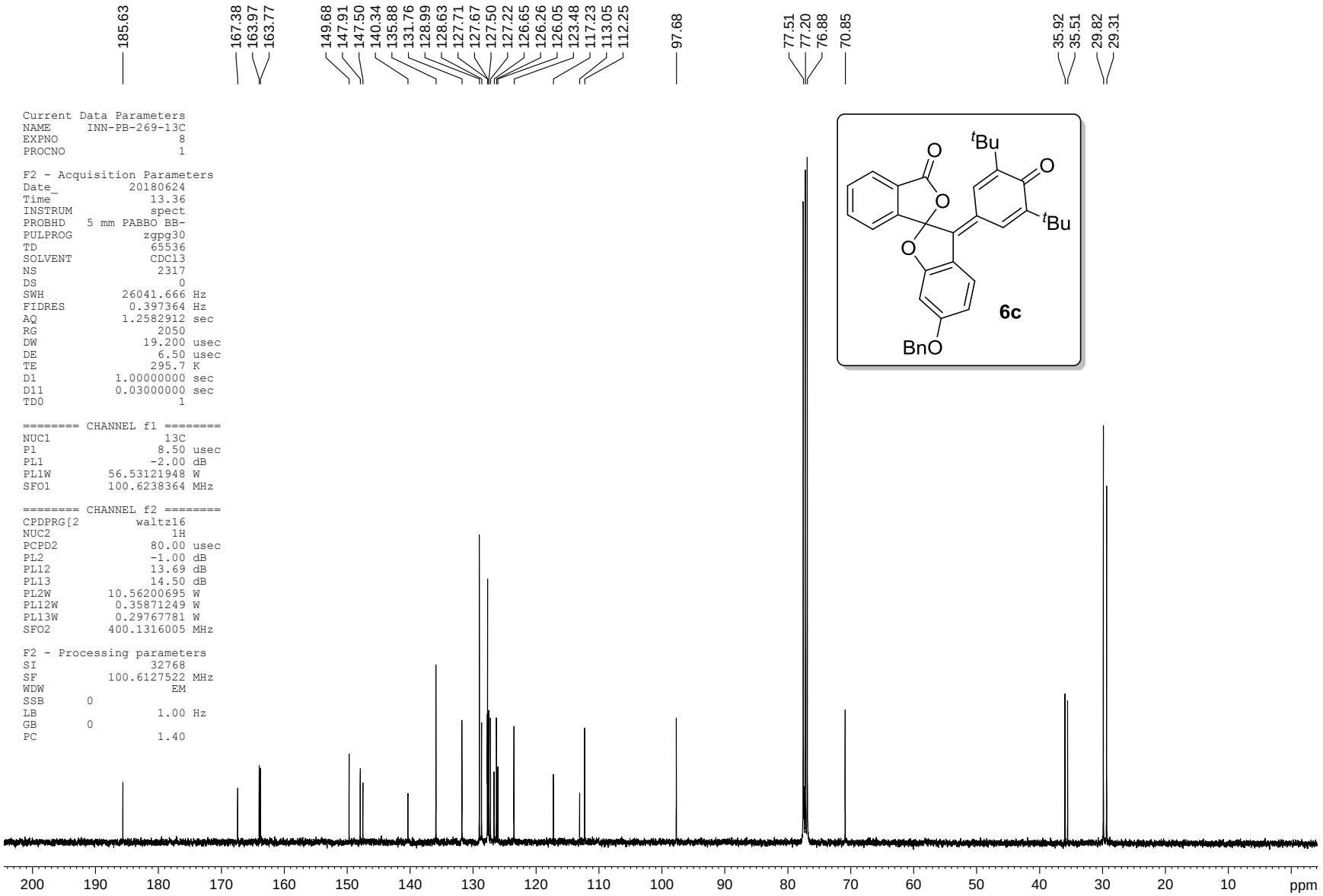


Figure S63. ^{13}C NMR Spectrum of 6c

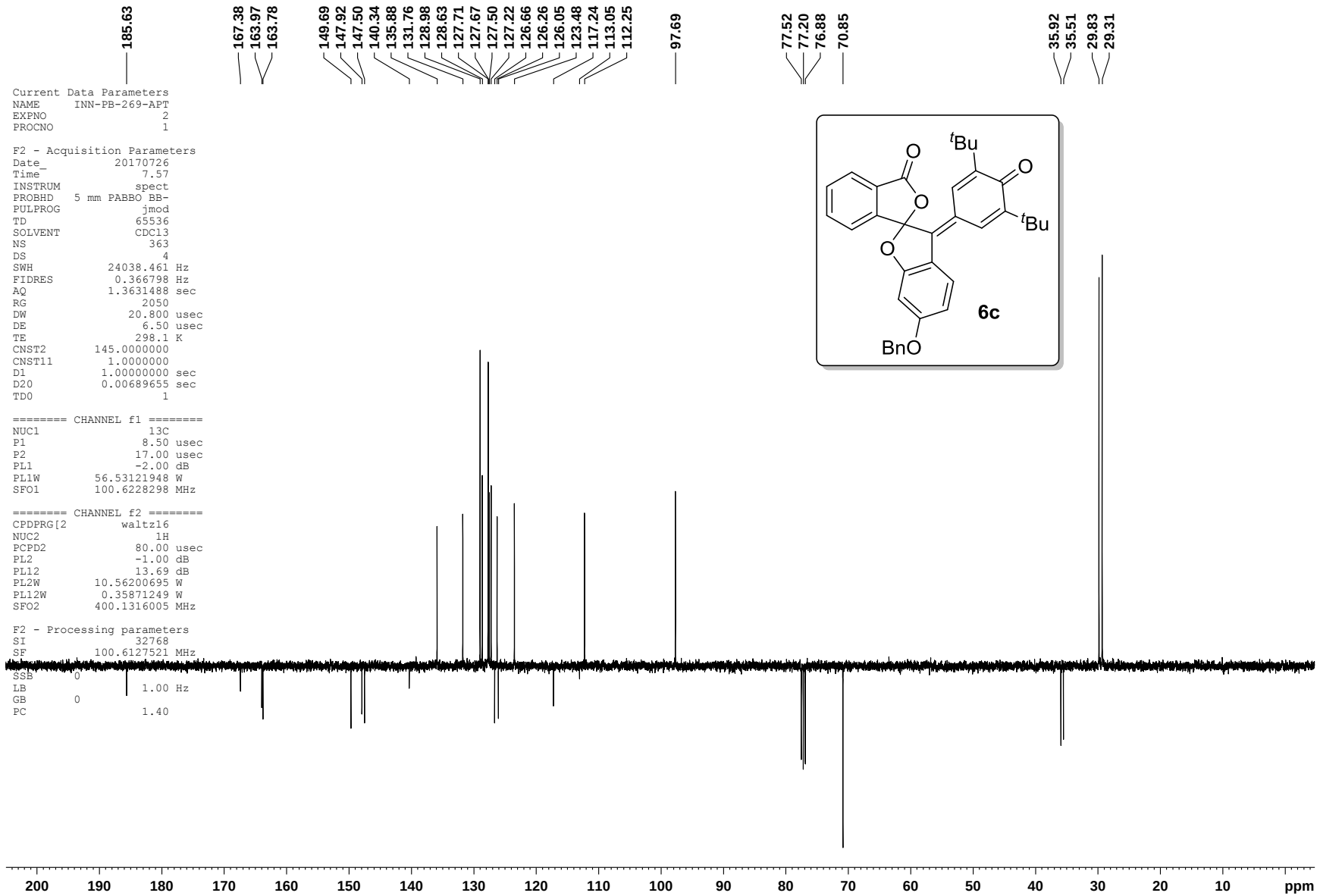


Figure S64. ^{13}C-APT NMR Spectrum of 6c

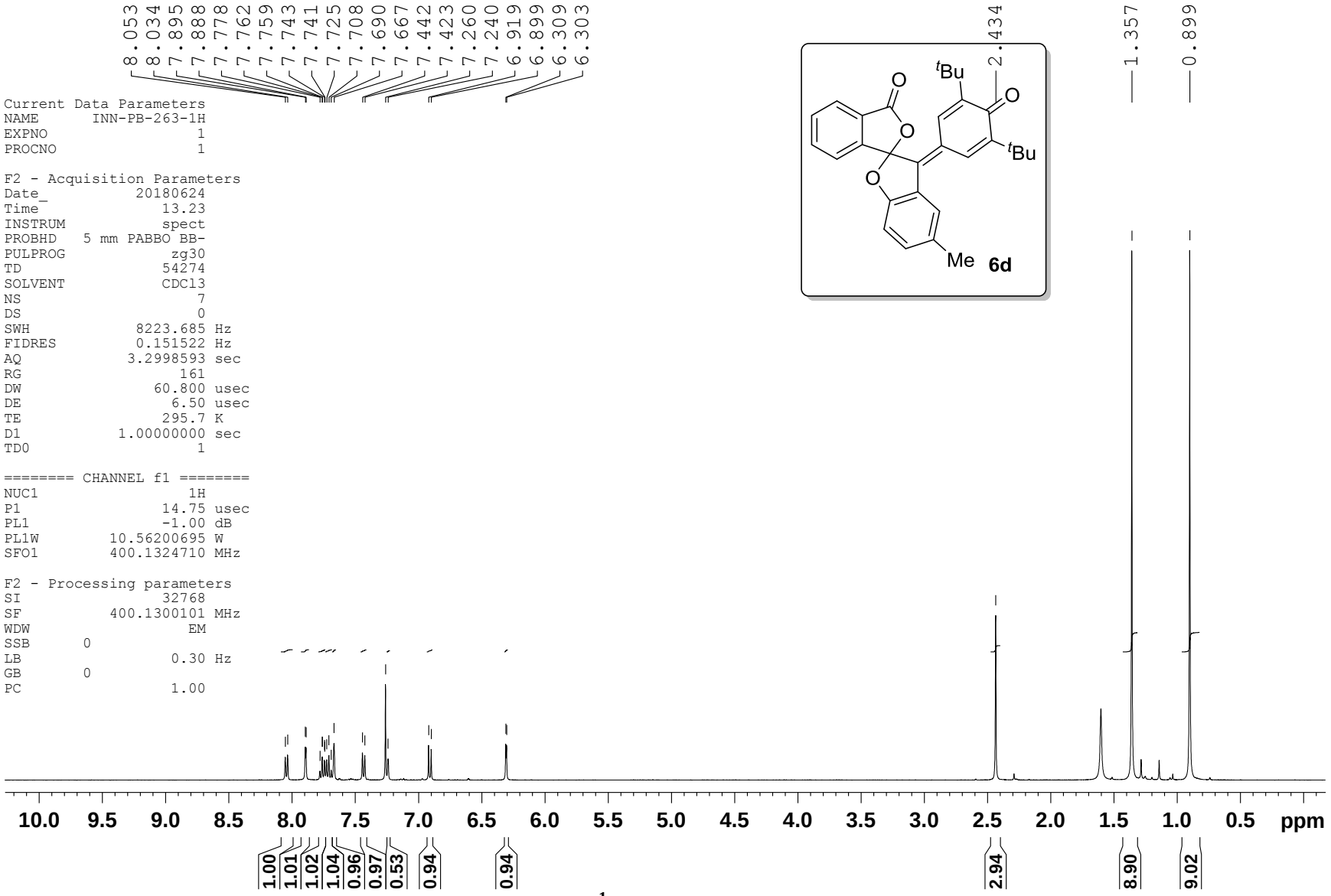


Figure S65. ^{1}H NMR Spectrum of 6d

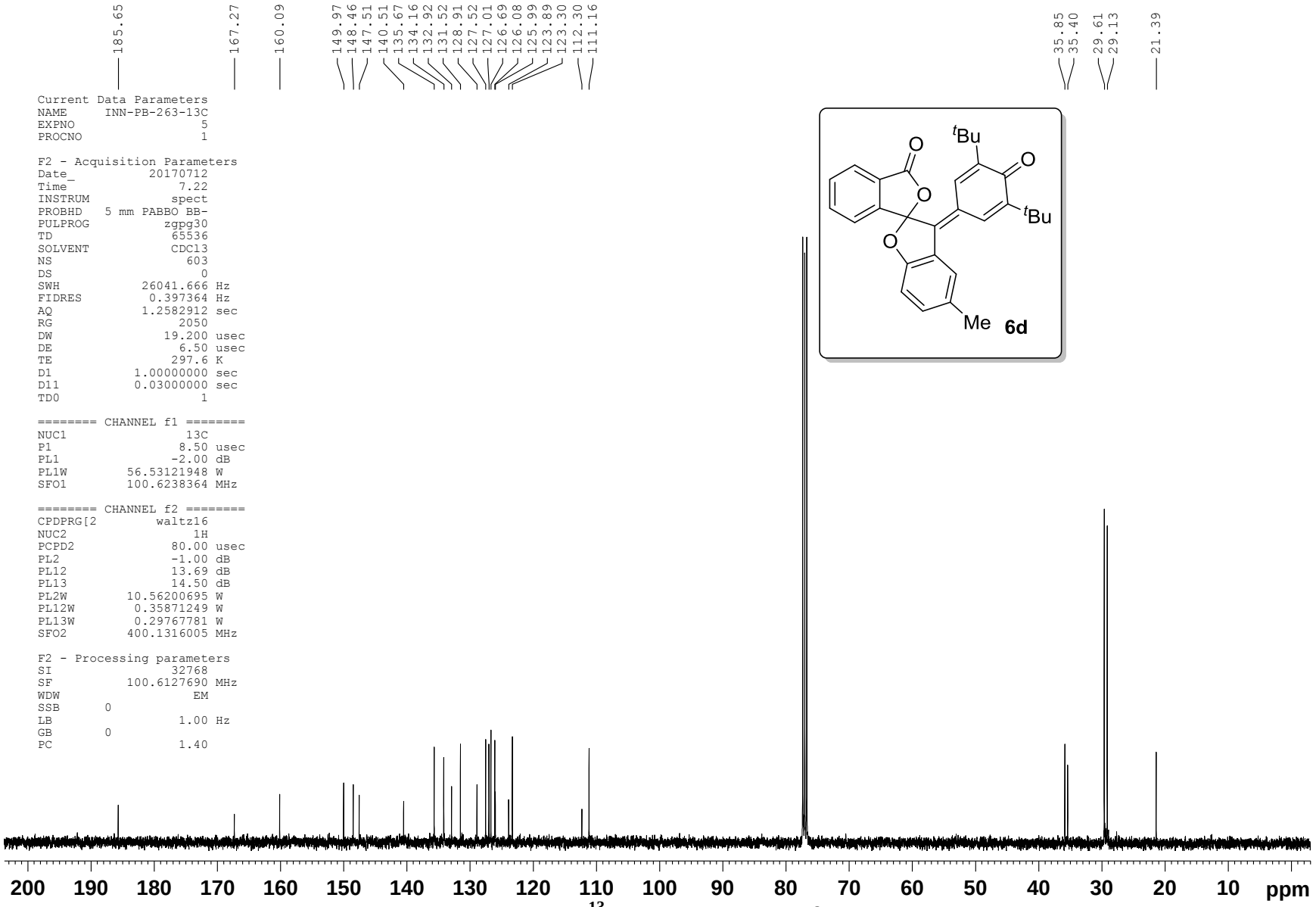


Figure S66. ^{13}C NMR Spectrum of 6d

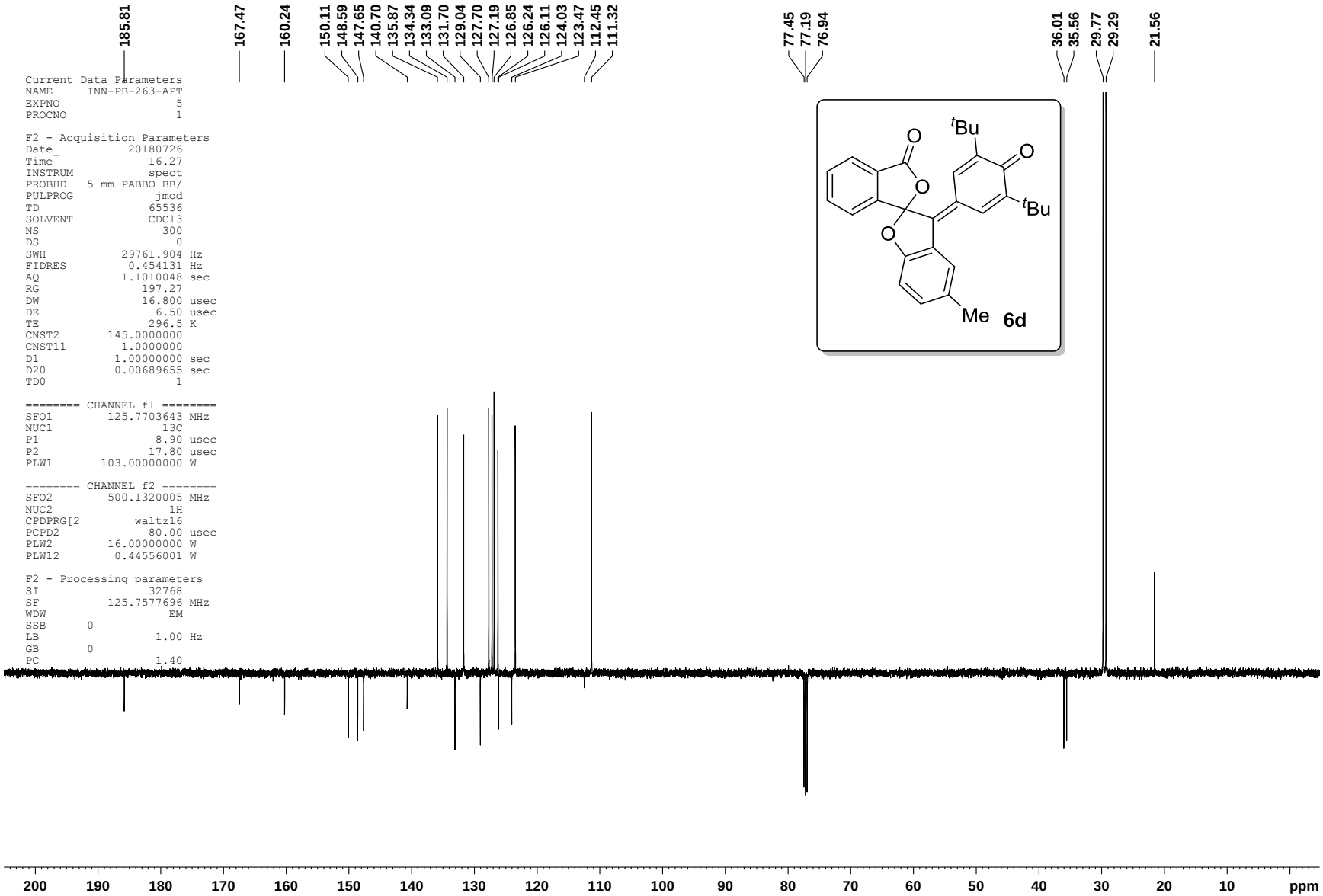


Figure S67. ^{13}C-APT NMR Spectrum of 6d

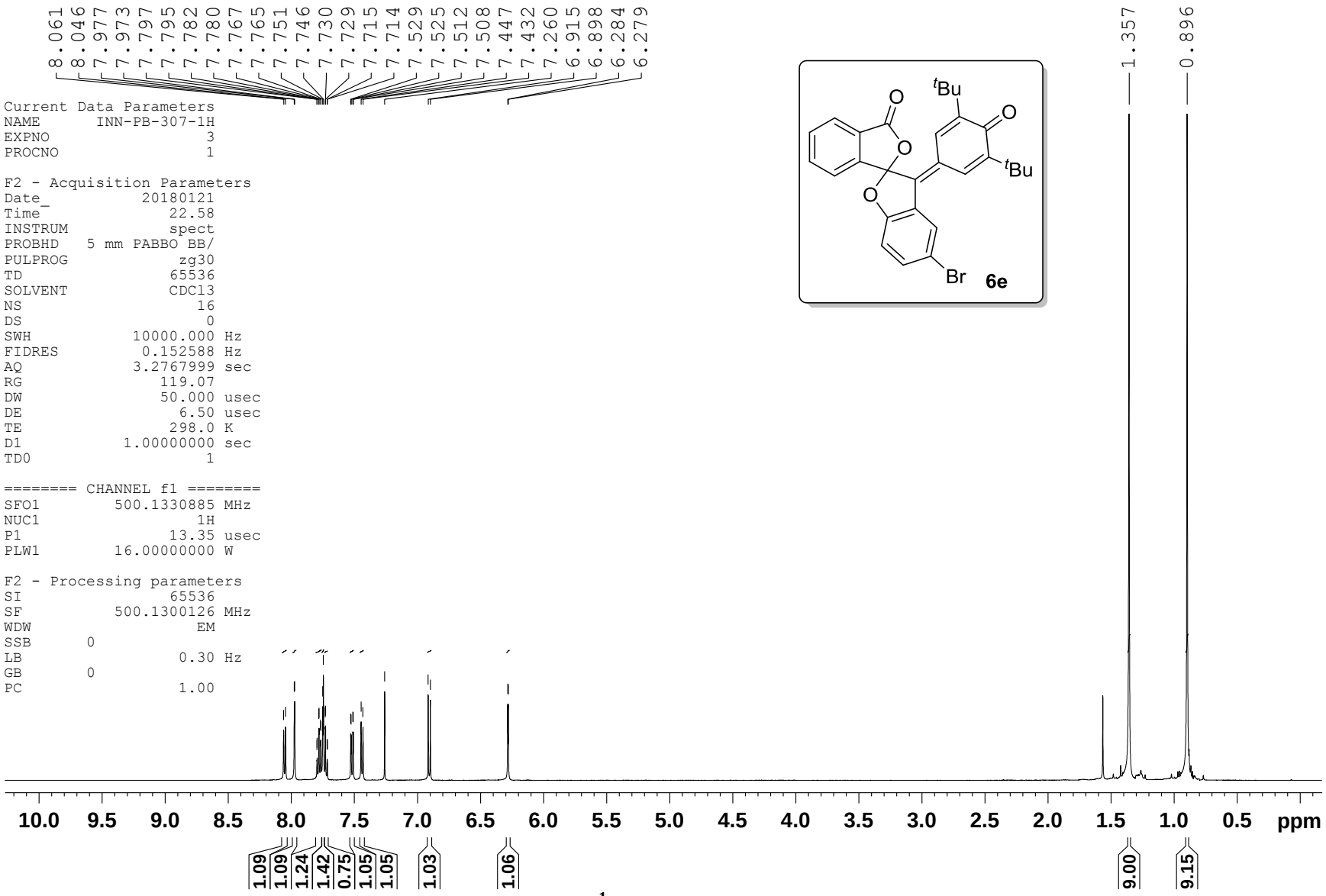


Figure S68. ^{1}H NMR Spectrum of 6e

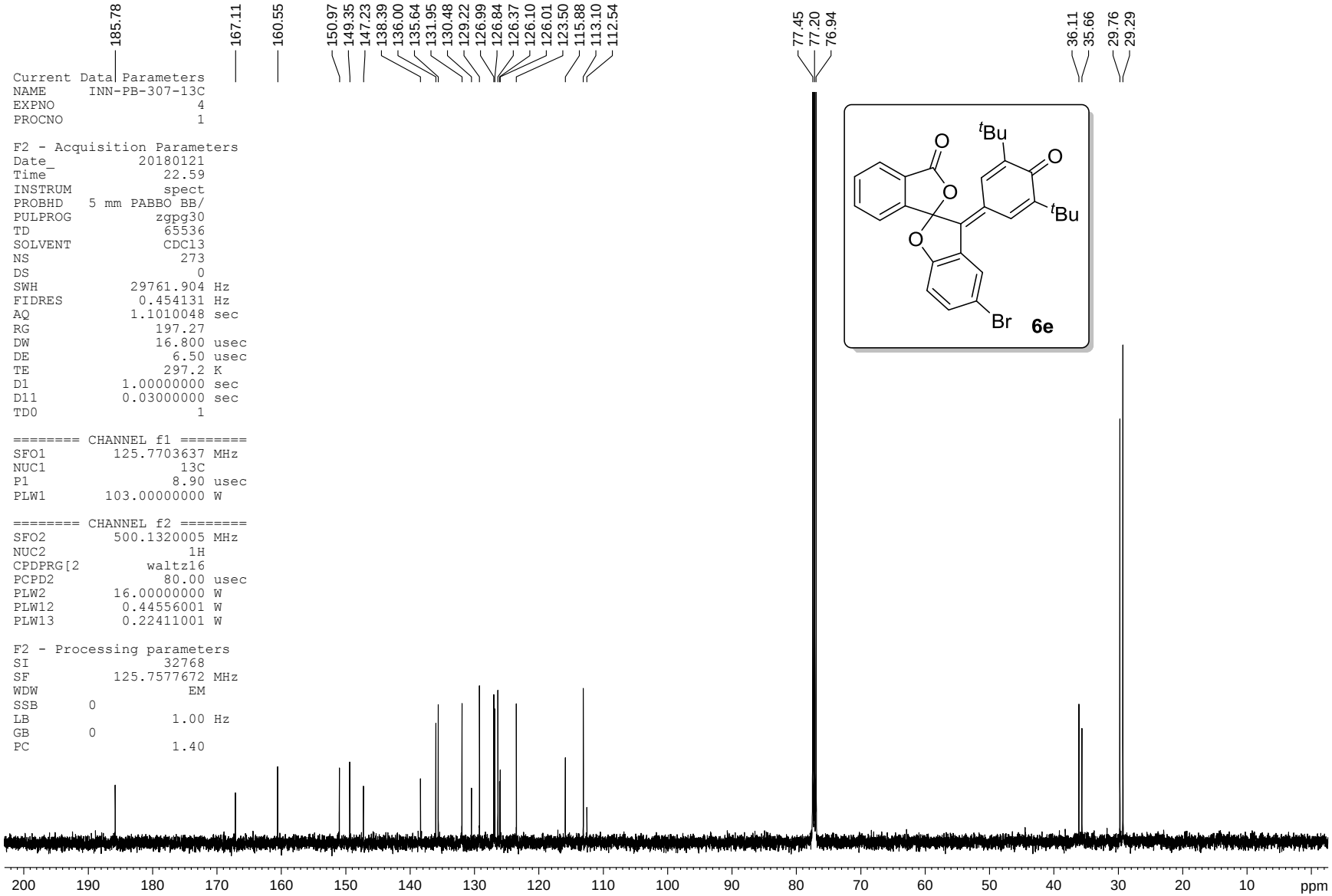


Figure S69. ^{13}C NMR Spectrum of 6e

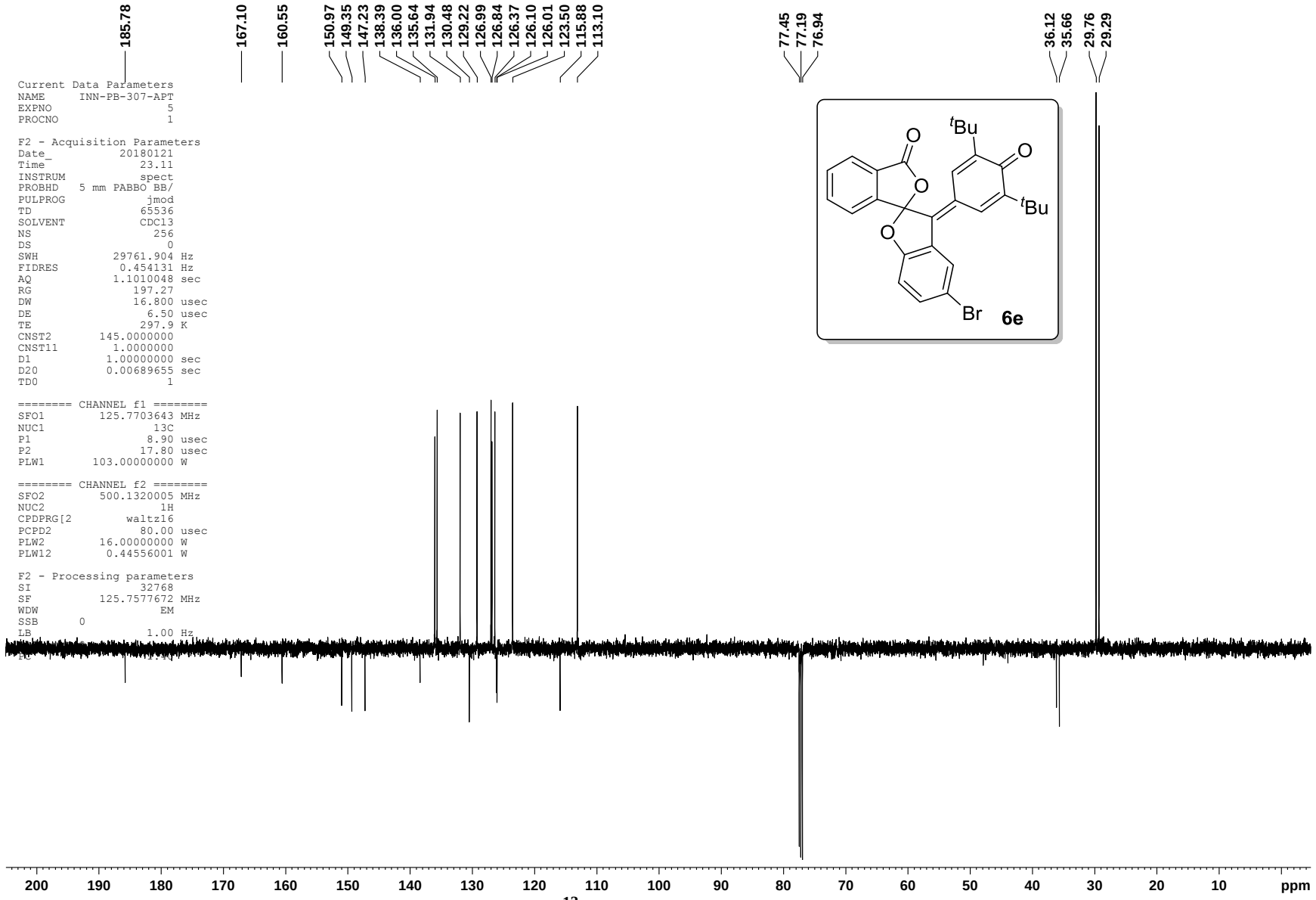


Figure S70. ^{13}C-APT NMR Spectrum of 6e

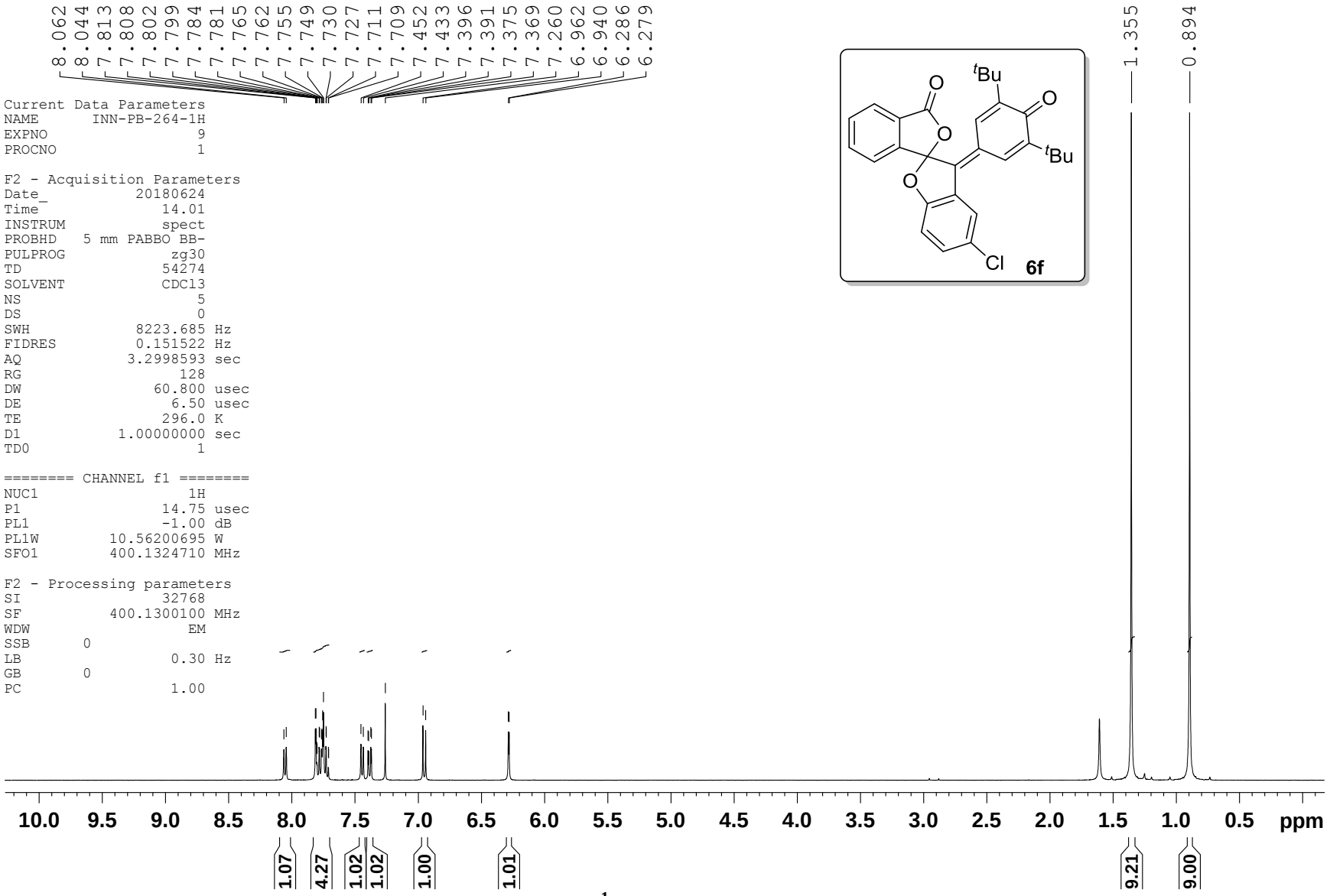


Figure S71. ^{1}H NMR Spectrum of 6f

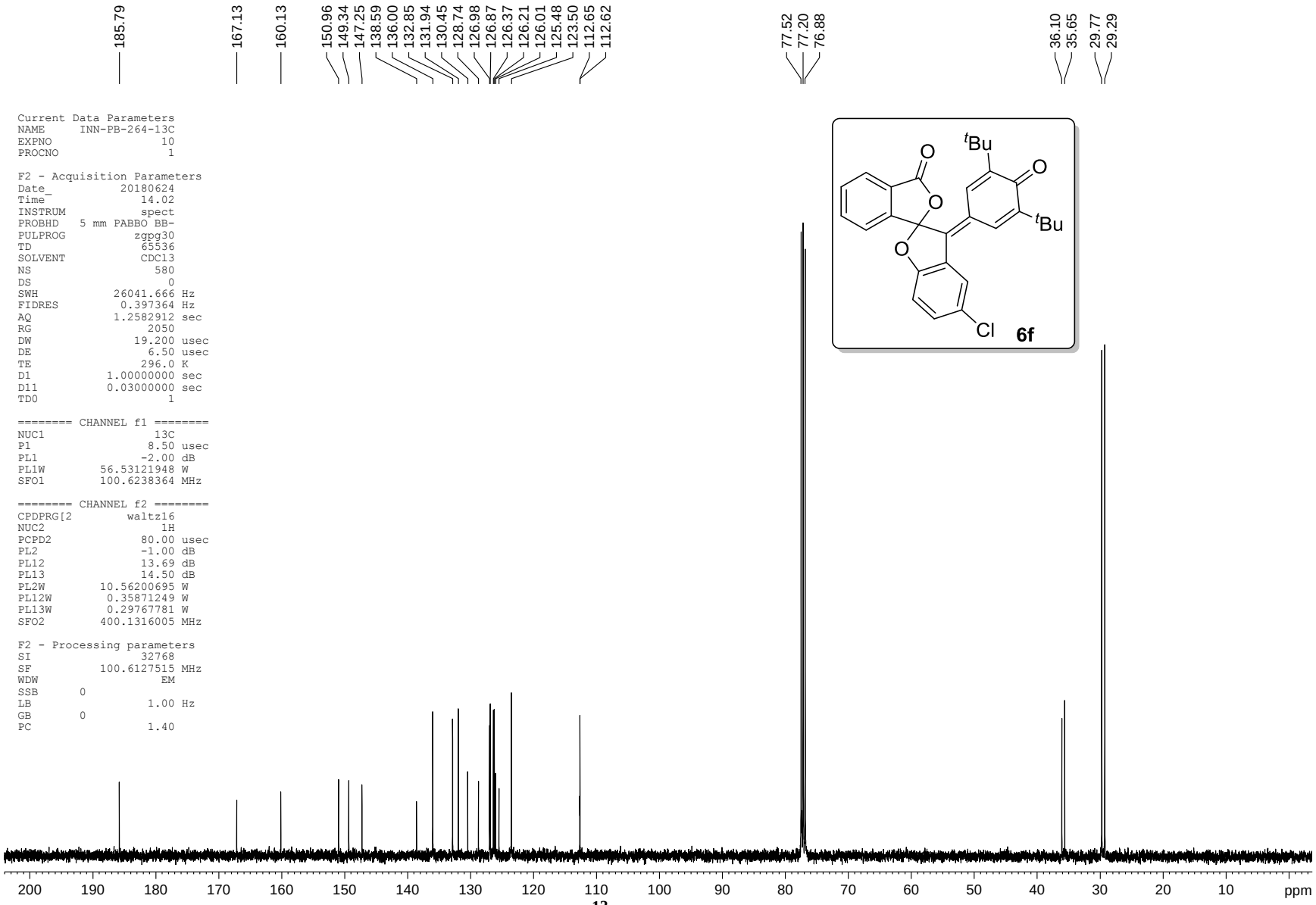


Figure S72. ^{13}C NMR Spectrum of 6f

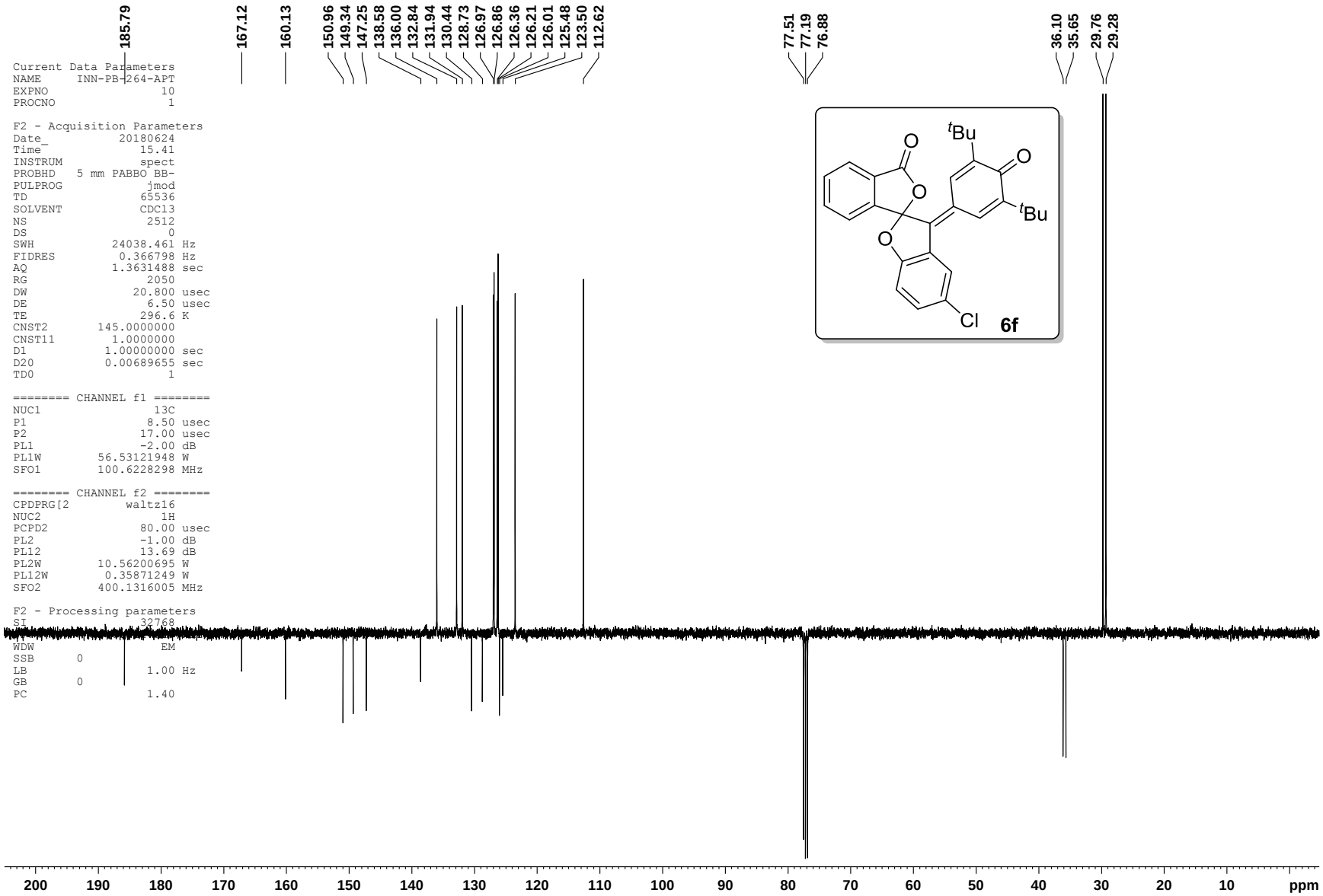


Figure S73. ^{13}C-APT NMR Spectrum of 6f

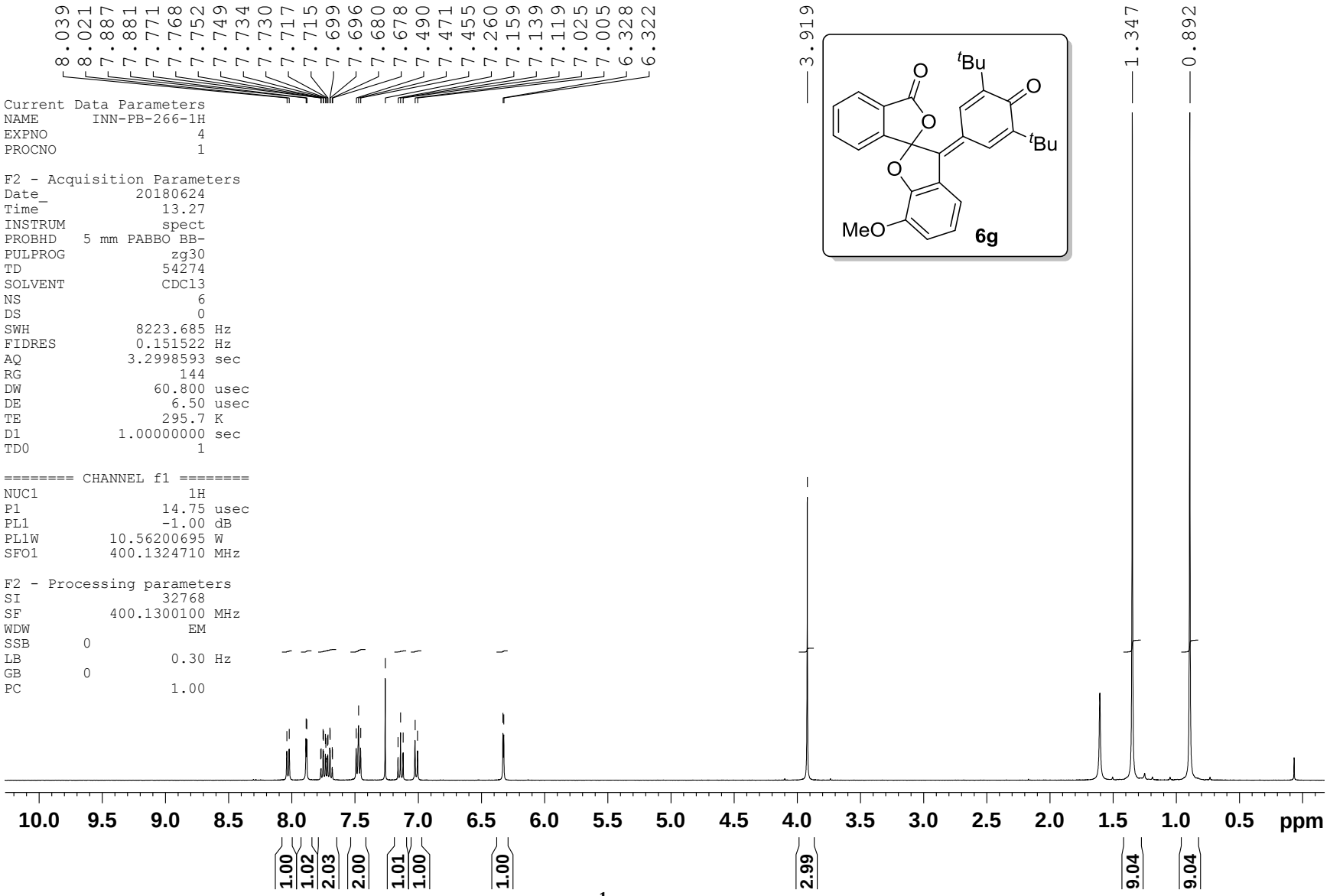


Figure S74. ^{1}H NMR Spectrum of 6g

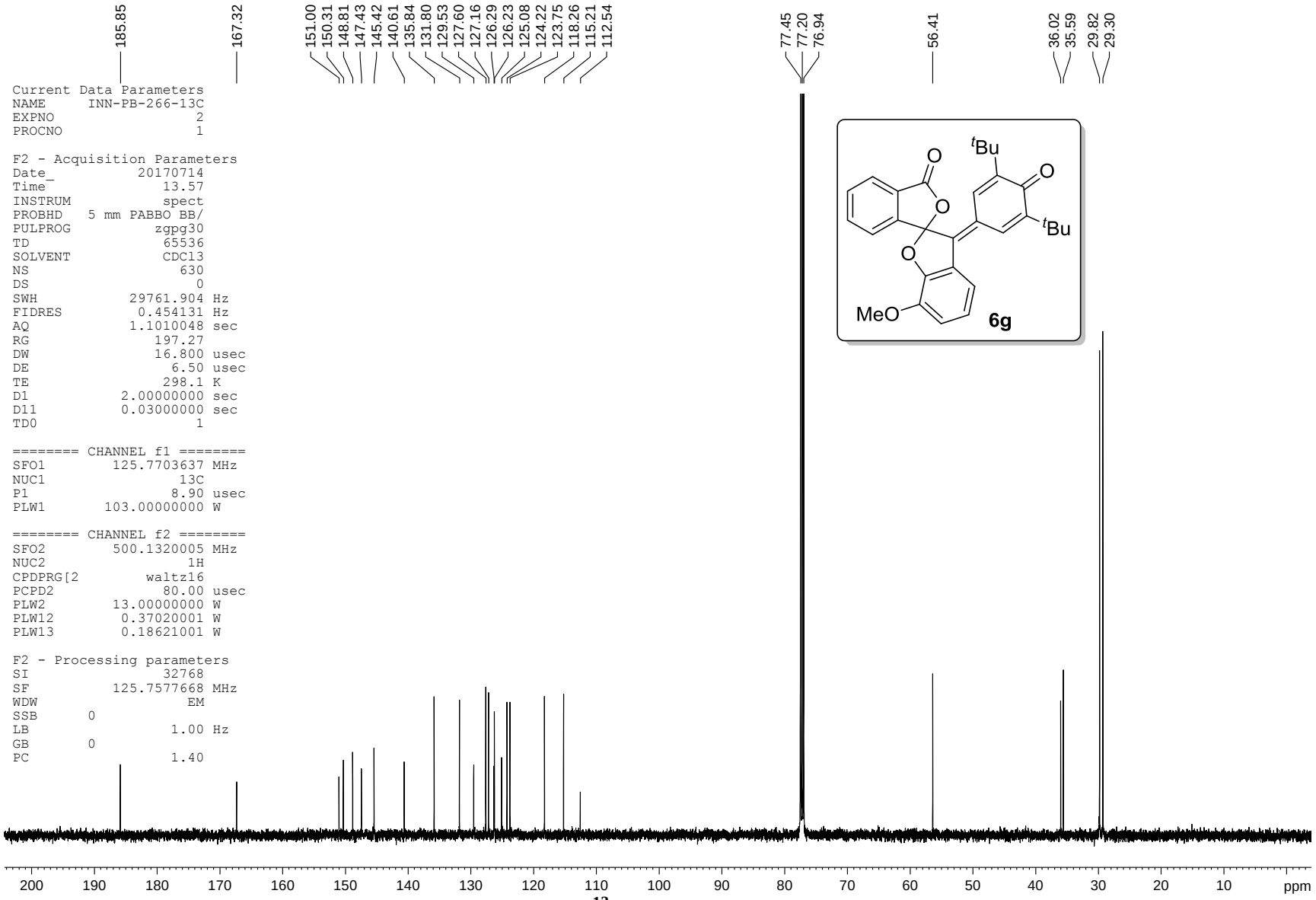


Figure S75. ^{13}C NMR Spectrum of 6g

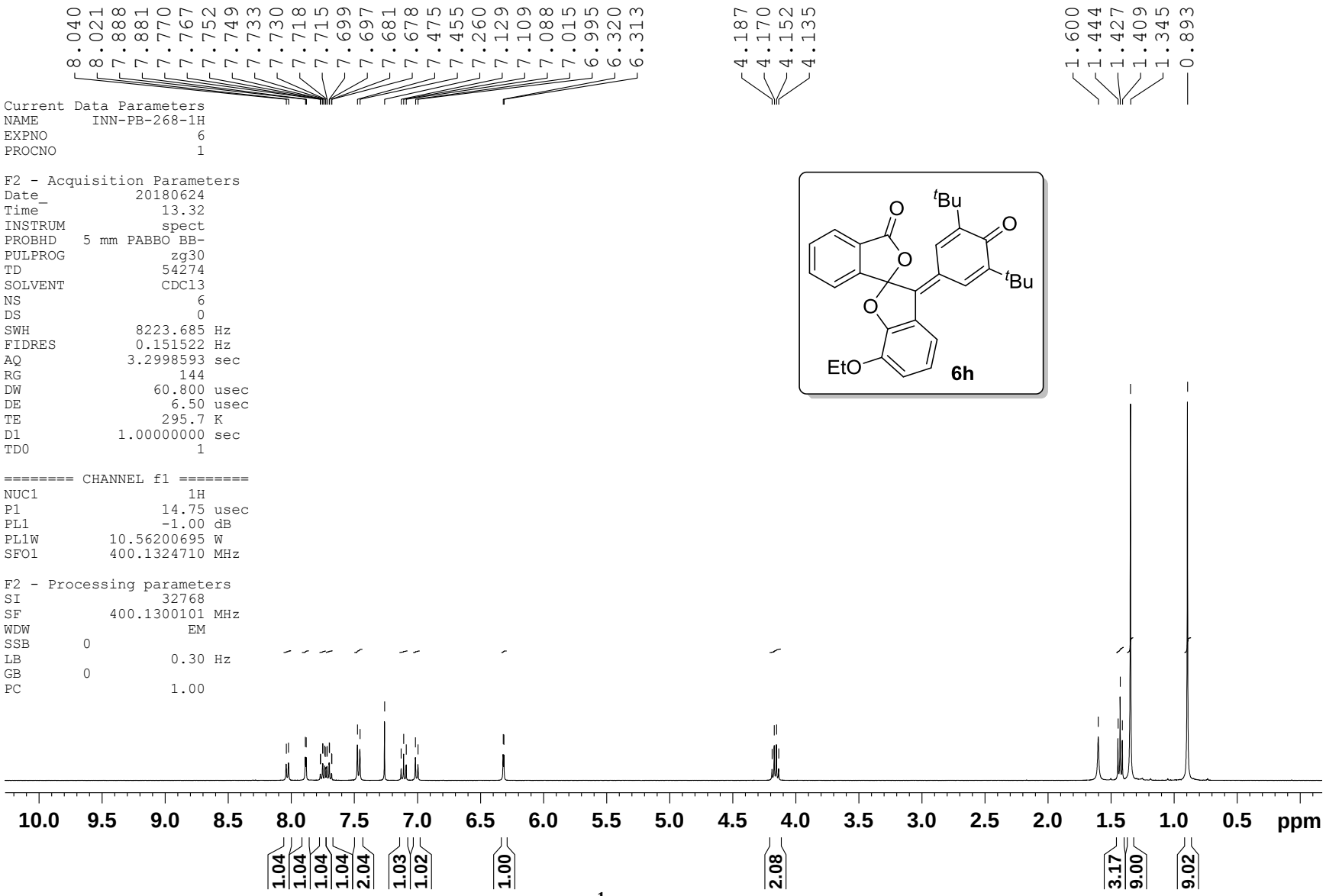


Figure S76. ^{1}H NMR Spectrum of 6h

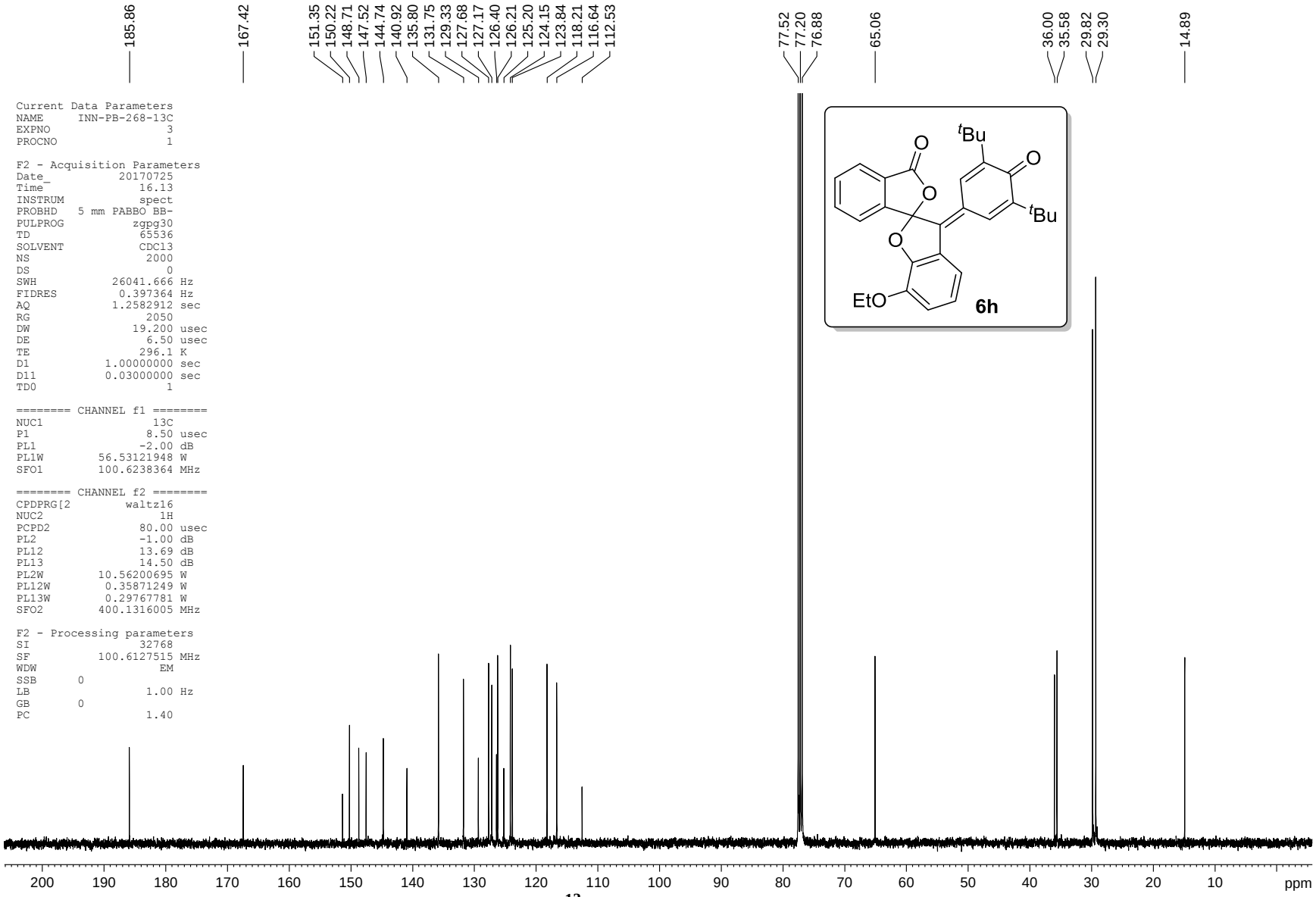
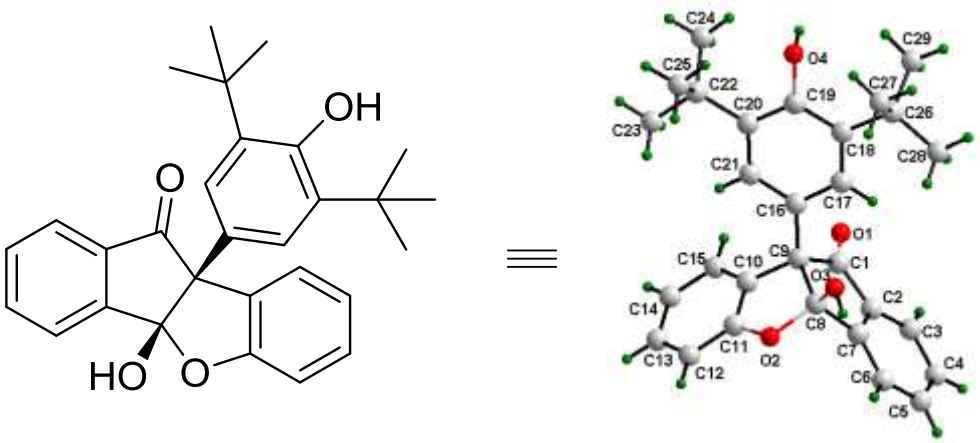


Figure S77. ^{13}C NMR Spectrum of 6h

Table S1. Selected X-ray data of 3a

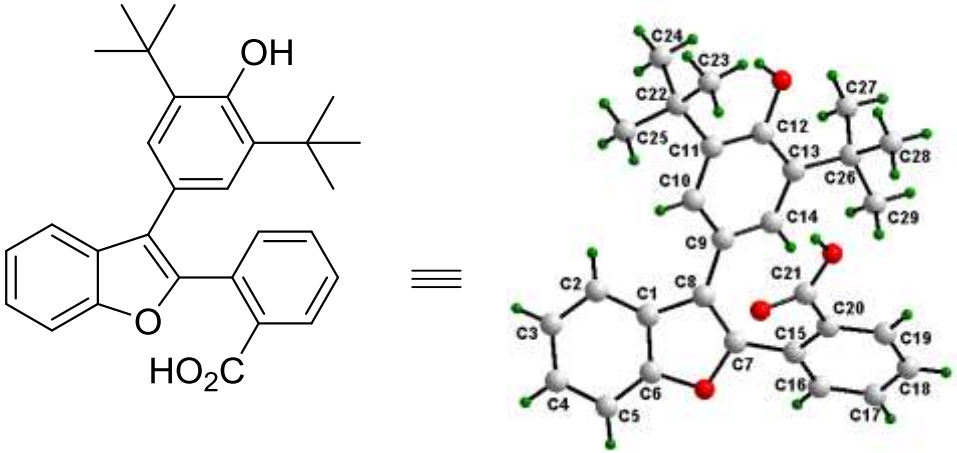


CCDC 1994862

Identification code	186-a_cifmo
Empirical formula	$C_{29}H_{30}O_4$
Formula weight	442.53
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.1334(13)
b/Å	10.3500(11)
c/Å	18.7632(18)
α/°	90
β/°	95.327(10)
γ/°	90
Volume/Å^3	2346.1(4)

Z	2
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	0.082
F(000)	944.0
Crystal size/mm^3	0.150 × 0.120 × 0.060
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.36 to 50
Index ranges	$-10 \leq h \leq 14$, $-8 \leq k \leq 12$, $-22 \leq l \leq 22$
Reflections collected	7750
Independent reflections	4048 [R_{int} = 0.0894, R_{sigma} = 0.1611]
Data/restraints/parameters	4048/3/305
Goodness-of-fit on F^2	1.006
Final R indexes [I>=2σ (I)]	R_1 = 0.0691, wR_2 = 0.1184
Final R indexes [all data]	R_1 = 0.1488, wR_2 = 0.1630
Largest diff. peak/hole / e Å^{-3}	0.31/-0.34

Table S2. Selected X-ray data of 4a

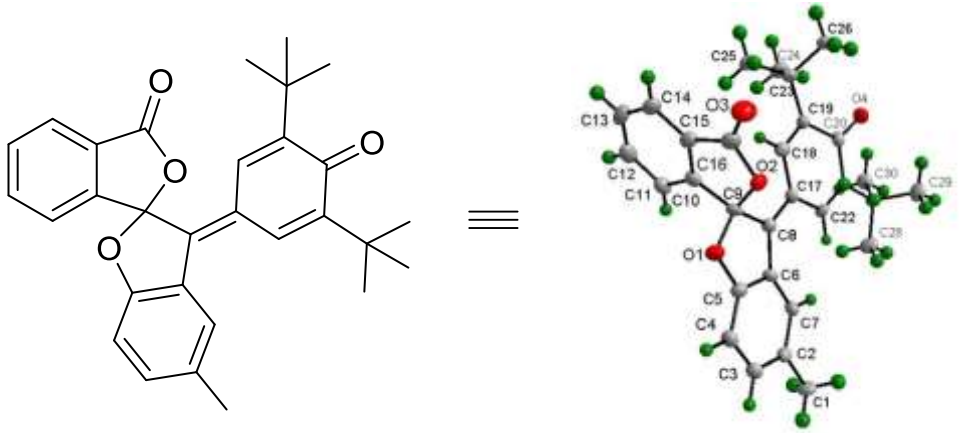


CCDC 1994867

Identification code	186-b_mo_cif
Empirical formula	$C_{29}H_{30}O_4$
Formula weight	442.53
Temperature/K	150(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	19.9040(6)
b/Å	11.4024(4)
c/Å	21.6619(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4916.2(3)
Z	8

ρ_{calc}g/cm^3	1.196
μ/mm^{-1}	0.078
F(000)	1888.0
Crystal size/mm^3	0.200 × 0.150 × 0.120
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.526 to 49.994
Index ranges	$-23 \leq h \leq 23$, $-13 \leq k \leq 12$, $-25 \leq l \leq 25$
Reflections collected	40196
Independent reflections	4323 [R_{int} = 0.0874, R_{sigma} = 0.0496]
Data/restraints/parameters	4323/0/305
Goodness-of-fit on F^2	1.164
Final R indexes [I>=2σ (I)]	R_1 = 0.0498, wR_2 = 0.1223
Final R indexes [all data]	R_1 = 0.0628, wR_2 = 0.1309
Largest diff. peak/hole / e Å^{-3}	0.37/-0.44

Table S3. Selected X-ray data of 6d



CCDC 1994868

Identification code	inn-pb-263_mo_sq
Empirical formula	$C_{30}H_{30}O_4$
Formula weight	454.54
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.6480(7)
b/Å	17.1737(13)
c/Å	18.0840(17)
α/°	90
β/°	98.244(8)
γ/°	90
Volume/Å^3	2658.0(4)

Z	4
ρ_{calc}g/cm^3	1.136
μ/mm^{-1}	0.074
F(000)	968.0
Crystal size/mm^3	0.200 × 0.150 × 0.120
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.286 to 49.996
Index ranges	$-7 \leq h \leq 10$, $-13 \leq k \leq 20$, $-21 \leq l \leq 21$
Reflections collected	9515
Independent reflections	4596 [R_{int} = 0.0757, R_{sigma} = 0.1219]
Data/restraints/parameters	4596/0/314
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0738, wR_2 = 0.1989
Final R indexes [all data]	R_1 = 0.1276, wR_2 = 0.2710
Largest diff. peak/hole / e Å^{-3}	0.39/-0.46