

Supporting Information

C(acyl)-C(sp²) and C(sp²)-C(sp²) Suzuki-Miyaura Cross-Coupling Reactions Using Nitrile-Functionalized NHC Palladium Complexes

Sinem Çakır,^a Serdar Batıkan Kavukcu,^a Hande Karabıyık,^b Senthil Rethinam,^{c,d} and Hayati Türkmen^{a*}

^aDepartment of Chemistry, Ege University, 35100 Bornova, Izmir, Turkey

^bDokuz Eylül University, Faculty of Science and Art, Department of Physics, Izmir, Turkey.

^cSchool of Natural and Applied Science, Ege University, 35100, Bornova, Izmir, Turkey.

^dSchool of Bio & Chemical Engineering, Sathyabama University, Chennai, 600 199, Tamilnadu, India.

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^1H - and ^{13}C - NMR spectra of the compound **1a-f**

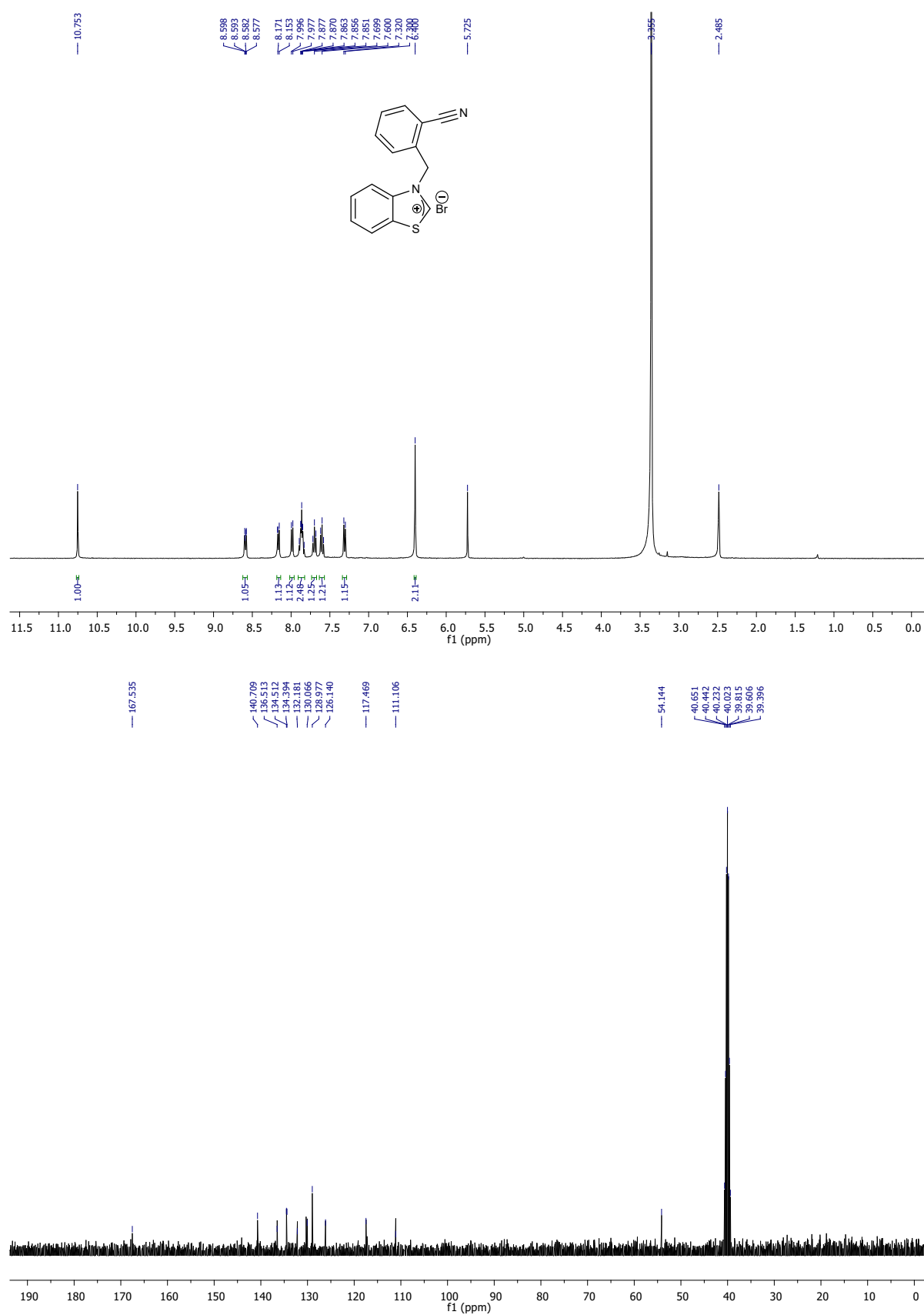


Figure S1. ^1H and ^{13}C NMR spectra of compound **1a** ($\text{DMSO-}d_6$).

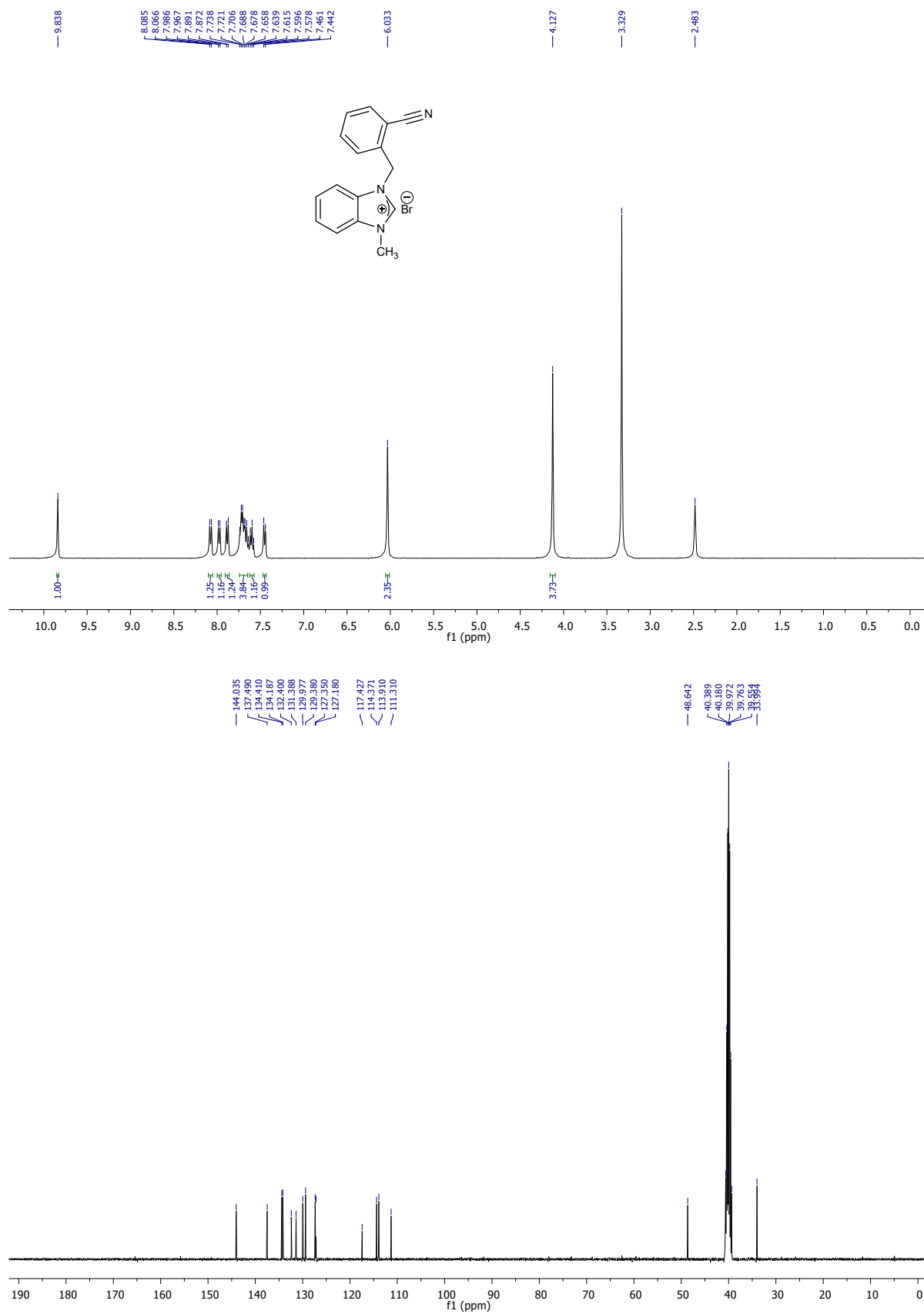


Figure S2. ¹H and ¹³C NMR spectra of compound **1b** (DMSO-*d*₆).

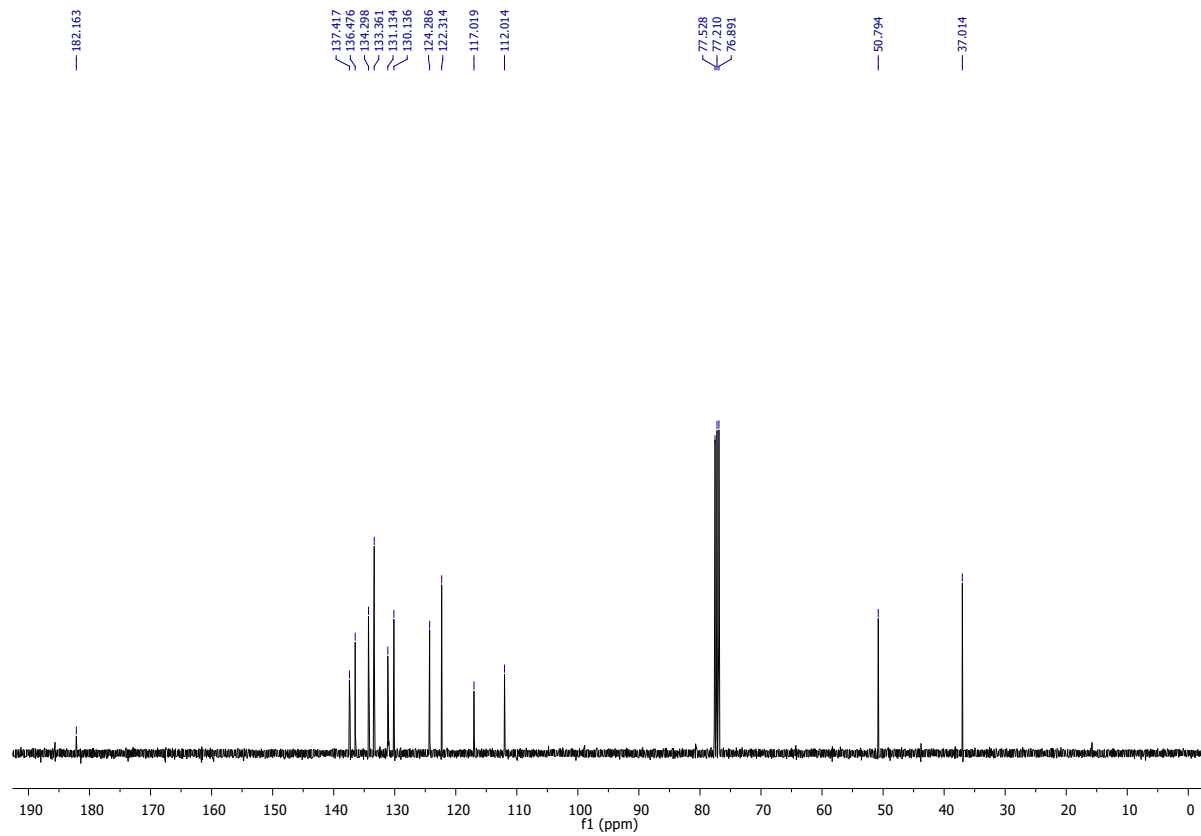
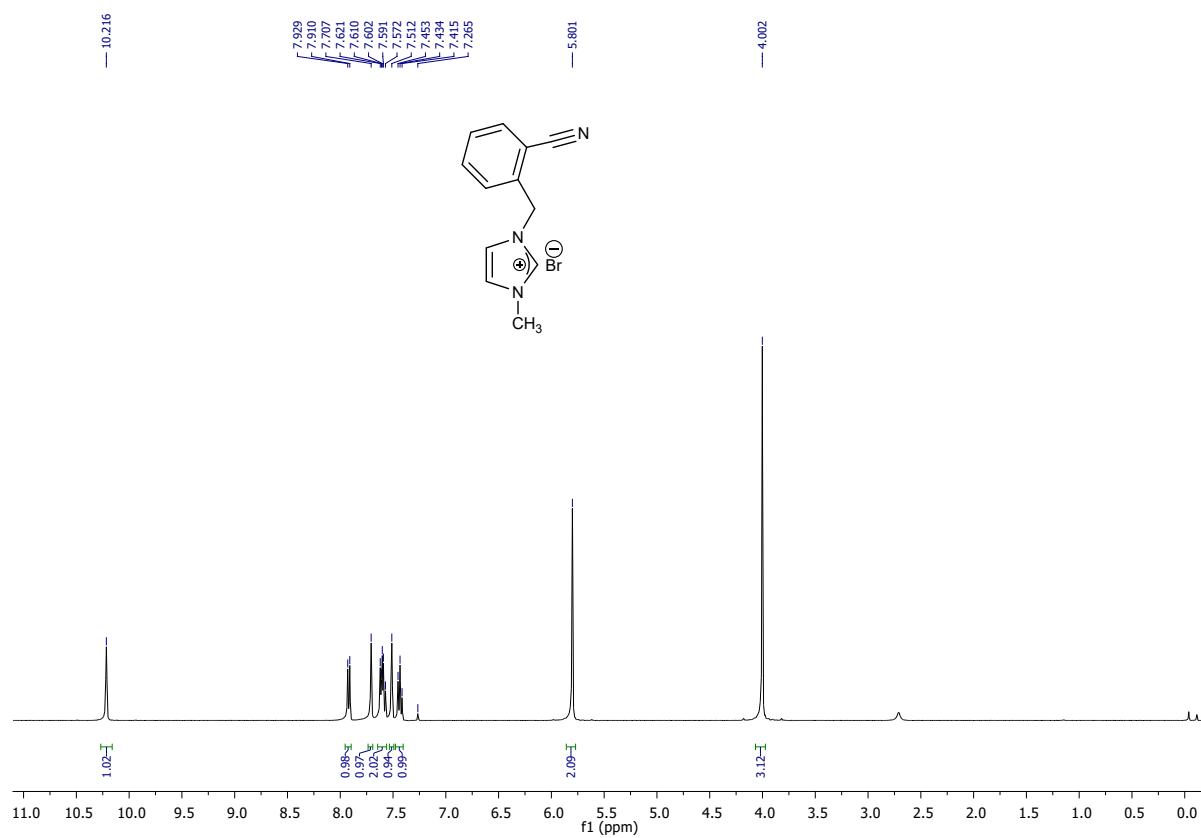


Figure S3. ¹H and ¹³C NMR spectra of compound **1c** (CDCl₃).

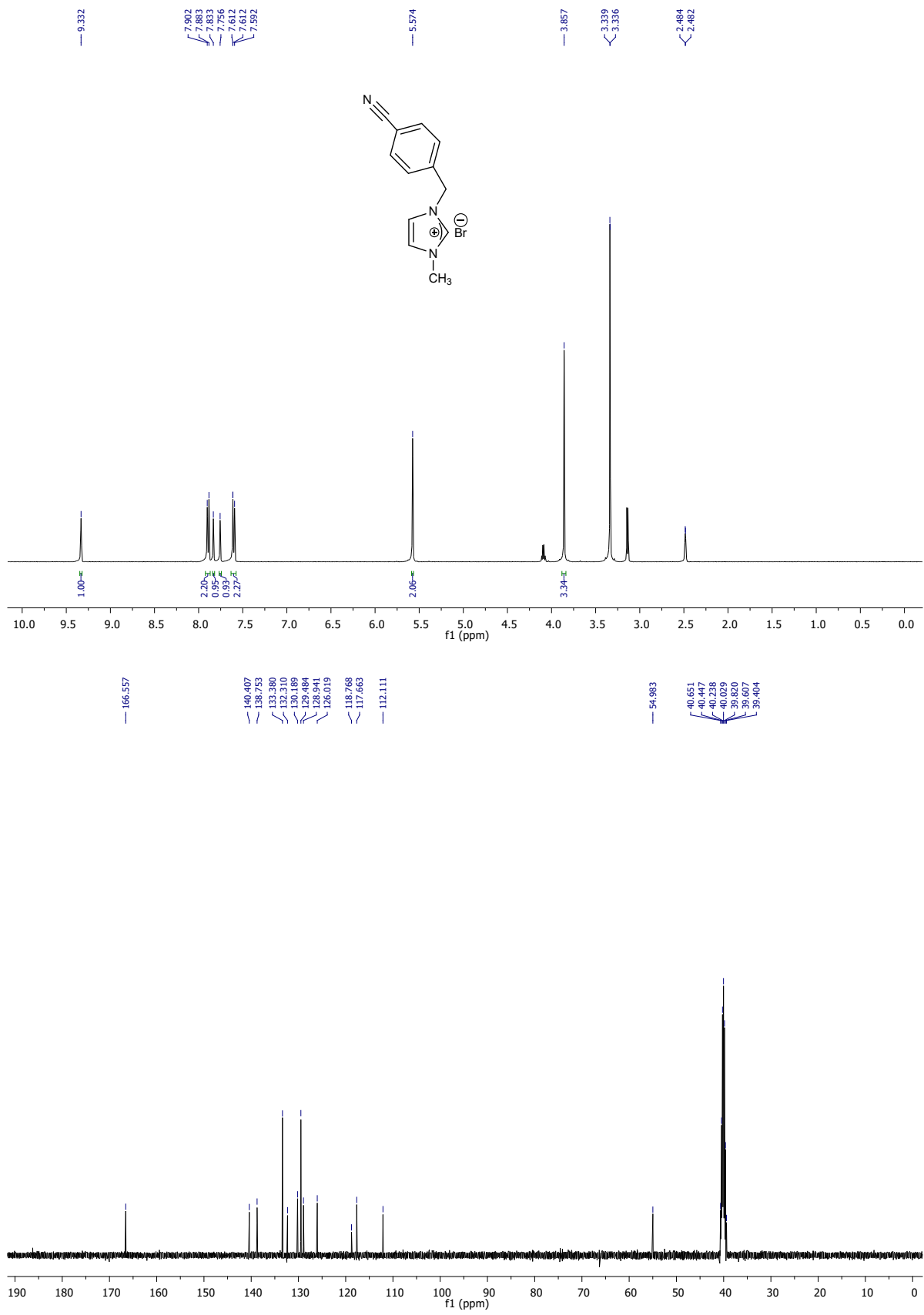


Figure S4. ¹H and ¹³C NMR spectra of compound **1d** (DMSO-*d*₆).

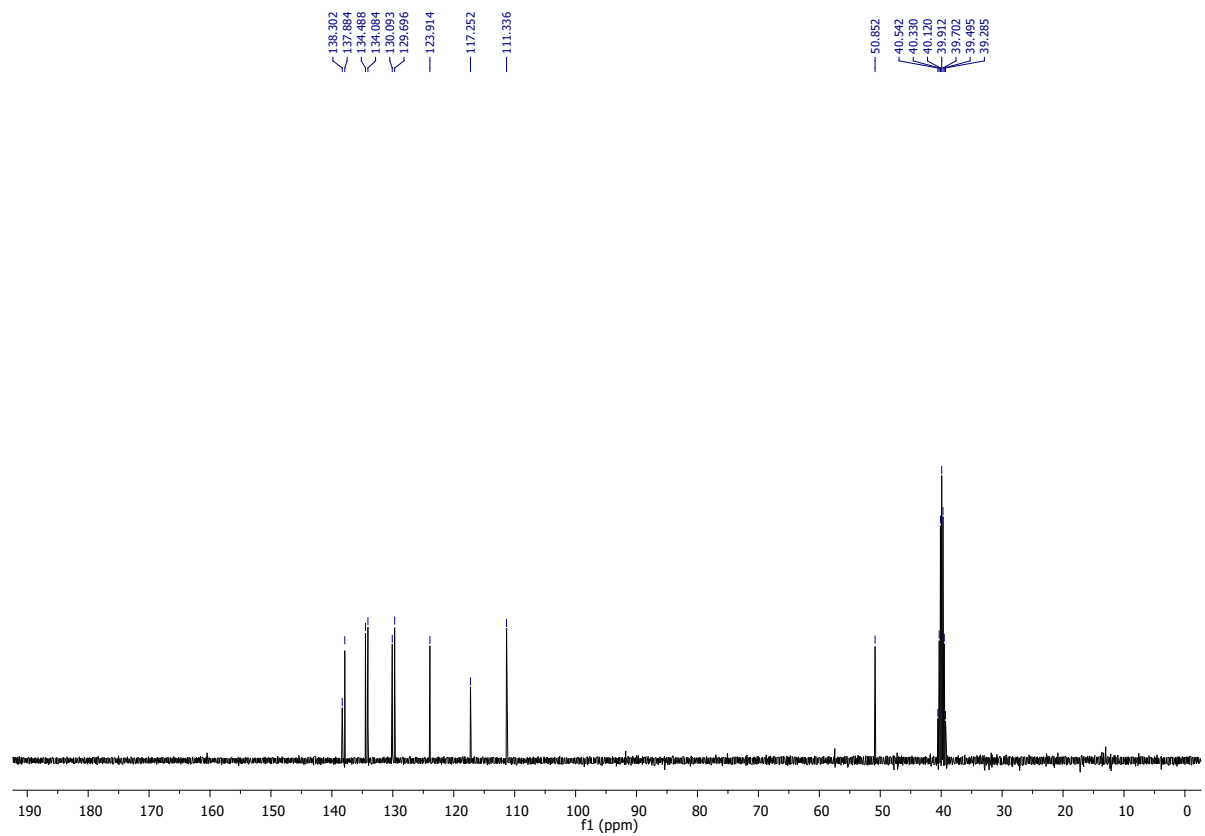
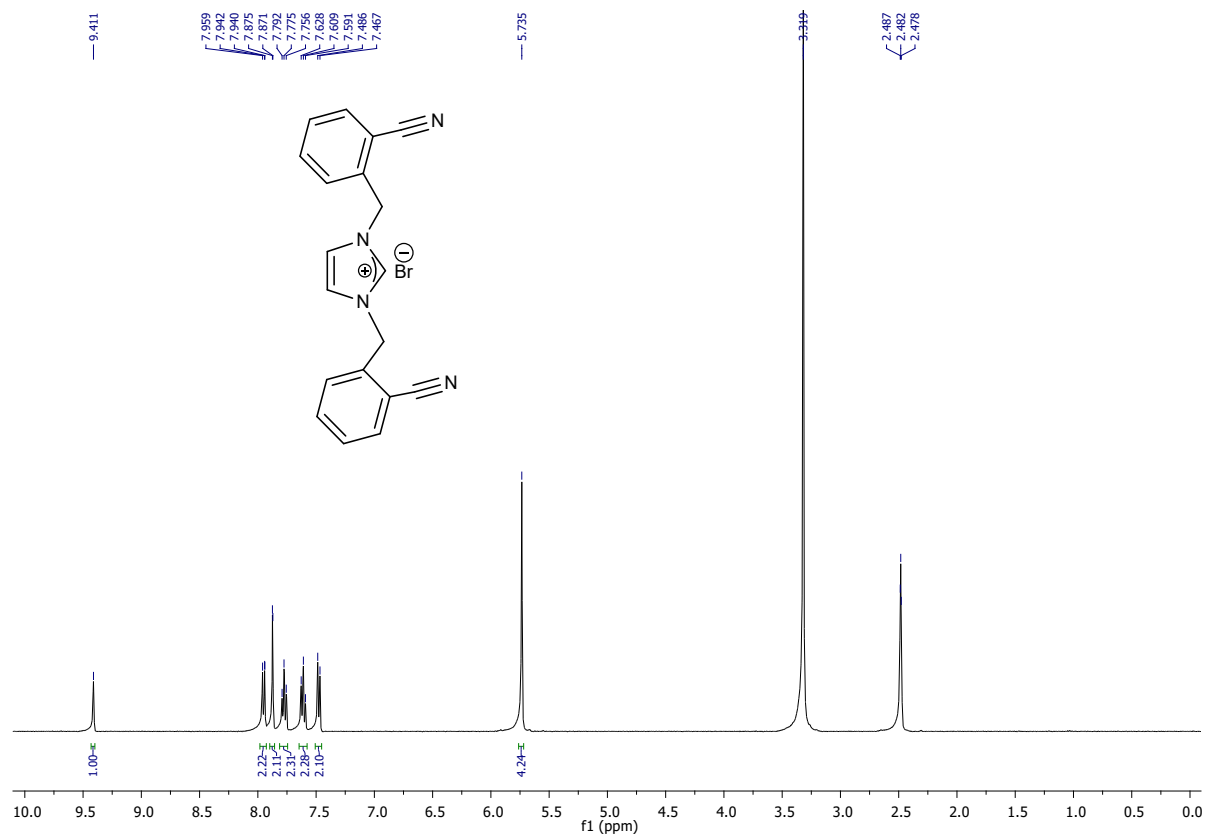


Figure S5. ¹H and ¹³C NMR spectra of compound **1e** (DMSO-*d*₆).

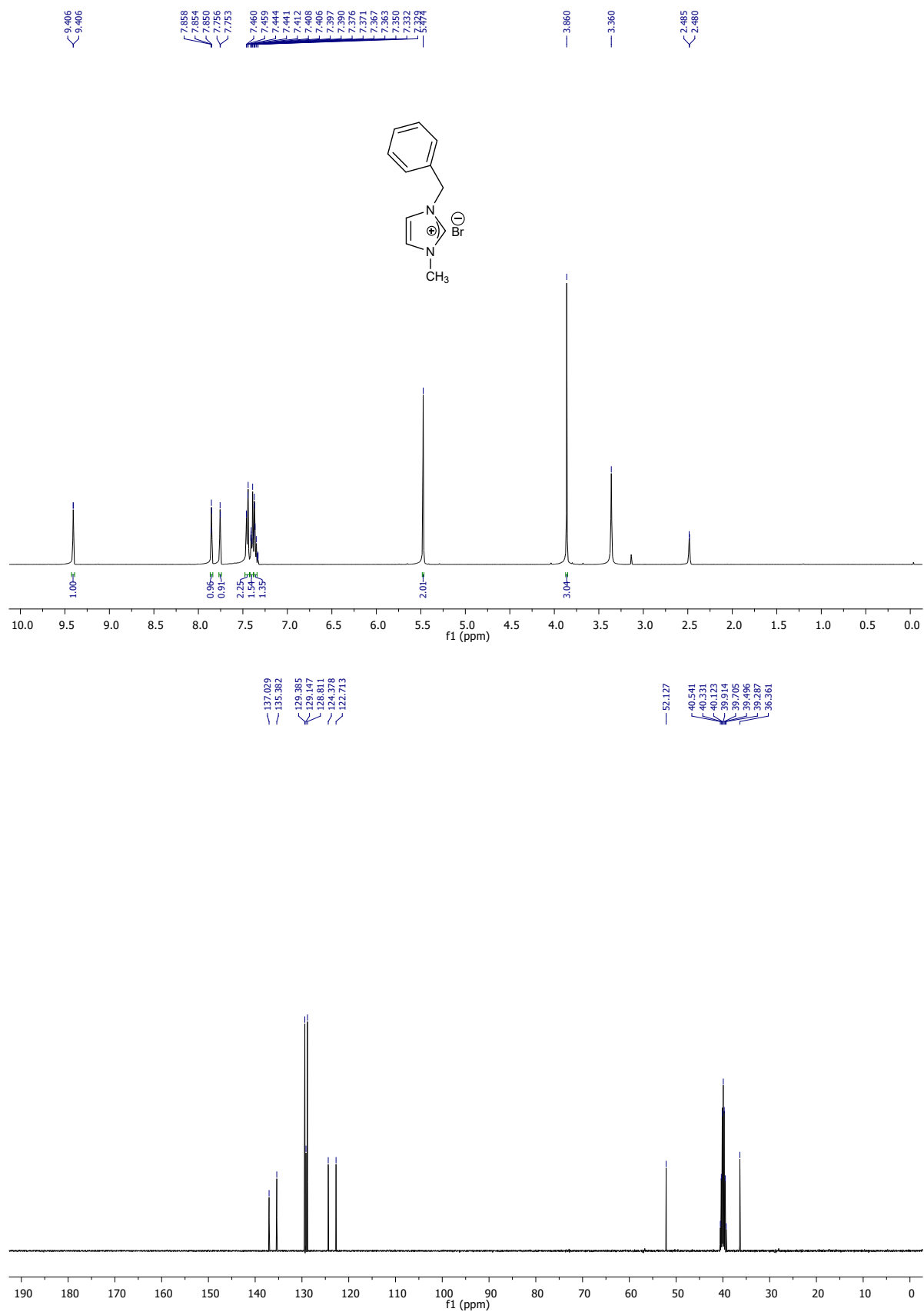


Figure S6. ¹H and ¹³C spectra of compound 1f (DMSO-*d*₆).

^1H - and ^{13}C - NMR spectra of the complexes **2a-c**, **3b-f** and **3b'**

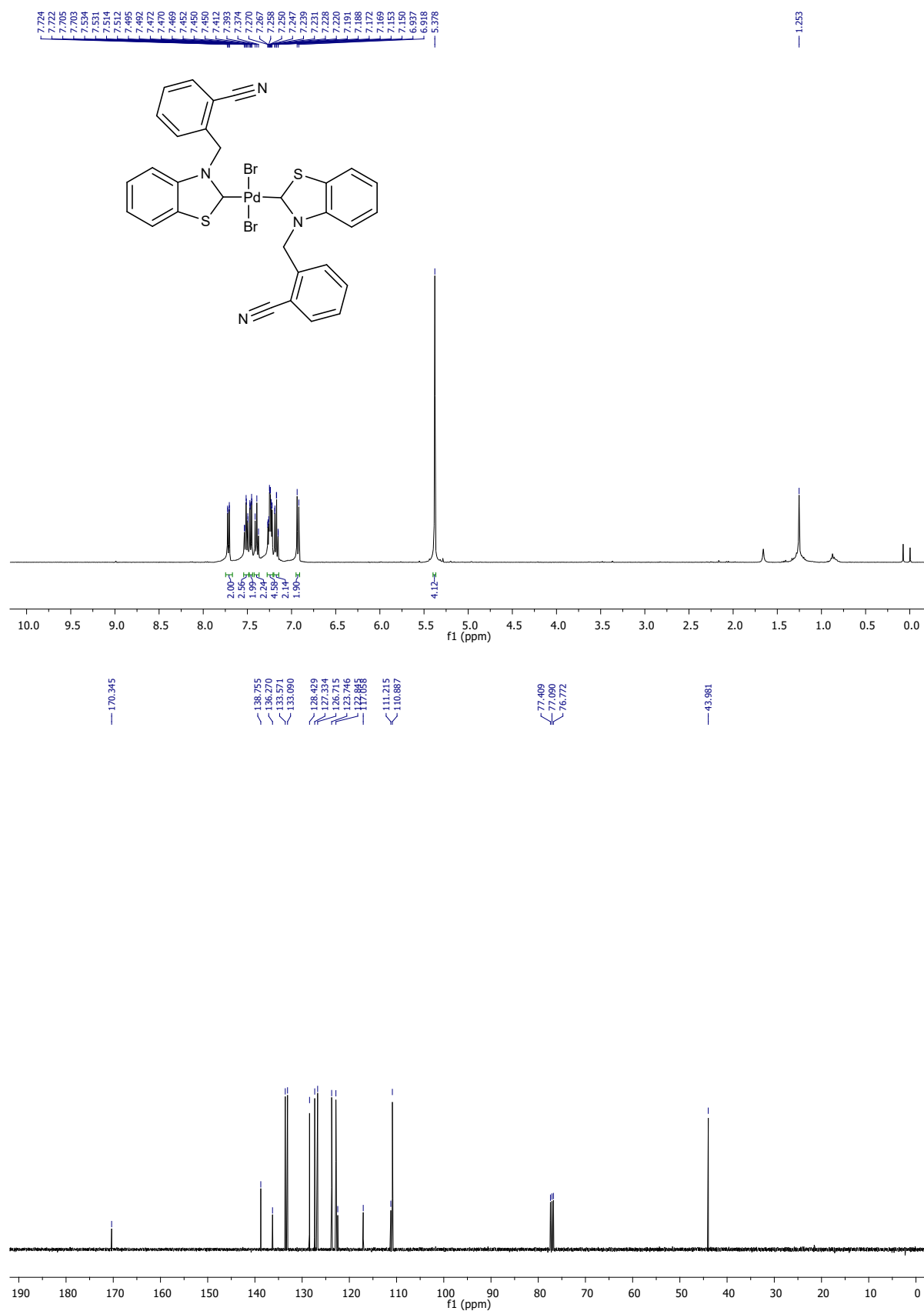


Figure S7. ^1H and ^{13}C NMR spectrums of complex **2a** (CDCl_3).

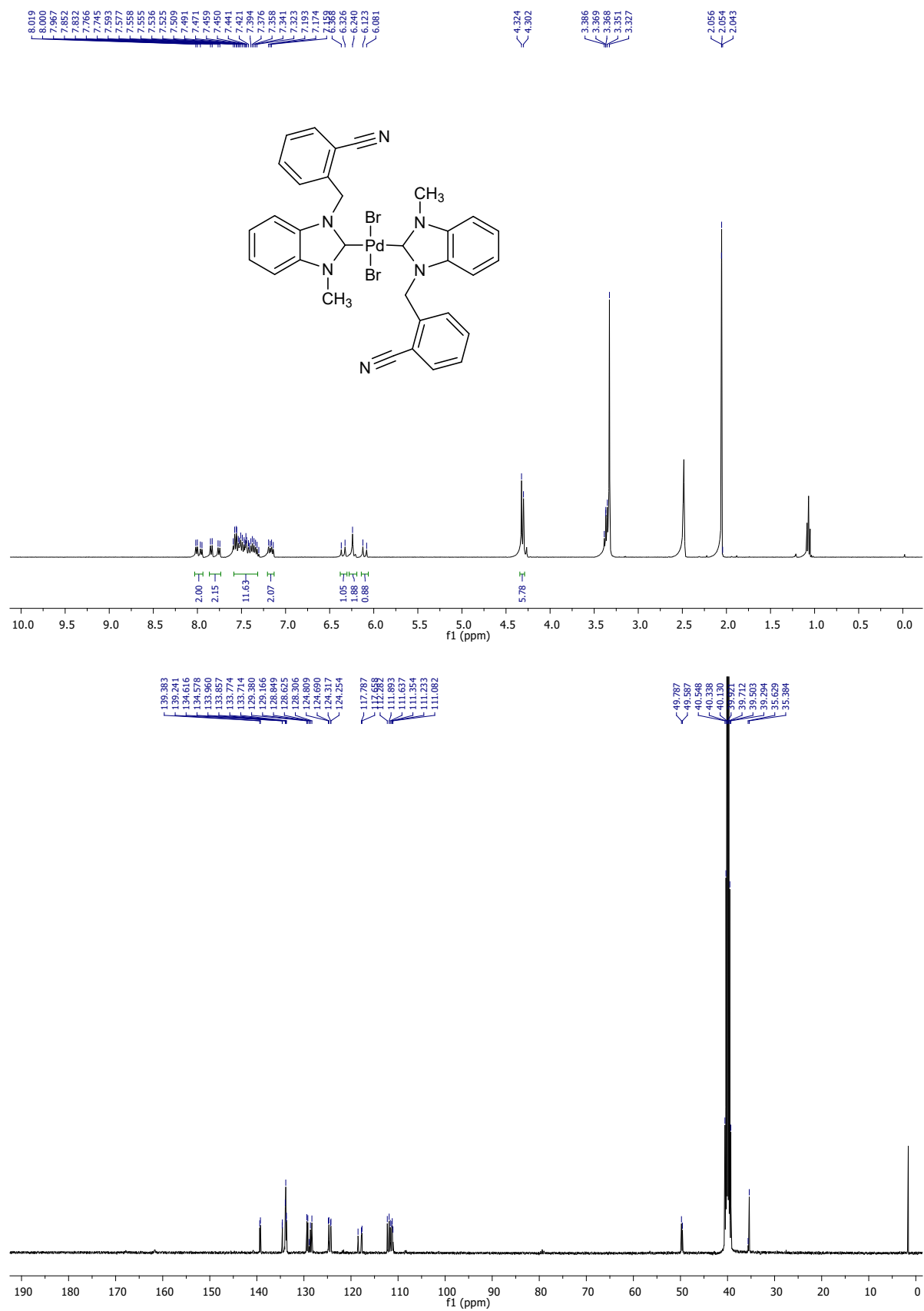


Figure S8. ¹H and ¹³C NMR spectra of complex **2b** (DMSO-*d*₆).

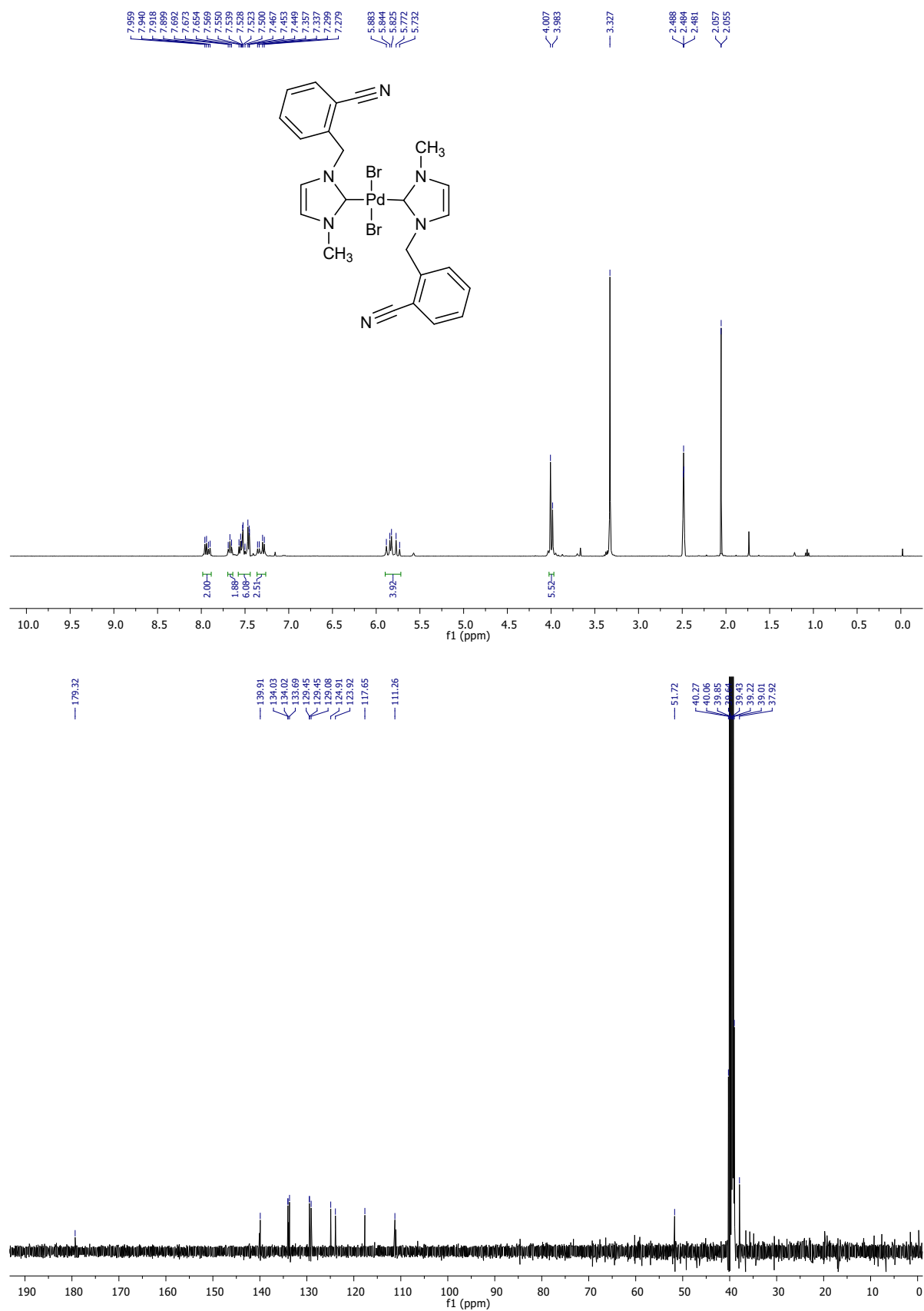


Figure S9. ¹H and ¹³C NMR spectrums of complex **2c** (DMSO-*d*₆).

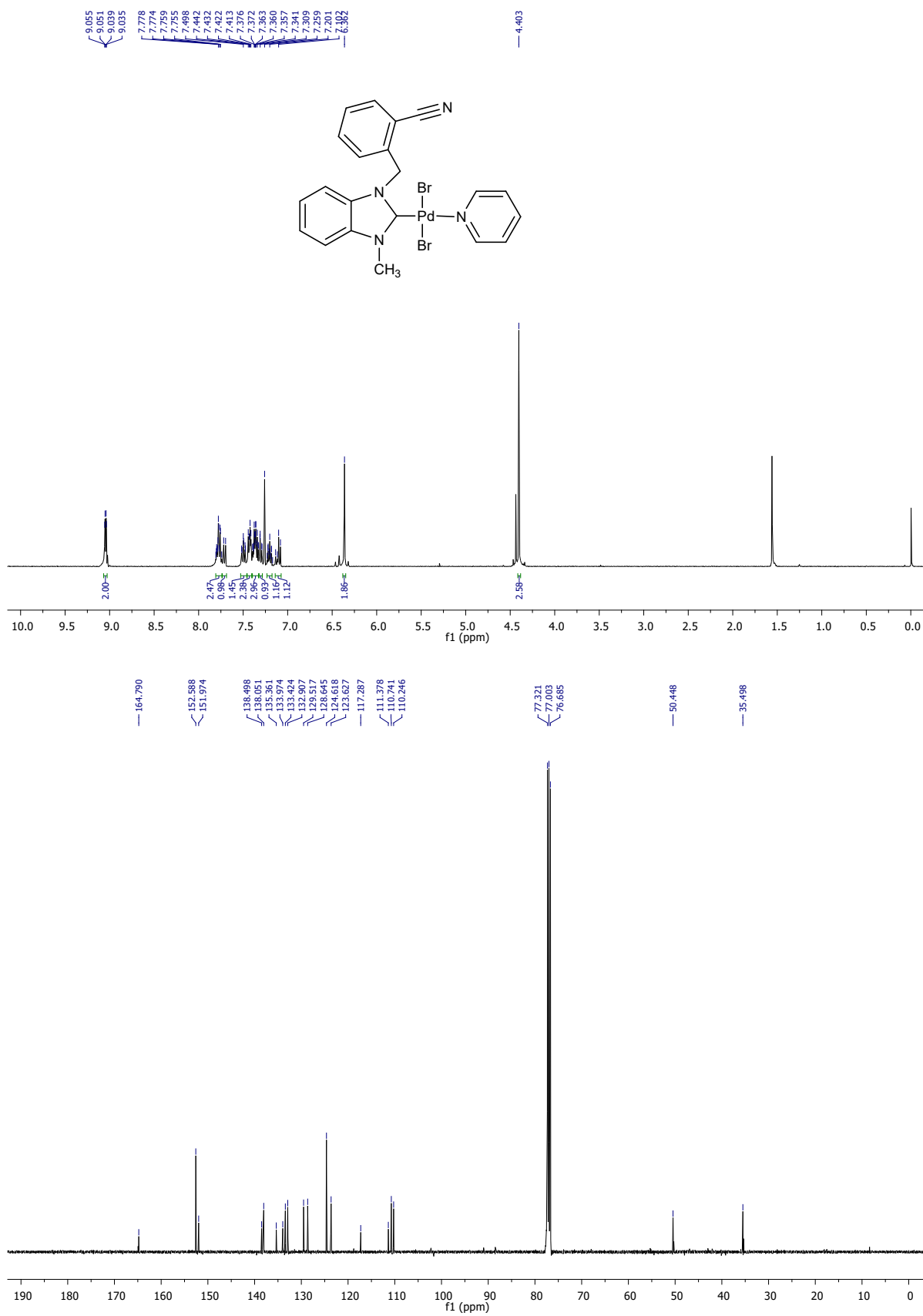


Figure S10. ¹H and ¹³C NMR spectra of complex **3b** (CDCl₃).

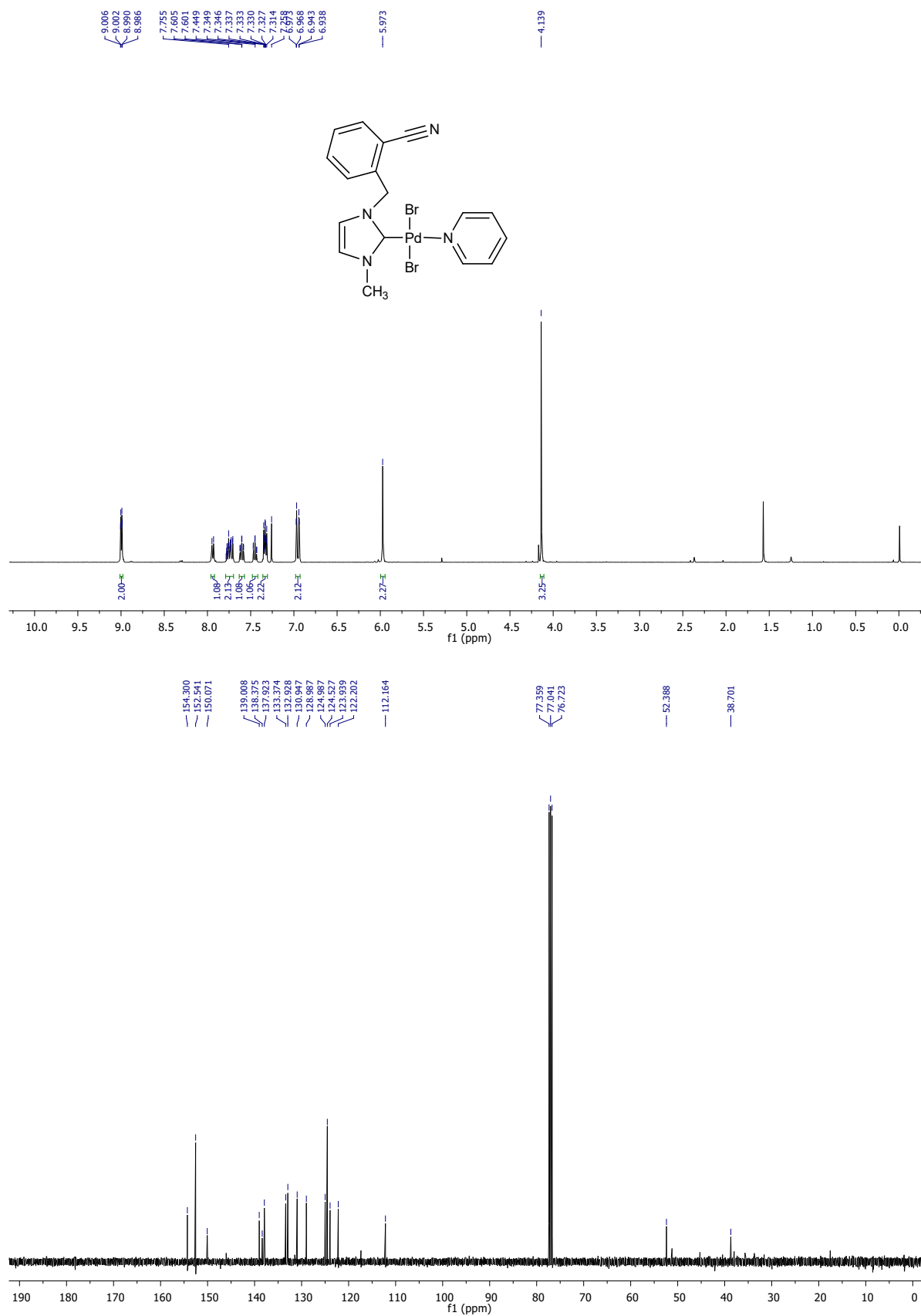


Figure S11. ¹H and ¹³C NMR spectra of complex **3c** (CDCl₃).

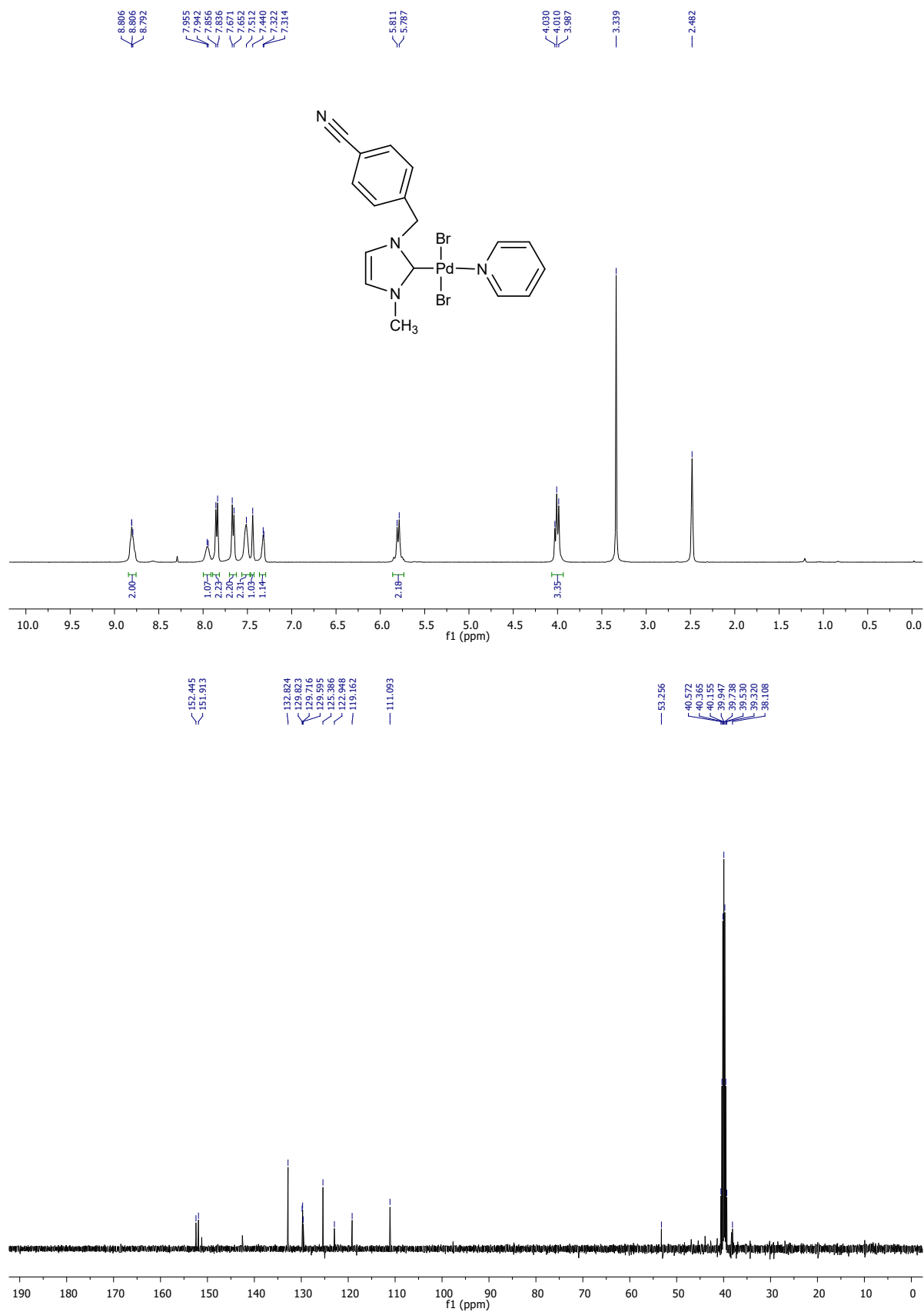


Figure S12. ¹H and ¹³C NMR spectra of complex **3d** (DMSO-*d*₆).

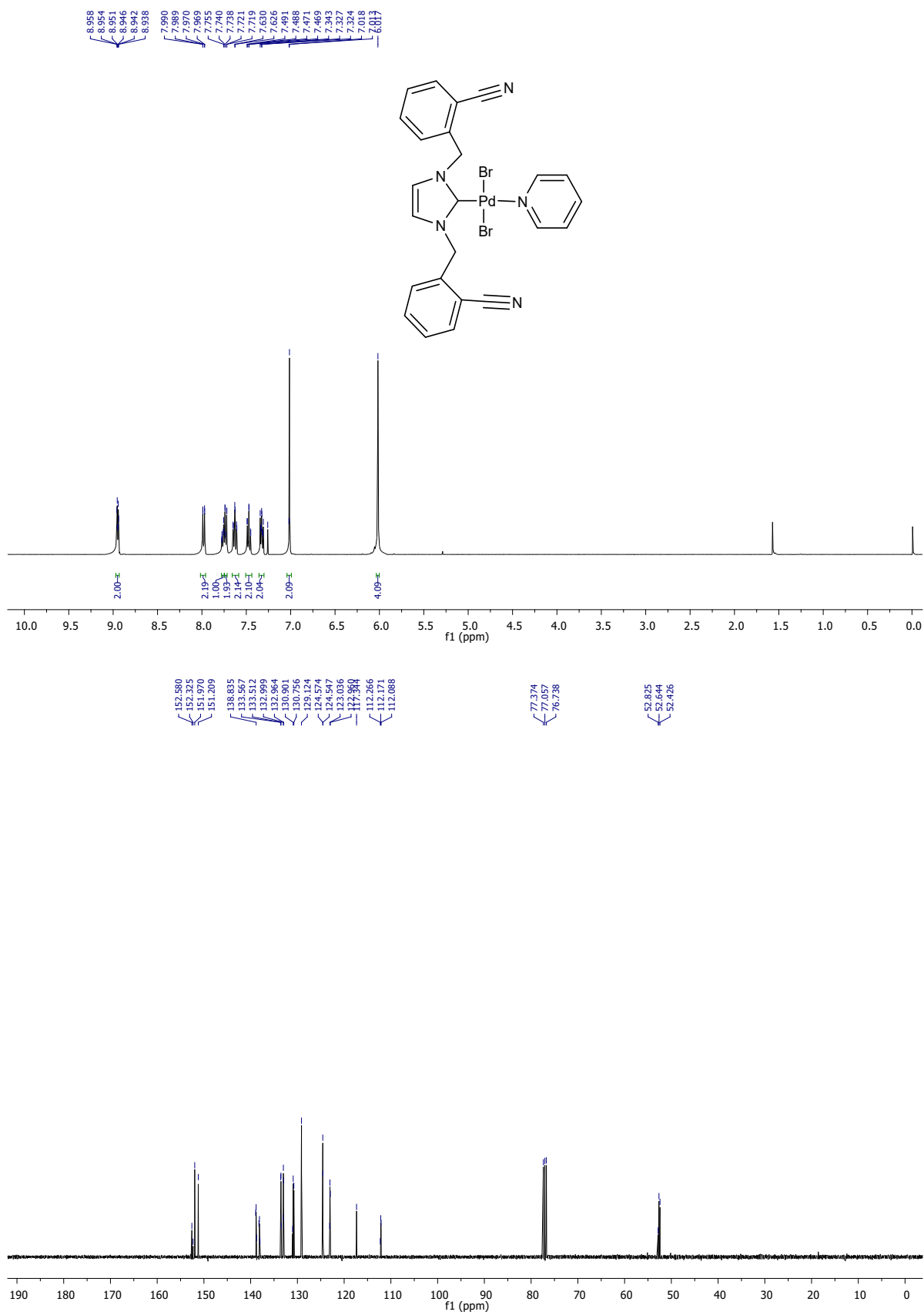


Figure S13. ¹H and ¹³C NMR spectra of complex **3e** (CDCl₃).

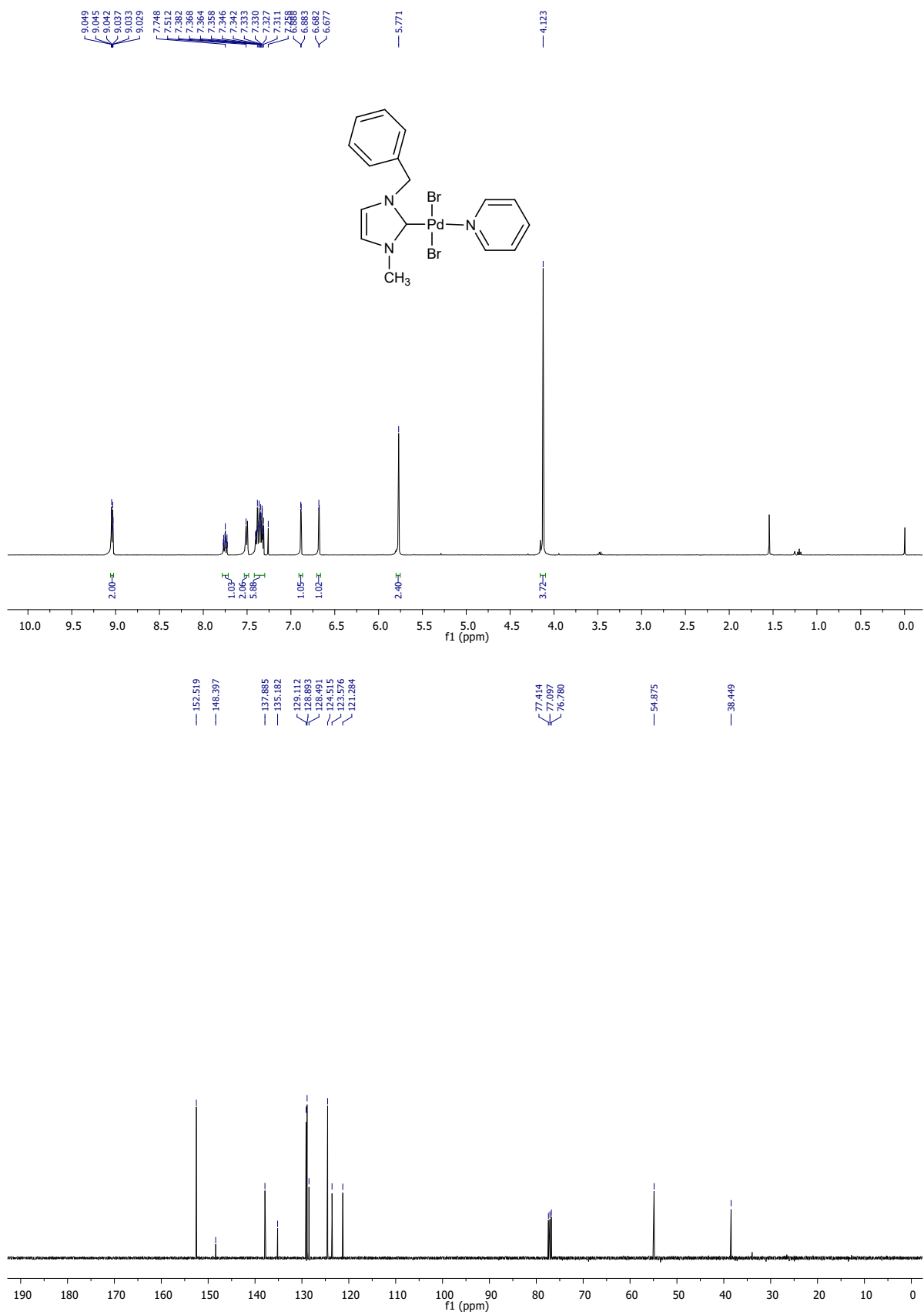


Figure S14. ¹H and ¹³C NMR spectrums of complex **3f** (CDCl₃).

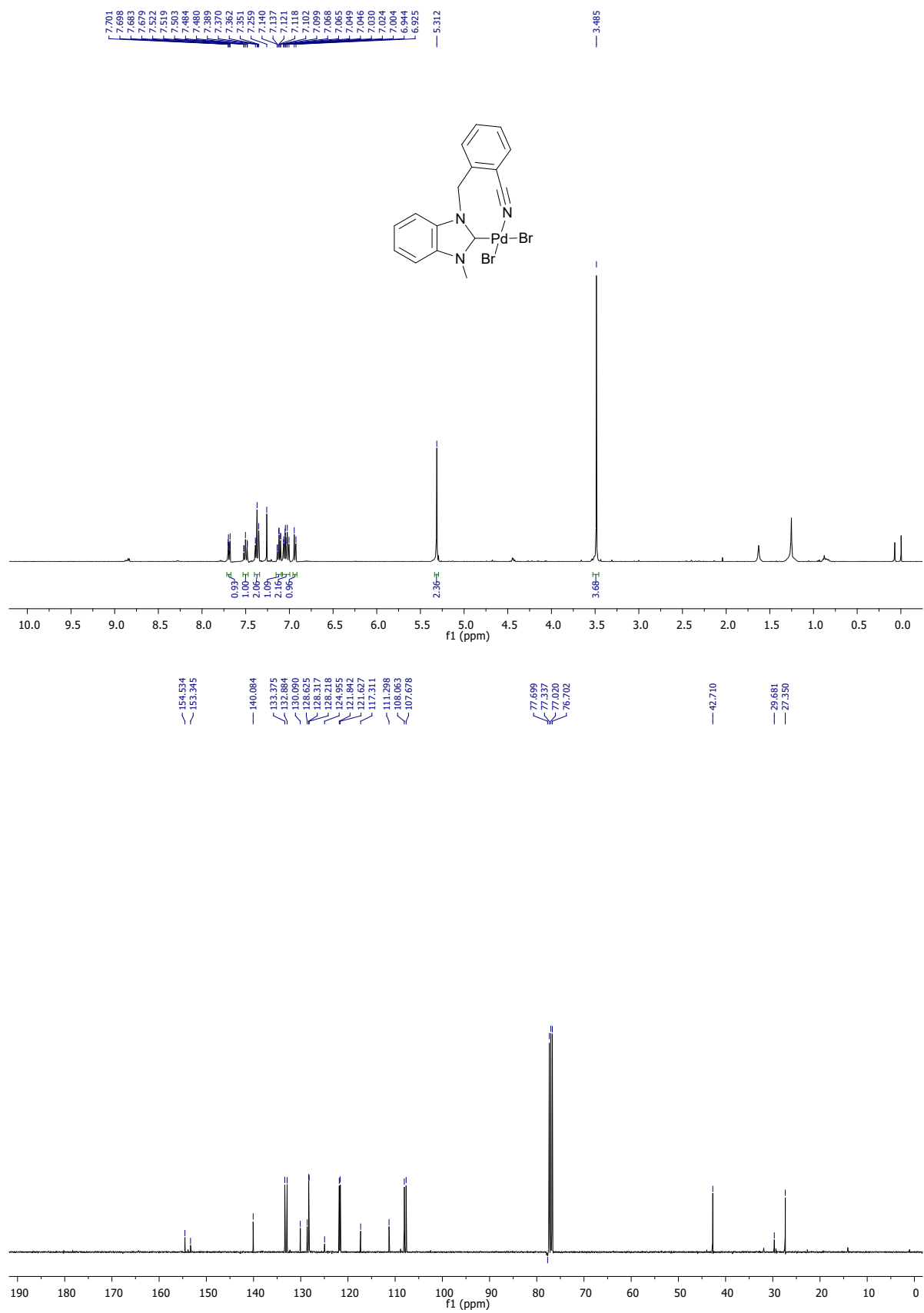


Figure S15. ¹H and ¹³C NMR spectra of complex **3b'** (CDCl₃).

^1H - and ^{13}C - NMR spectras of Acylative Suzuki products

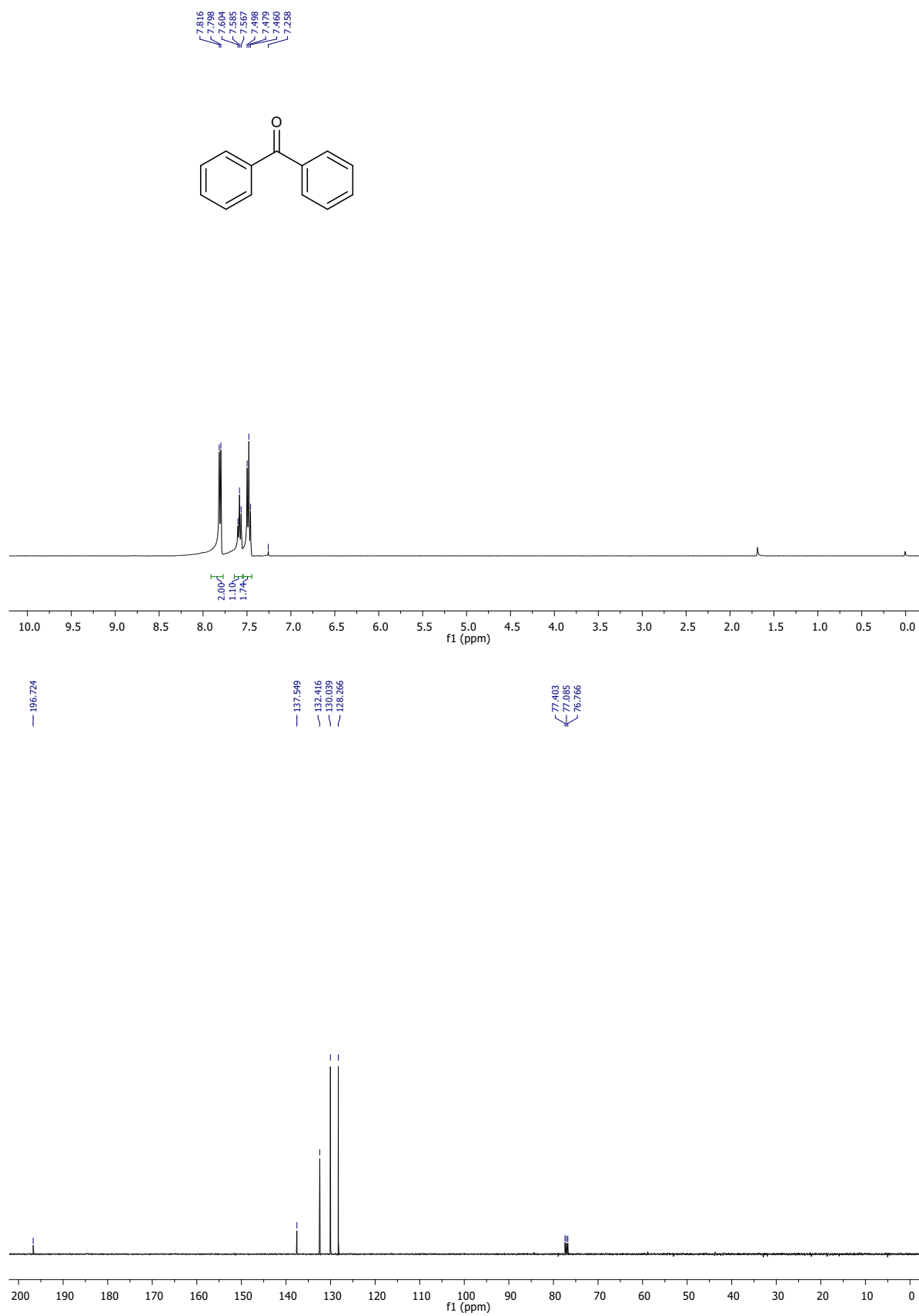


Figure S16. ^1H and ^{13}C NMR spectras of Benzophenone (CDCl_3).

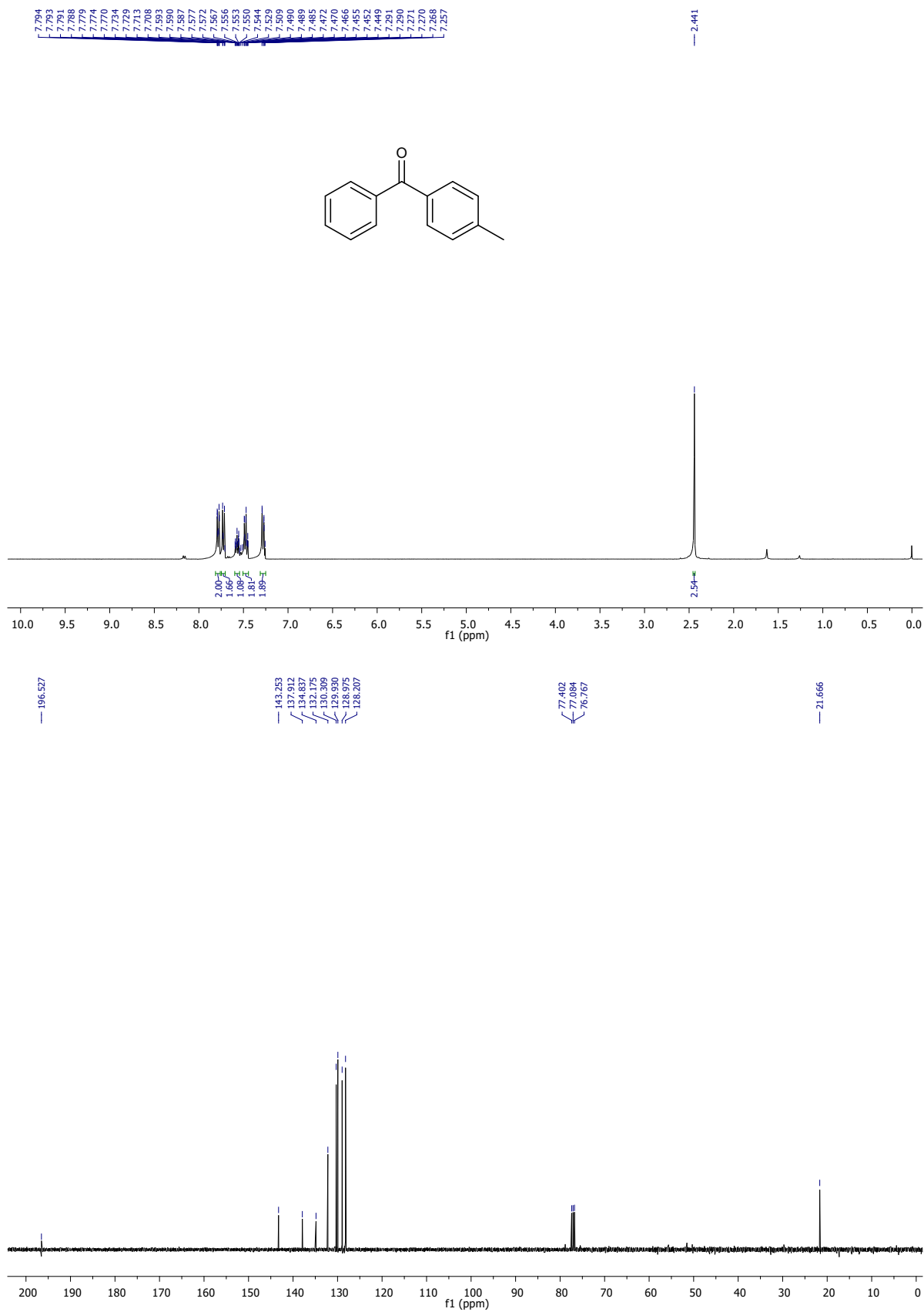


Figure S17. ¹H and ¹³C NMR spectra of 4-Methylbenzophenone (CDCl₃).

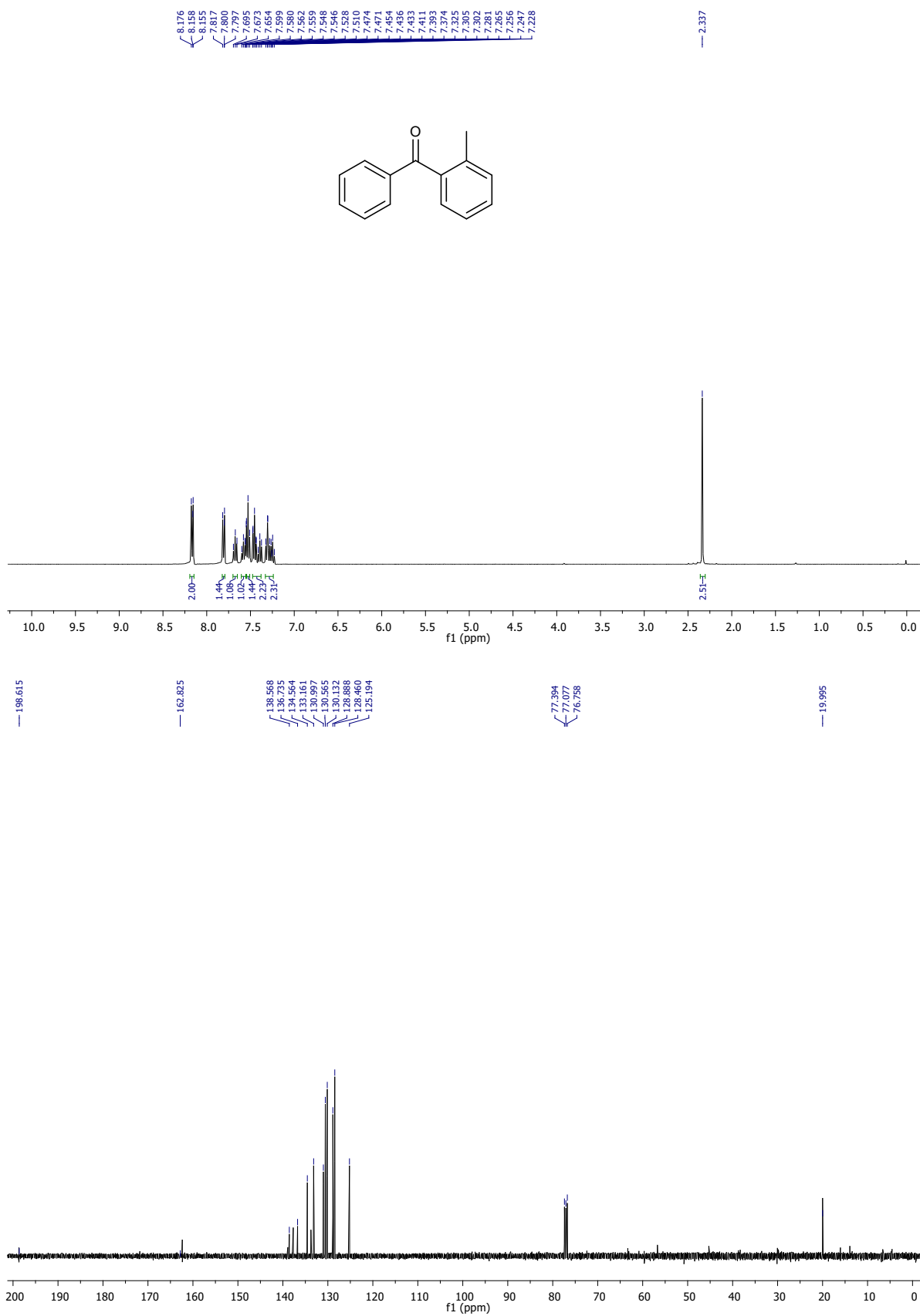


Figure S18. ^1H and ^{13}C NMR spectra of 2-Methylbenzophenone (CDCl_3).

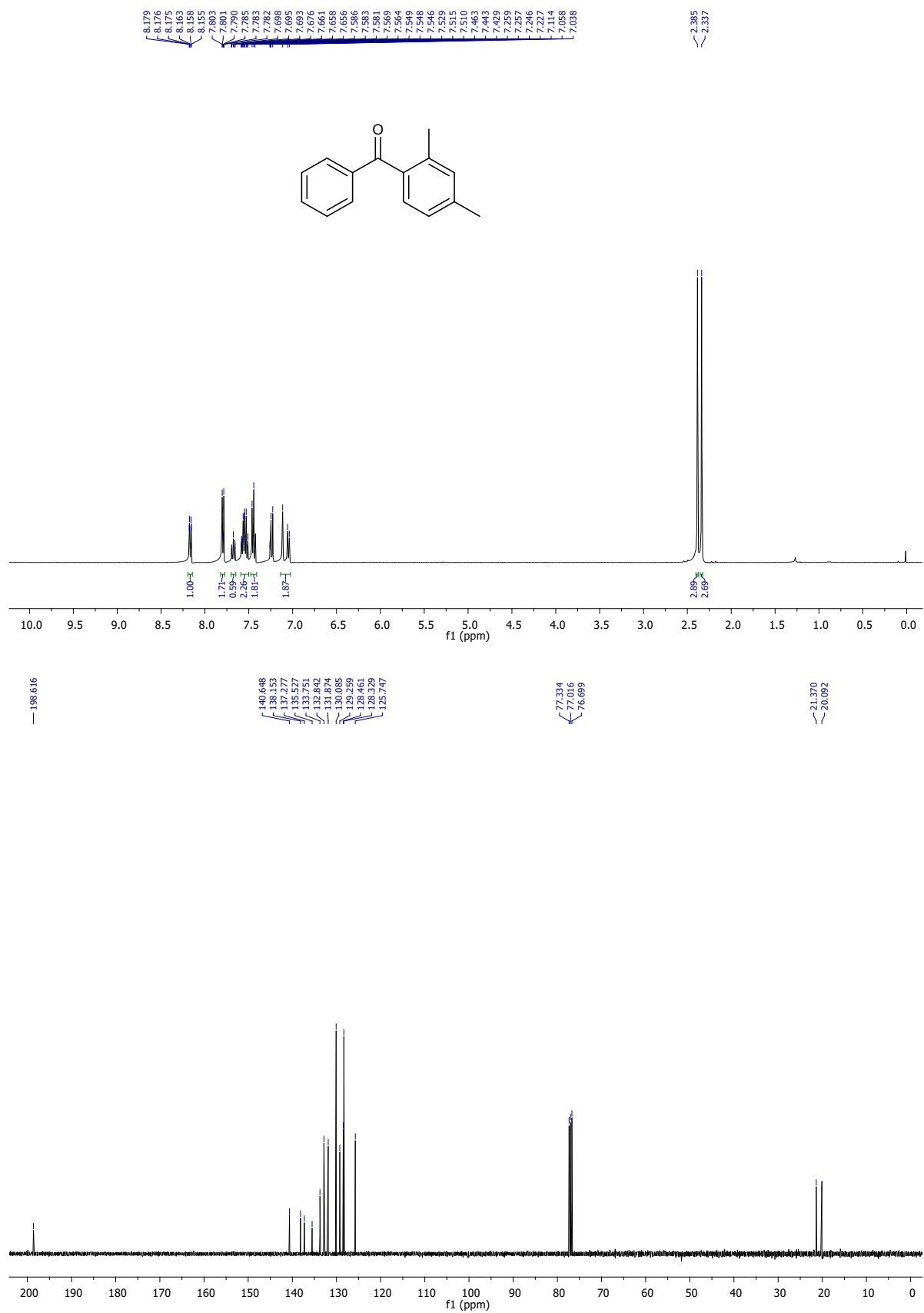


Figure S19. ¹H and ¹³C NMR spectra of 2,4-dimethylbenzophenone (CDCl₃).

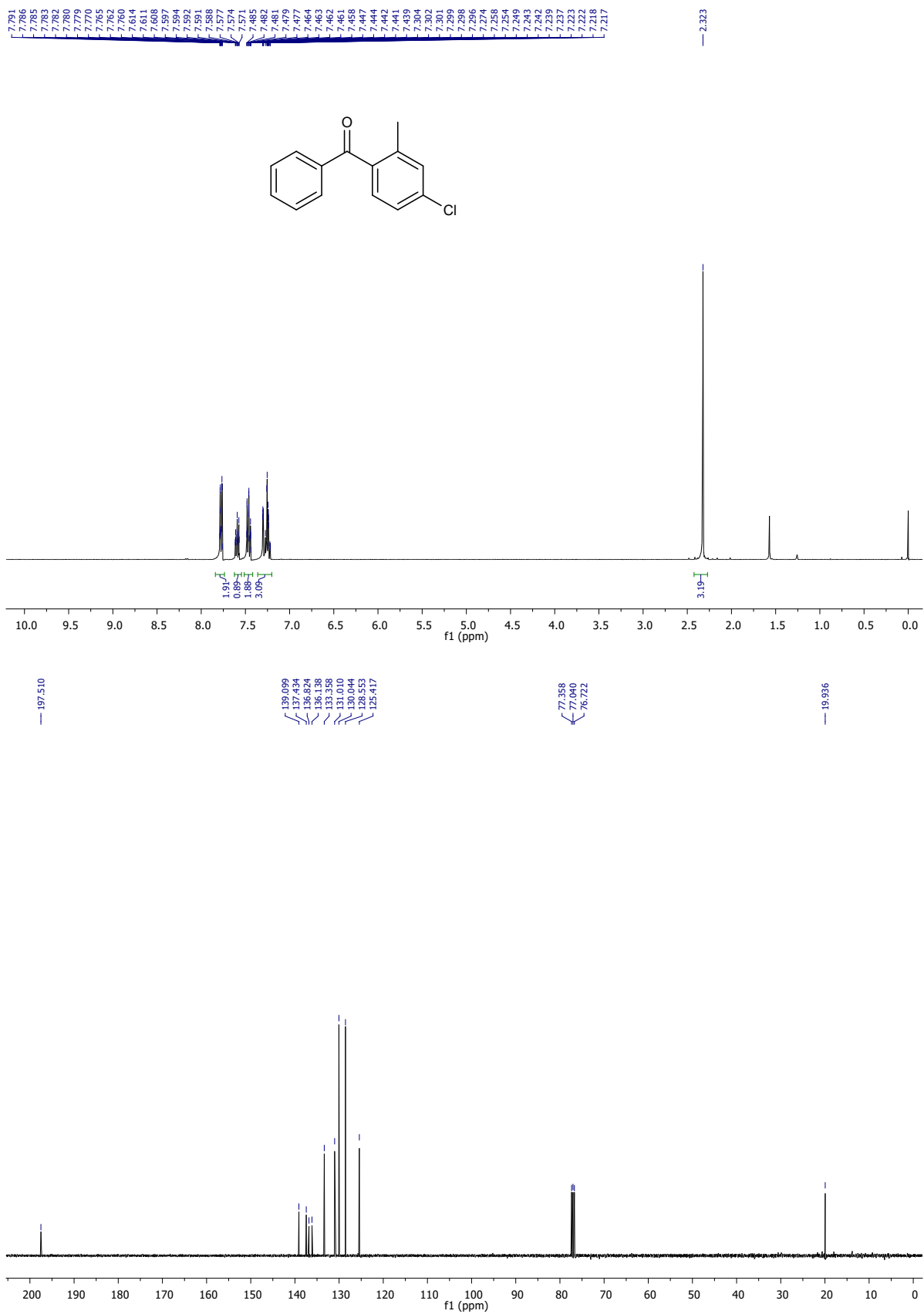
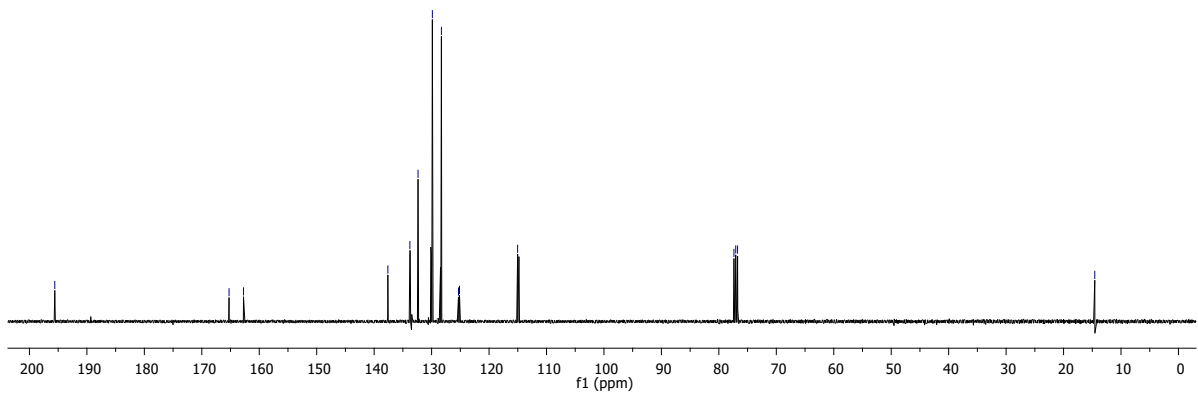
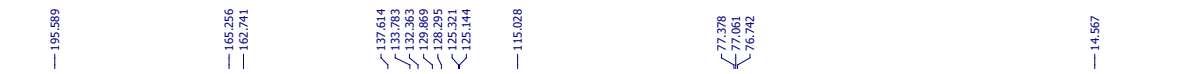
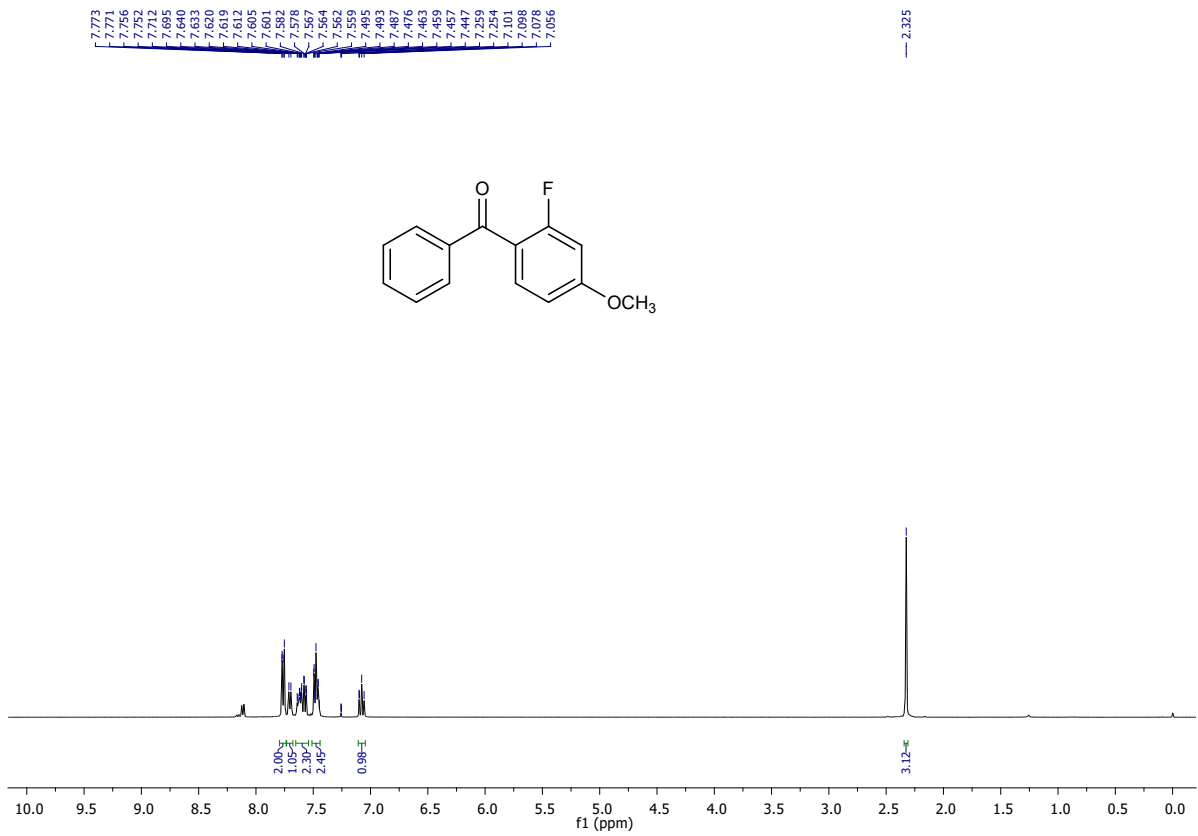


Figure S20. ¹H and ¹³C NMR spectra of 4-Chloro-2-methylbenzophenone (CDCl₃).



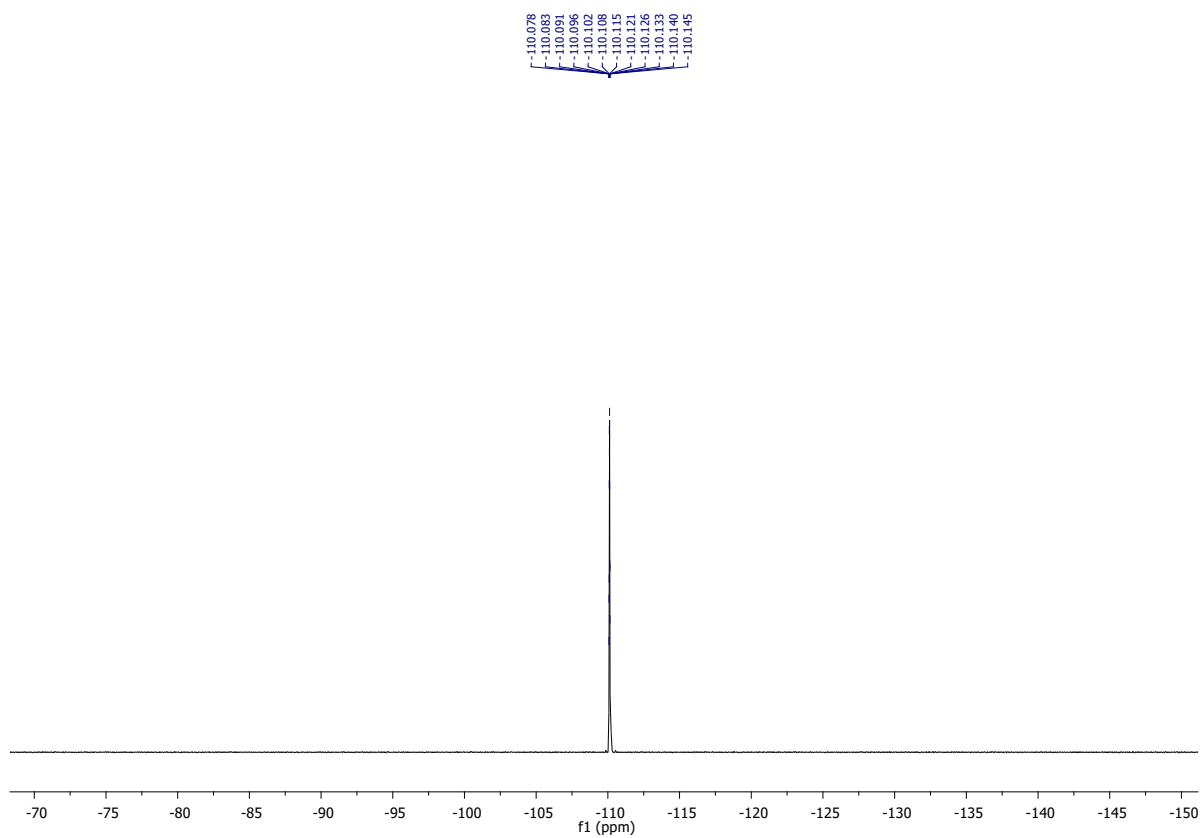


Figure S21. ^1H , ^{13}C and ^{19}F NMR spectrums of 2-Fluoro,4-methoxybenzophenone (CDCl_3).

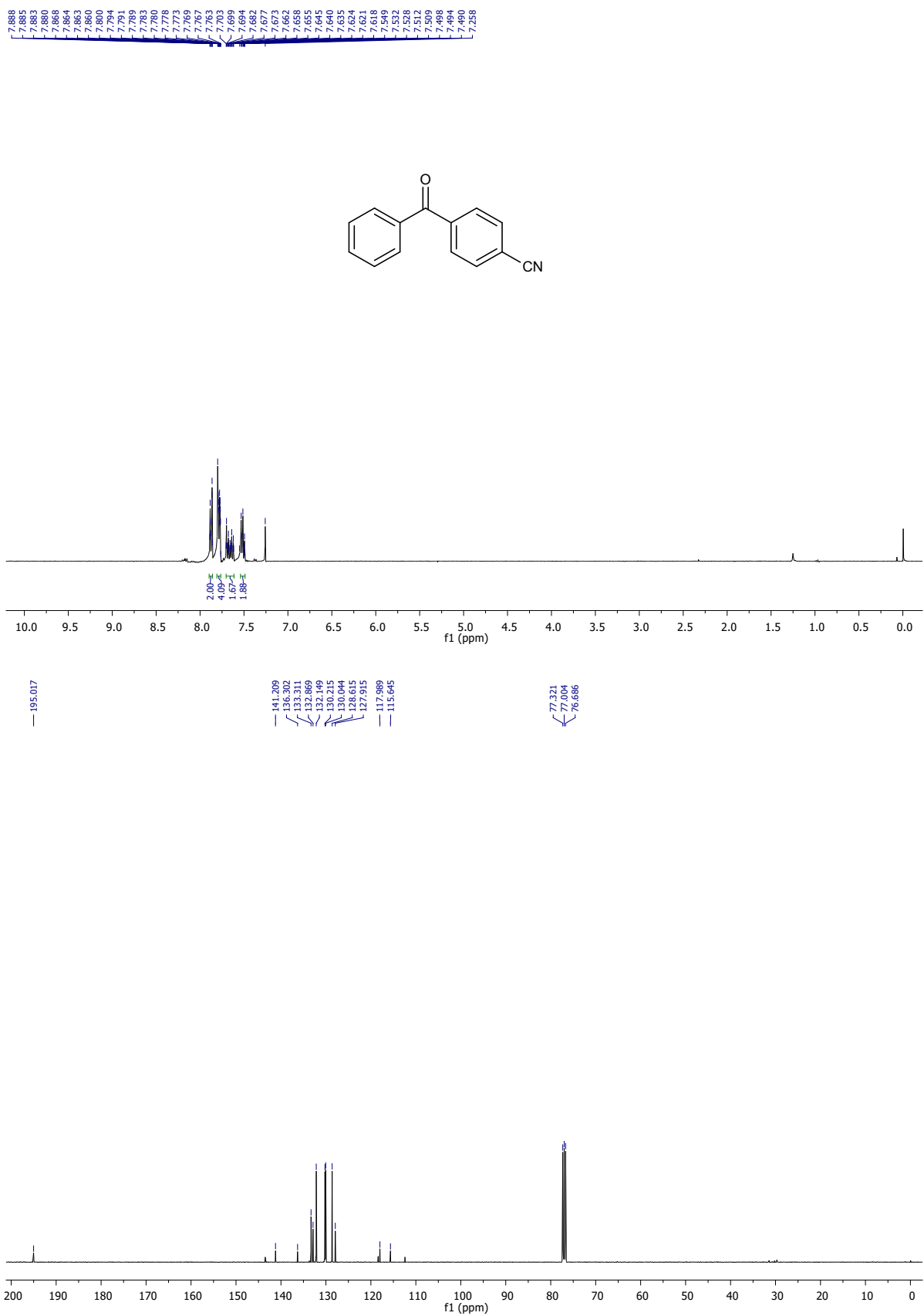
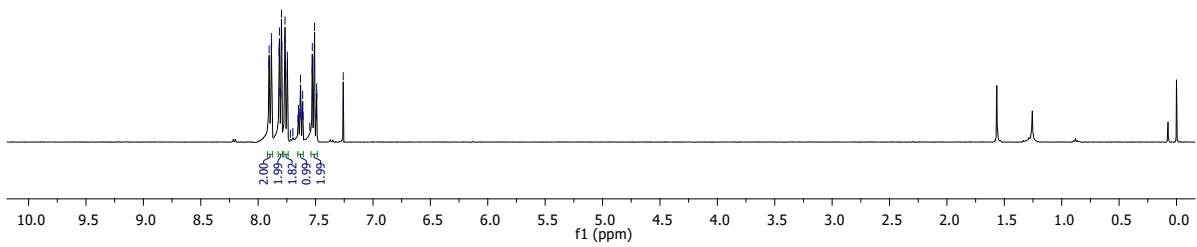
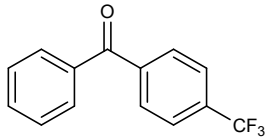


Figure S22. ¹H and ¹³C NMR spectra of 4-Cyanobenzophenone (CDCl₃).

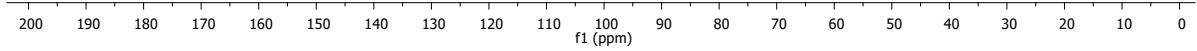
7.906
7.905
7.903
7.895
7.883
7.818
7.817
7.815
7.813
7.811
7.803
7.797
7.794
7.766
7.766
7.747
7.746
7.744
7.719
7.719
7.683
7.653
7.649
7.648
7.646
7.636
7.632
7.631
7.626
7.615
7.614
7.612
7.609
7.550
7.529
7.528
7.527
7.525
7.511
7.495
7.495
7.493
7.490
7.489
7.259
7.258



195.517

140.694
140.682
136.686
133.078
130.124
130.087
128.378
125.304

77.339
77.021
76.703



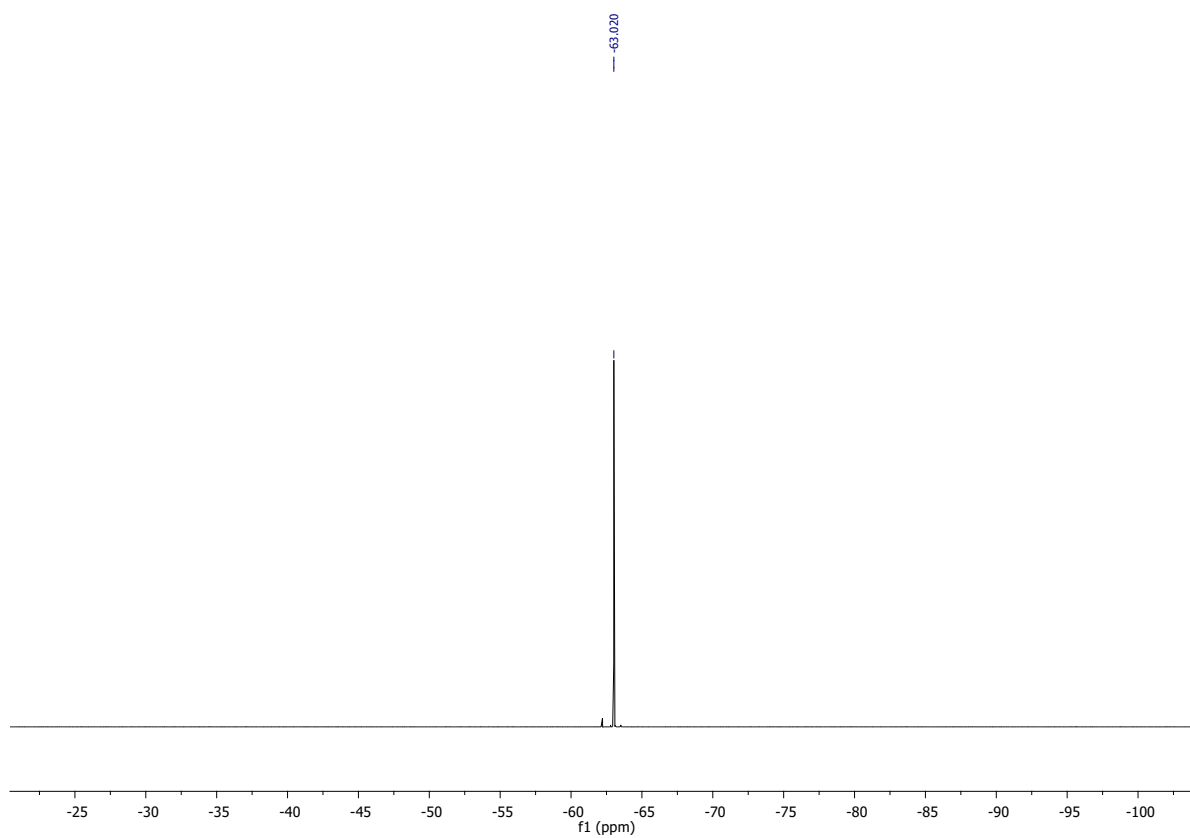


Figure S23. ^1H , ^{13}C and ^{19}F NMR spectrums of 4-(Trifluoromethyl)benzophenone (CDCl_3).

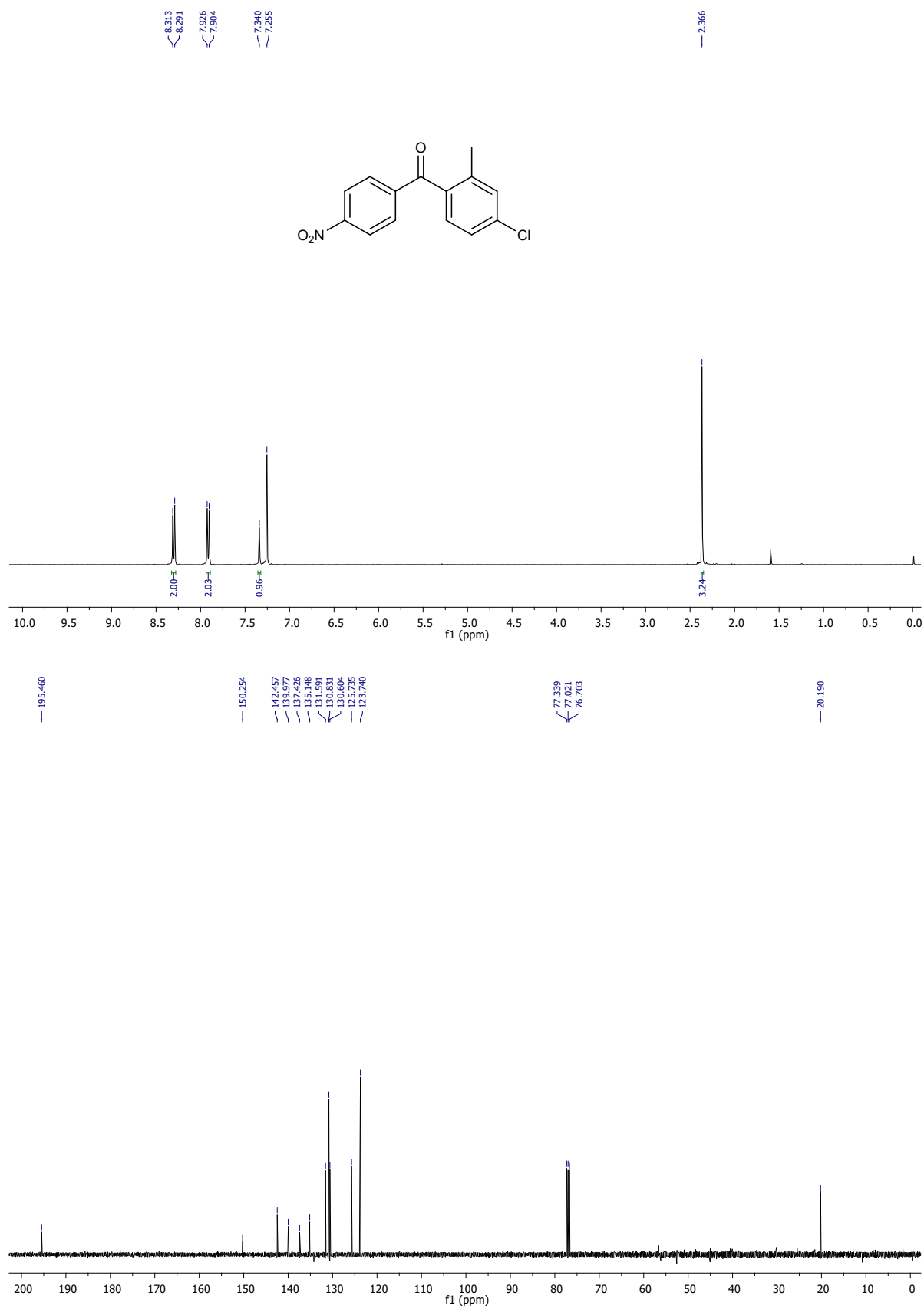
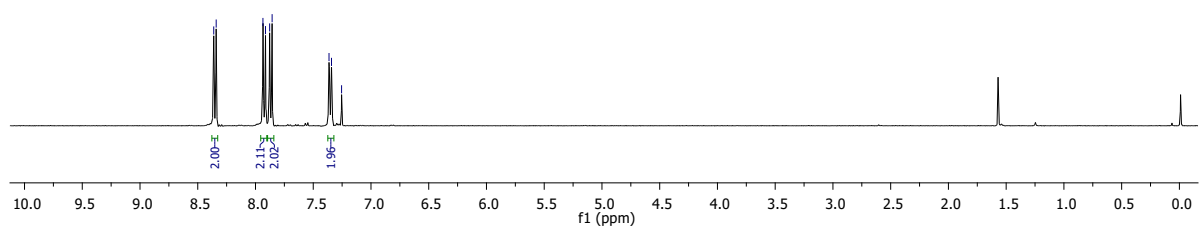
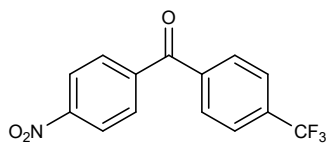
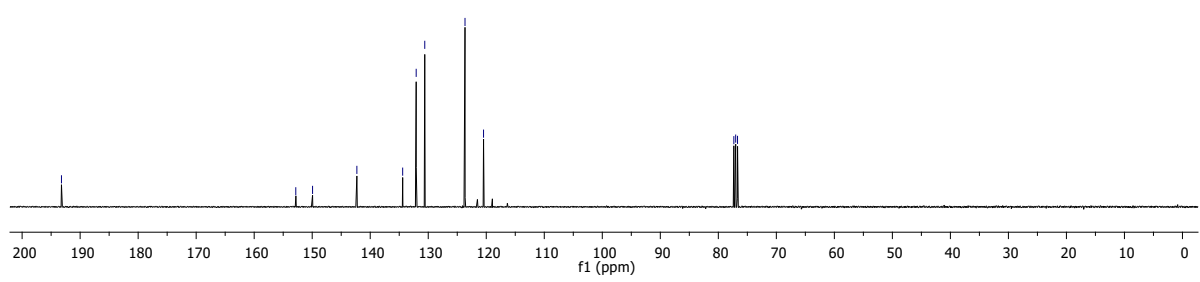


Figure S24. ¹H and ¹³C NMR spectra of 4-Chloro-2-methyl-4'-nitrobenzophenone (CDCl₃).

8.362
8.340
7.936
7.913
7.878
7.856
7.383
7.342
7.255



193.218
152.829
149.937
142.300
134.406
132.677
130.599
123.661
120.467
77.325
77.007
76.689



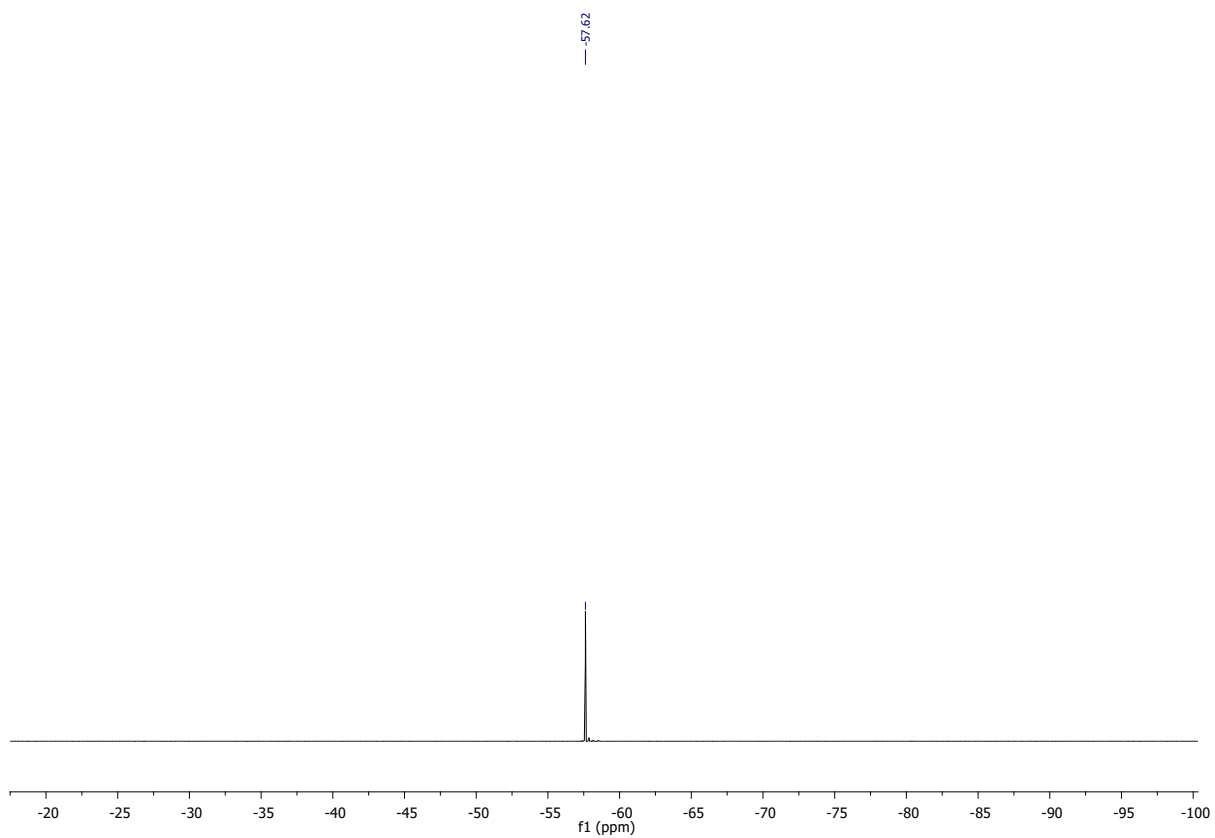


Figure S25. ^1H , ^{13}C and ^{19}F NMR spectra of 4-Trifluoromethyl-4'-nitrobenzophenone (CDCl_3).

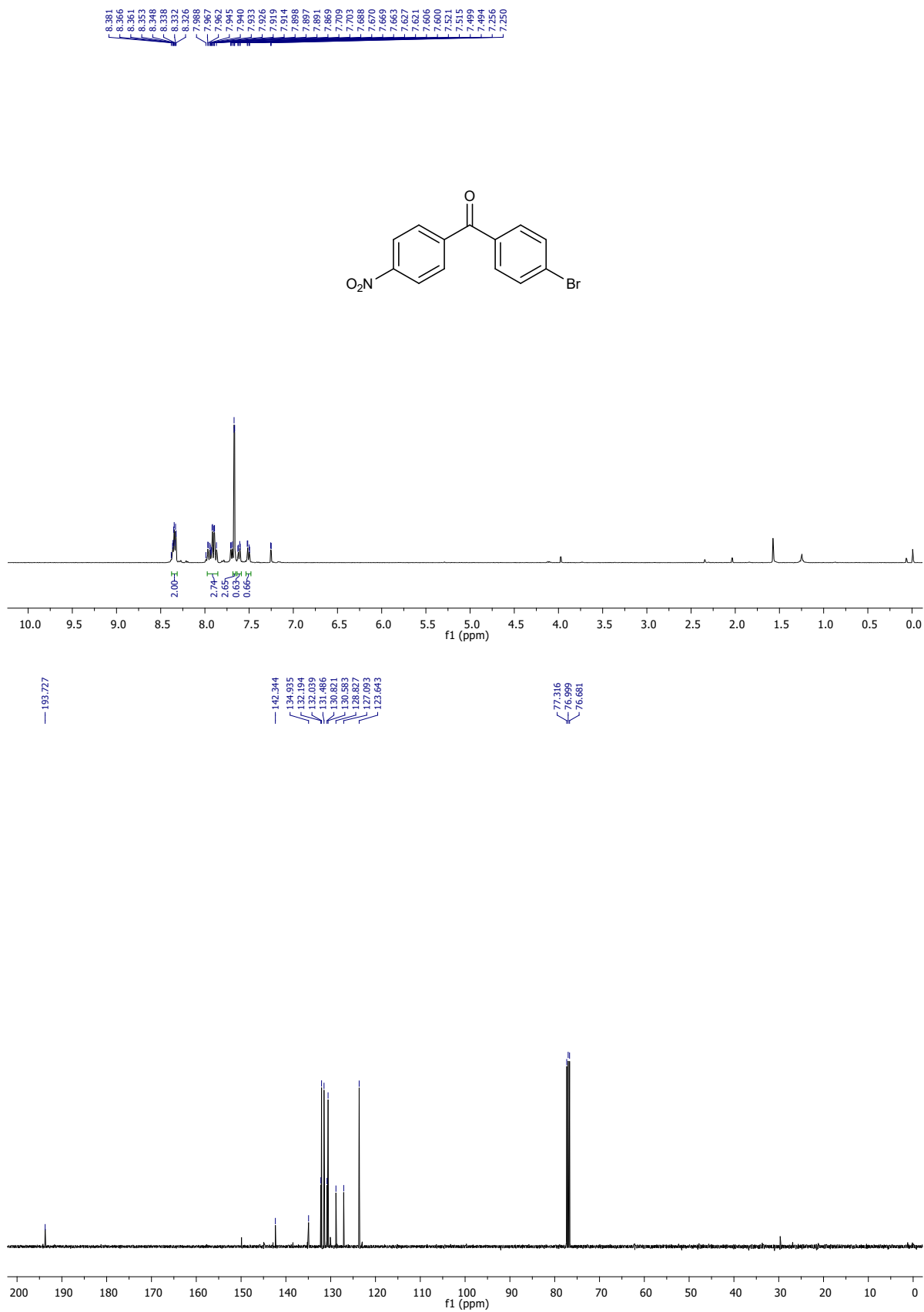


Figure S26. ¹H and ¹³C NMR spectra of 4-Bromo-4'-nitrobenzophenone (CDCl₃).

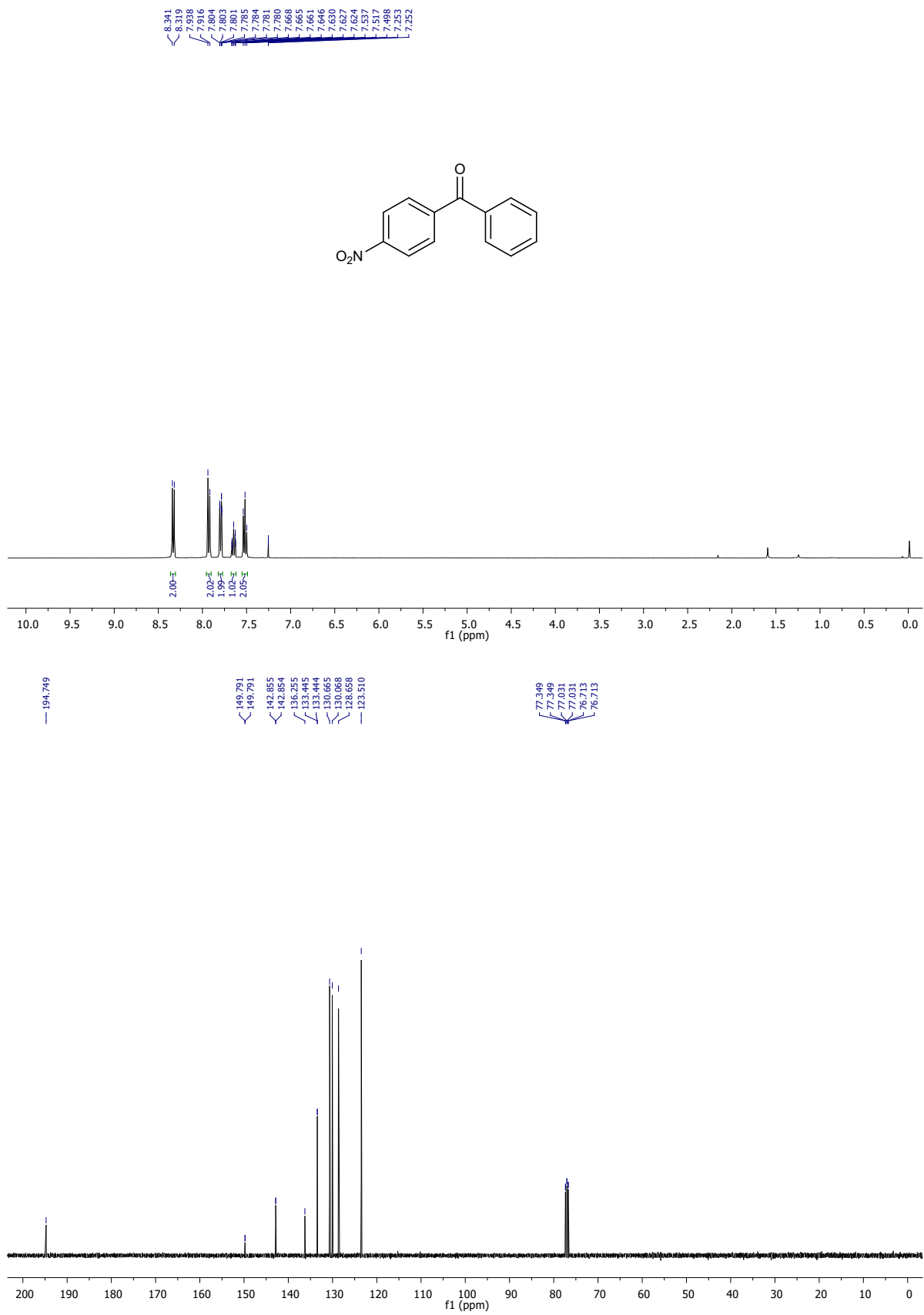


Figure S27. ¹H and ¹³C NMR spectra of 4'-nitrobenzophenone (CDCl₃).

^1H - and ^{13}C - NMR spectras of Suzuki products

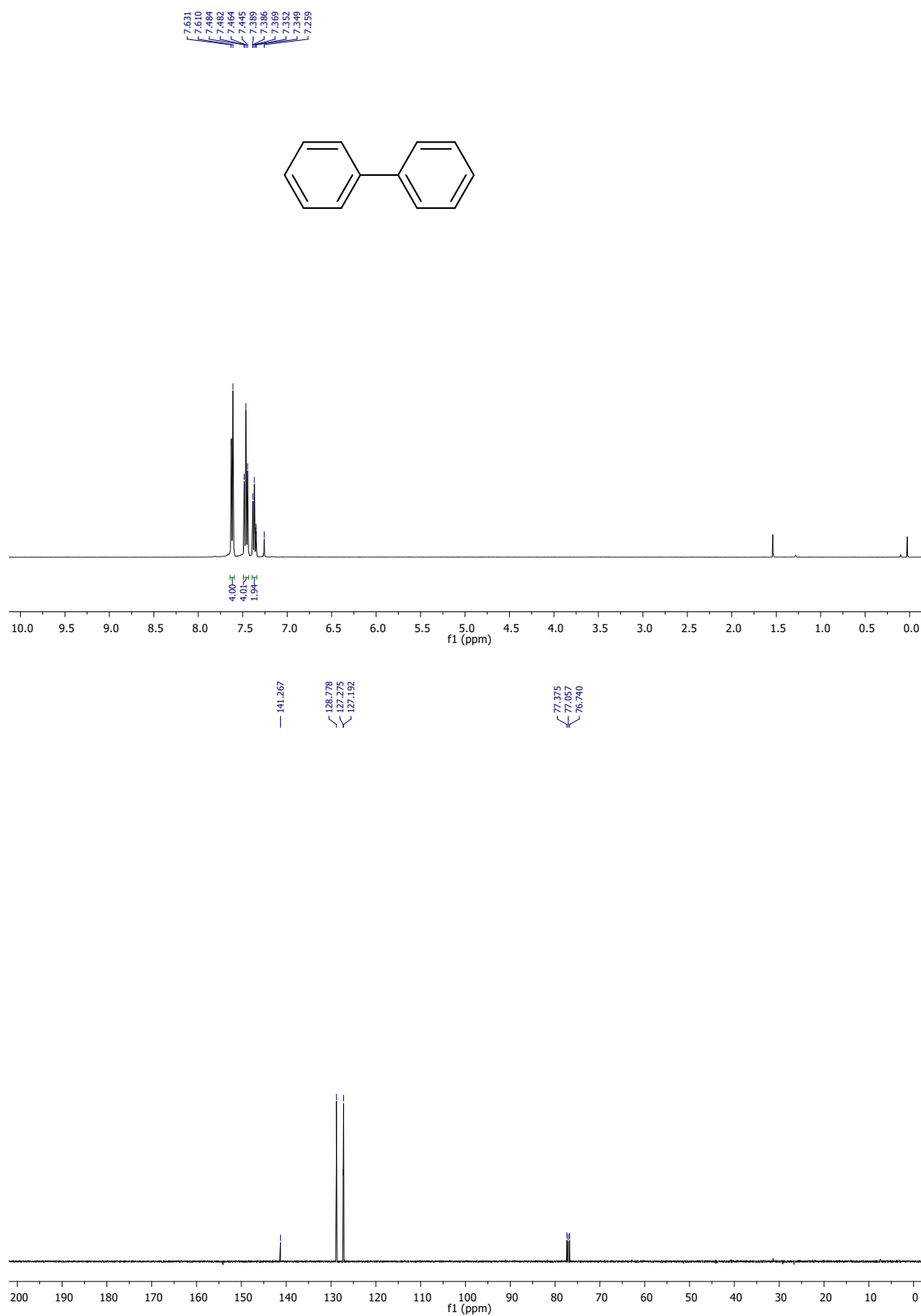


Figure S28. ^1H and ^{13}C NMR spectras of Biphenyl (CDCl_3).

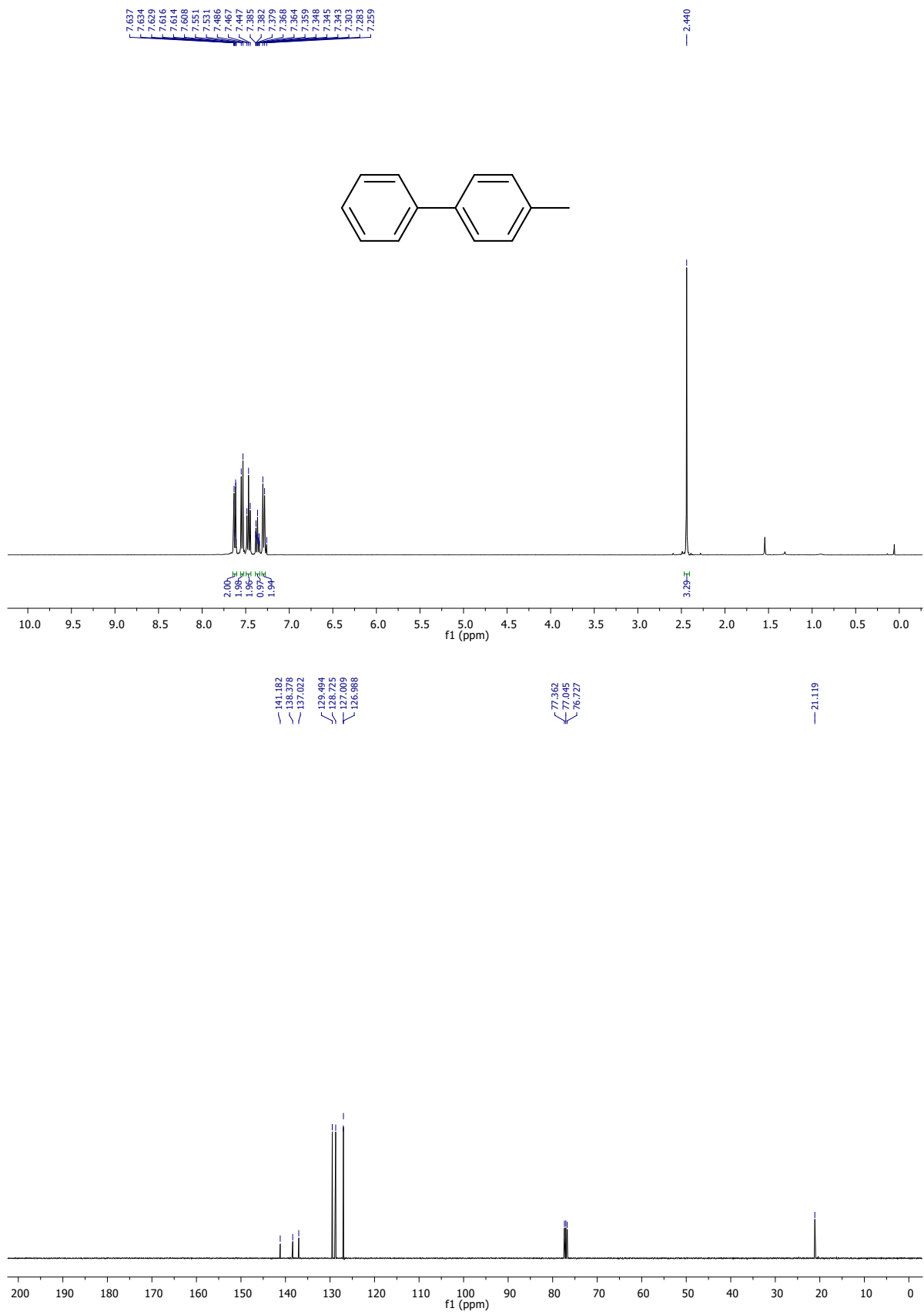


Figure S29. ¹H and ¹³C NMR spectra of 4-Methylbiphenyl (CDCl₃).



Figure S30. ¹H and ¹³C NMR spectra of 4-Tert-butylbiphenyl (CDCl₃).

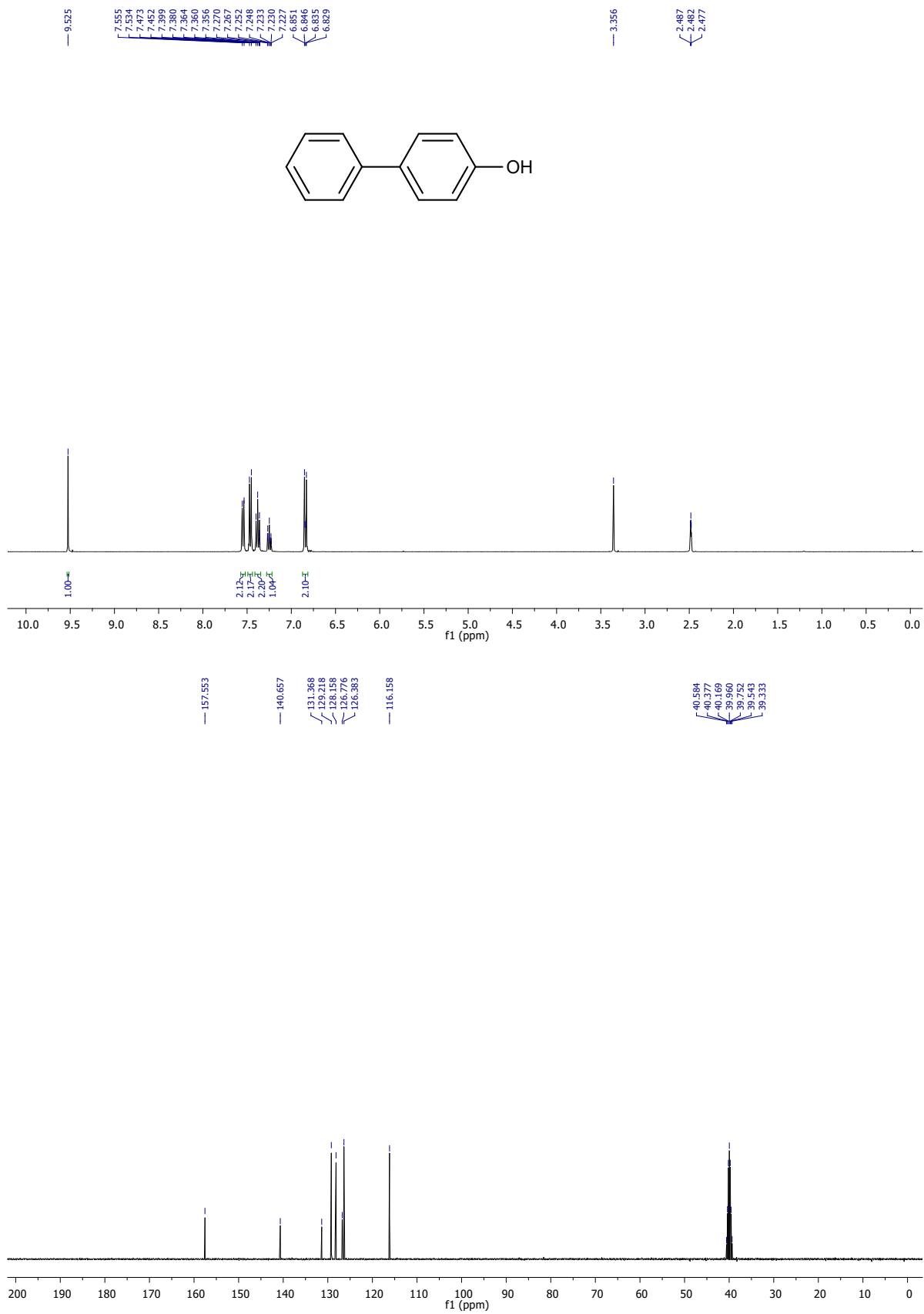


Figure S31. ¹H and ¹³C NMR spectra of 4-Hydroxybiphenyl (DMSO-*d*₆).

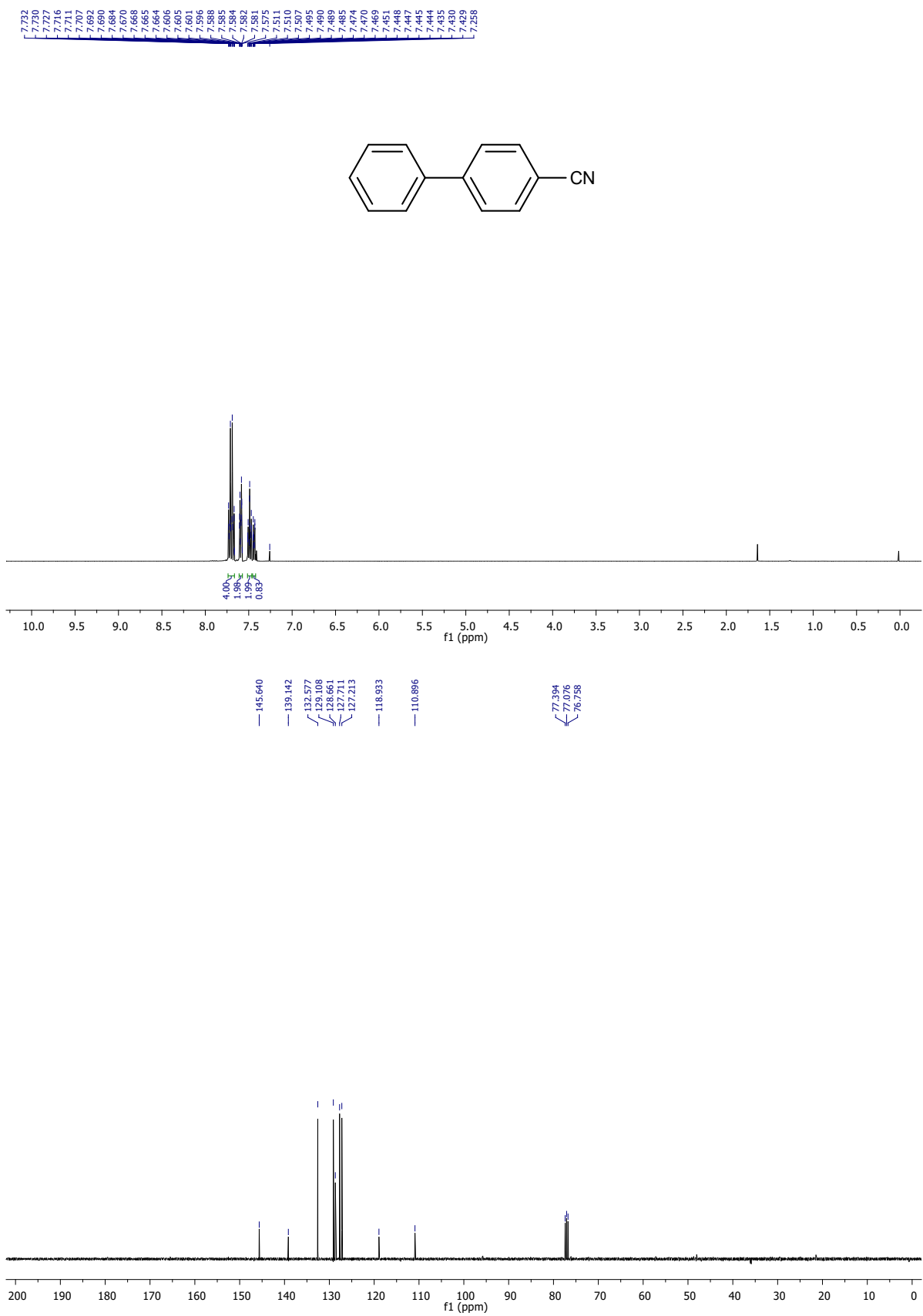
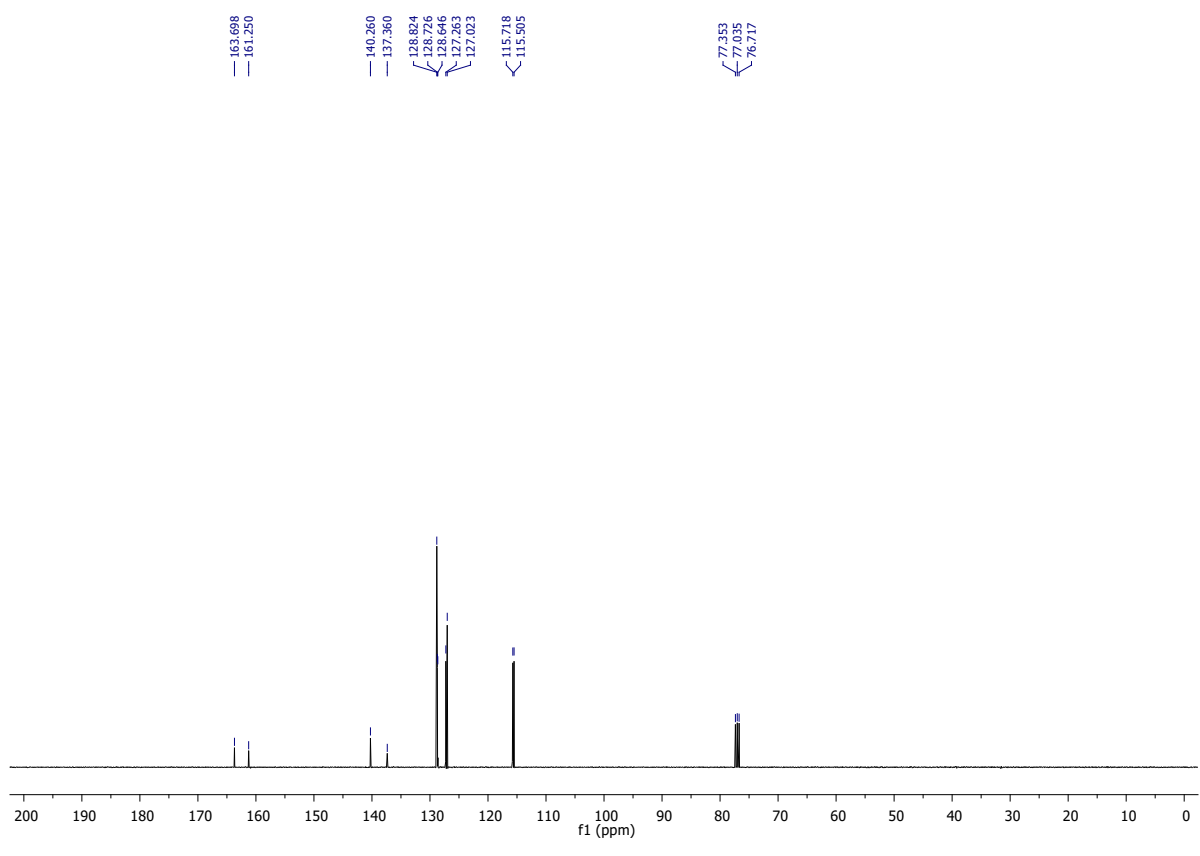
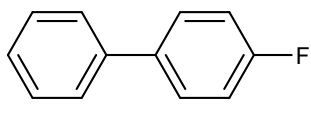
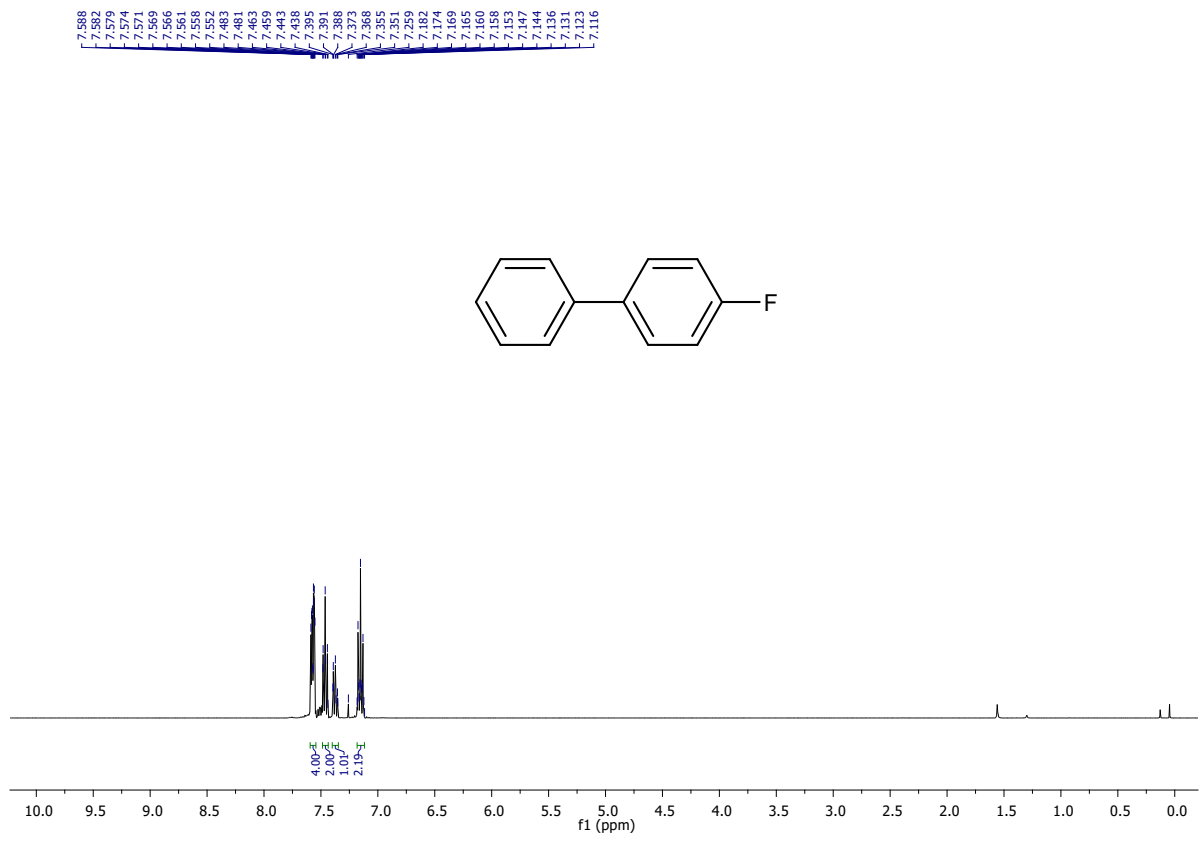


Figure S32. ¹H and ¹³C NMR spectra of 4-Cyanobiphenyl (CDCl₃).



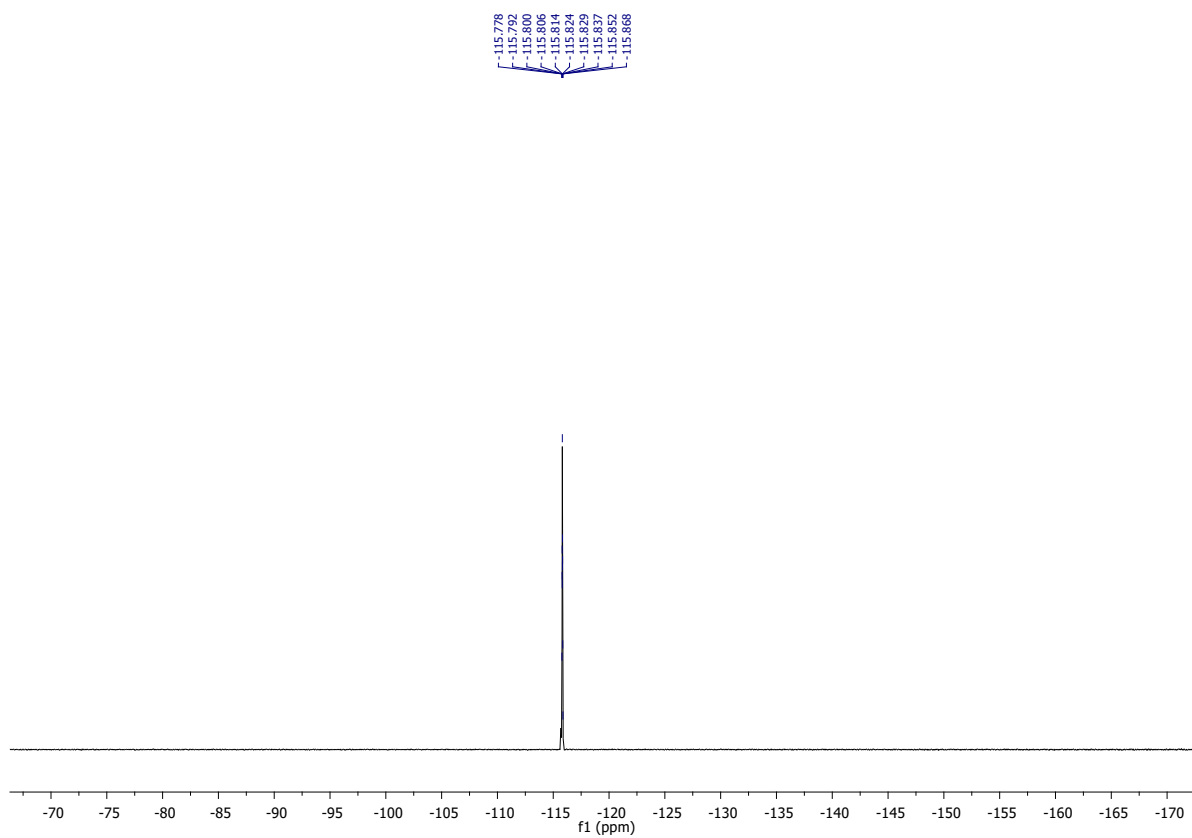
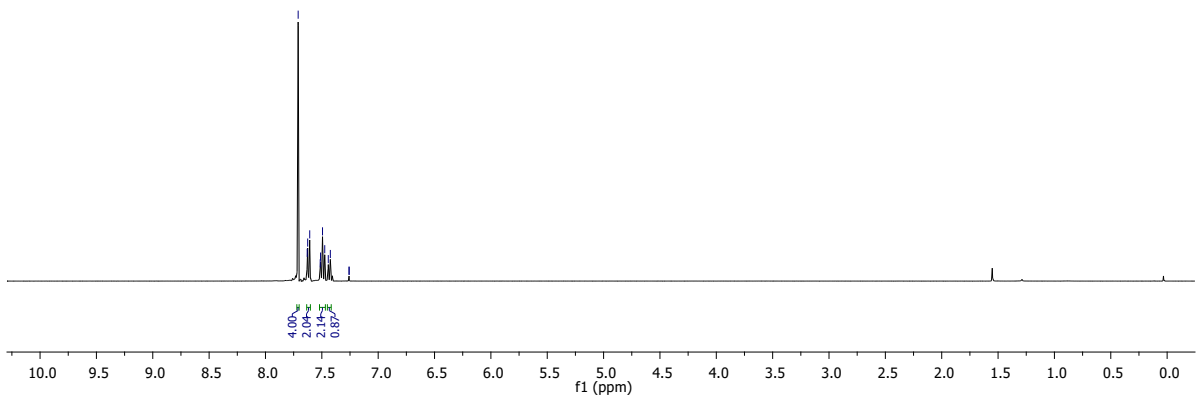
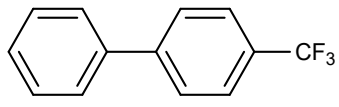
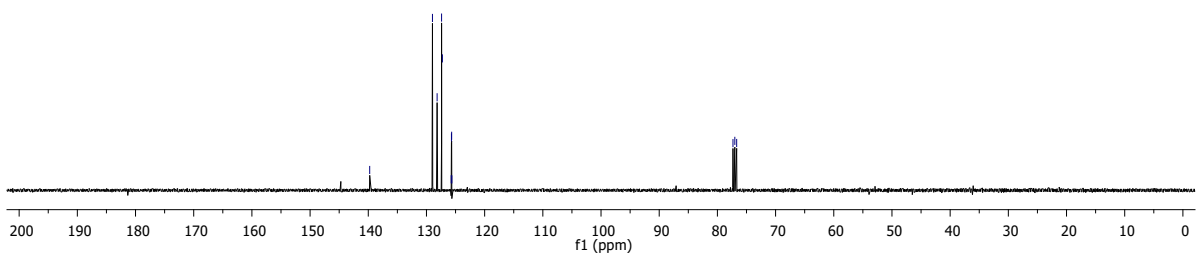


Figure S33. ^1H , ^{13}C and ^{19}F NMR spectra of 4-Fluorobiphenyl (CDCl_3).

7.710
7.630
7.625
7.607
7.514
7.381
7.374
7.443
7.424
7.258



139.755
128.969
128.169
127.402
127.262
125.746
125.708
125.670
125.632
77.324
77.006
76.688



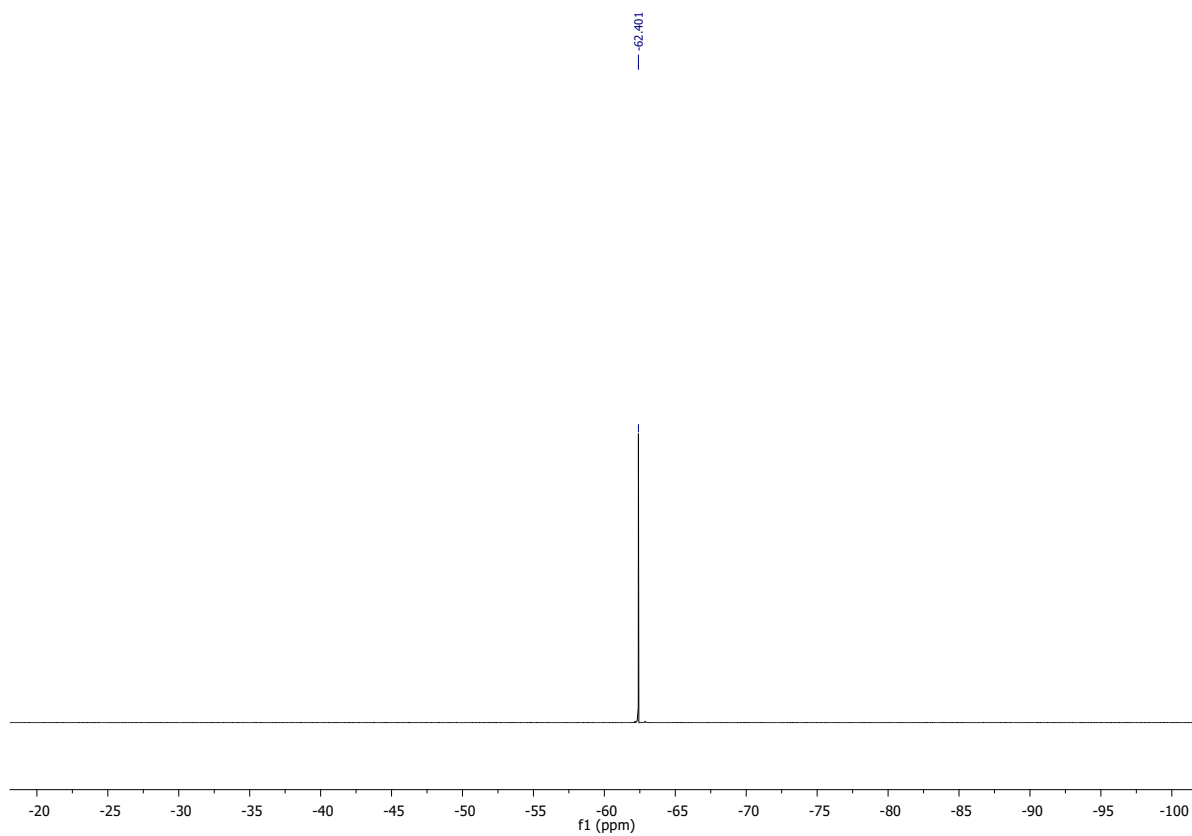
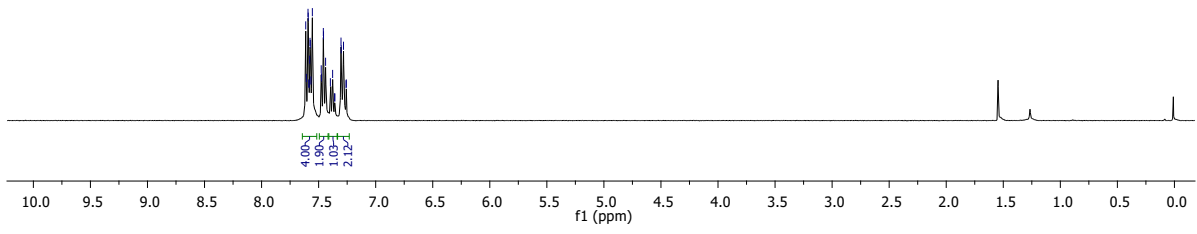
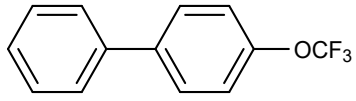


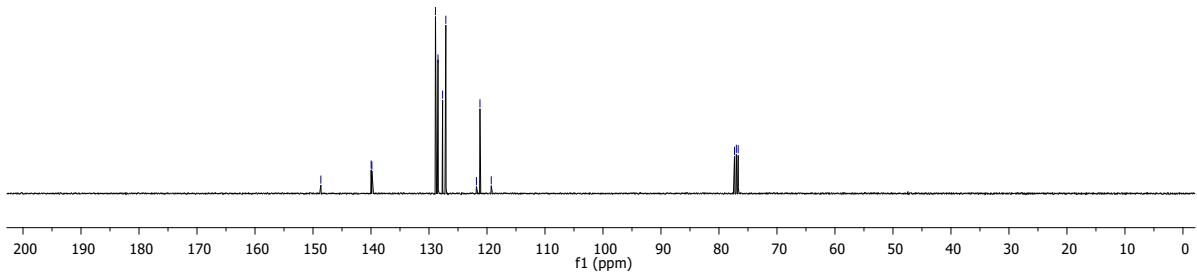
Figure S34. ^1H , ^{13}C and ^{19}F NMR spectrums of 4-(Trifluoromethyl)biphenyl (CDCl_3).

7.613
7.608
7.593
7.591
7.586
7.584
7.578
7.575
7.563
7.562
7.555
7.477
7.475
7.459
7.457
7.439
7.397
7.377
7.366
7.358
7.304
7.302
7.282
7.260
7.257



148.649
139.675
139.642
128.881
127.654
127.097
121.821
121.209
119.266

77.321
77.003
76.686



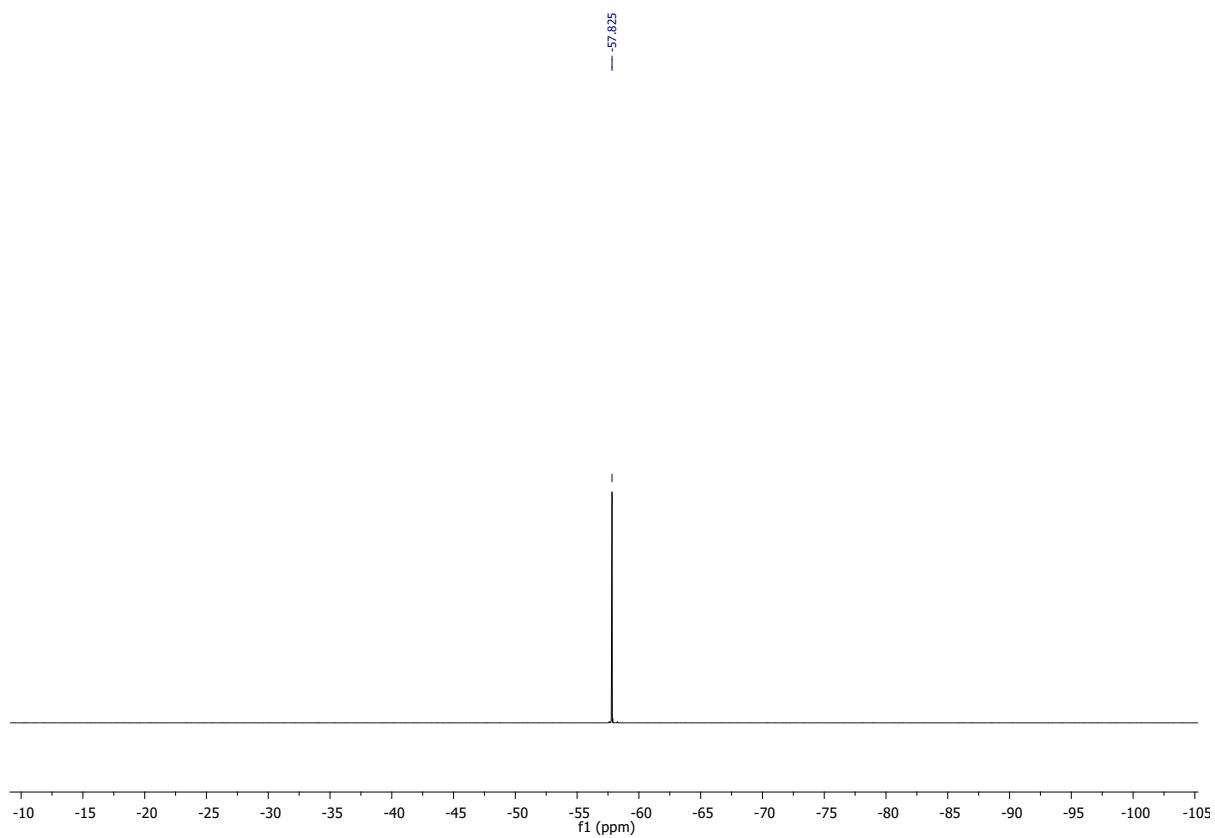


Figure S35. ^1H , ^{13}C and ^{19}F NMR spectrums of 4-(Trifluoromethoxy)biphenyl (CDCl_3).

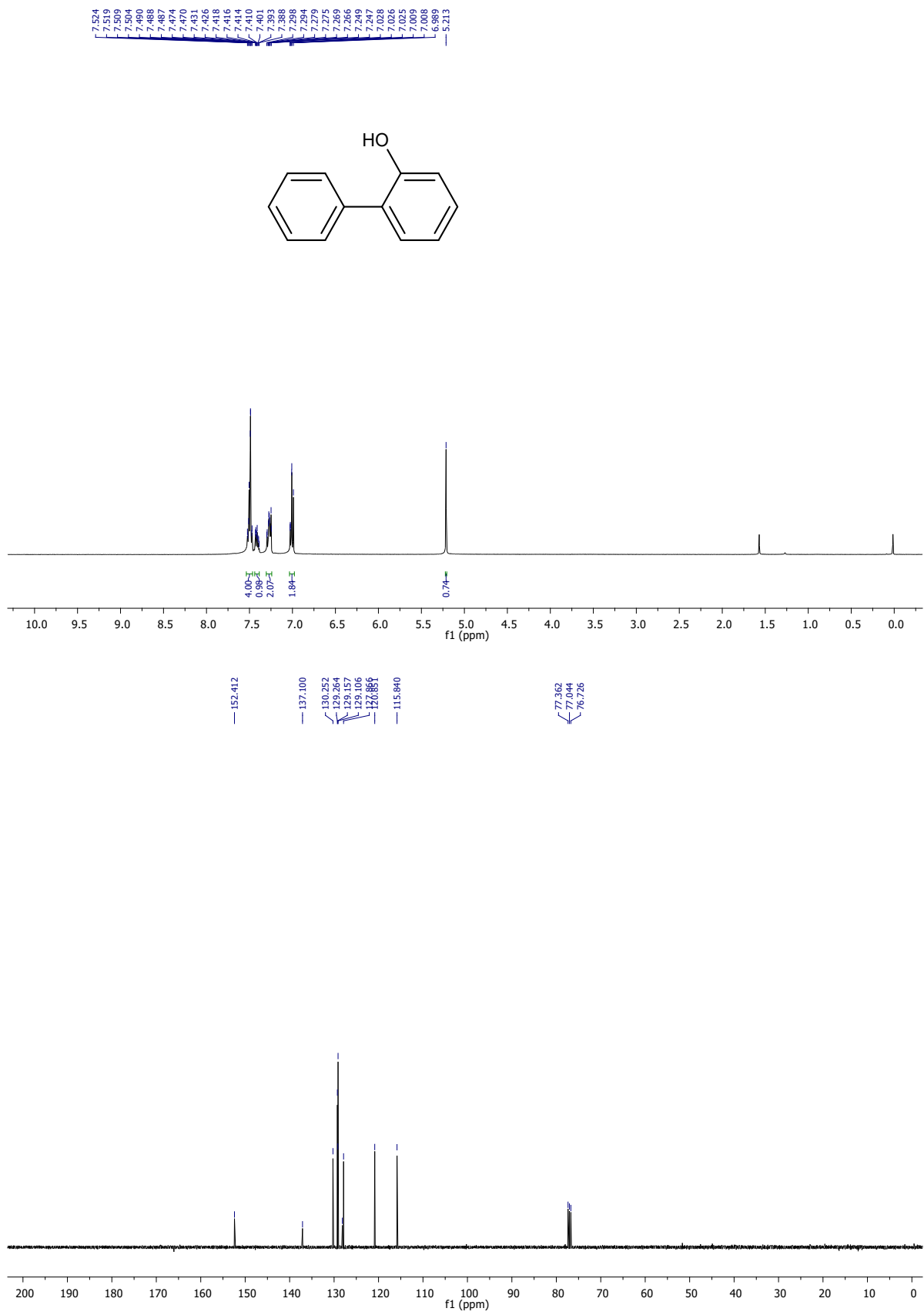


Figure S36. ¹H and ¹³C NMR spectra of 2-Hydroxybiphenyl (CDCl₃).

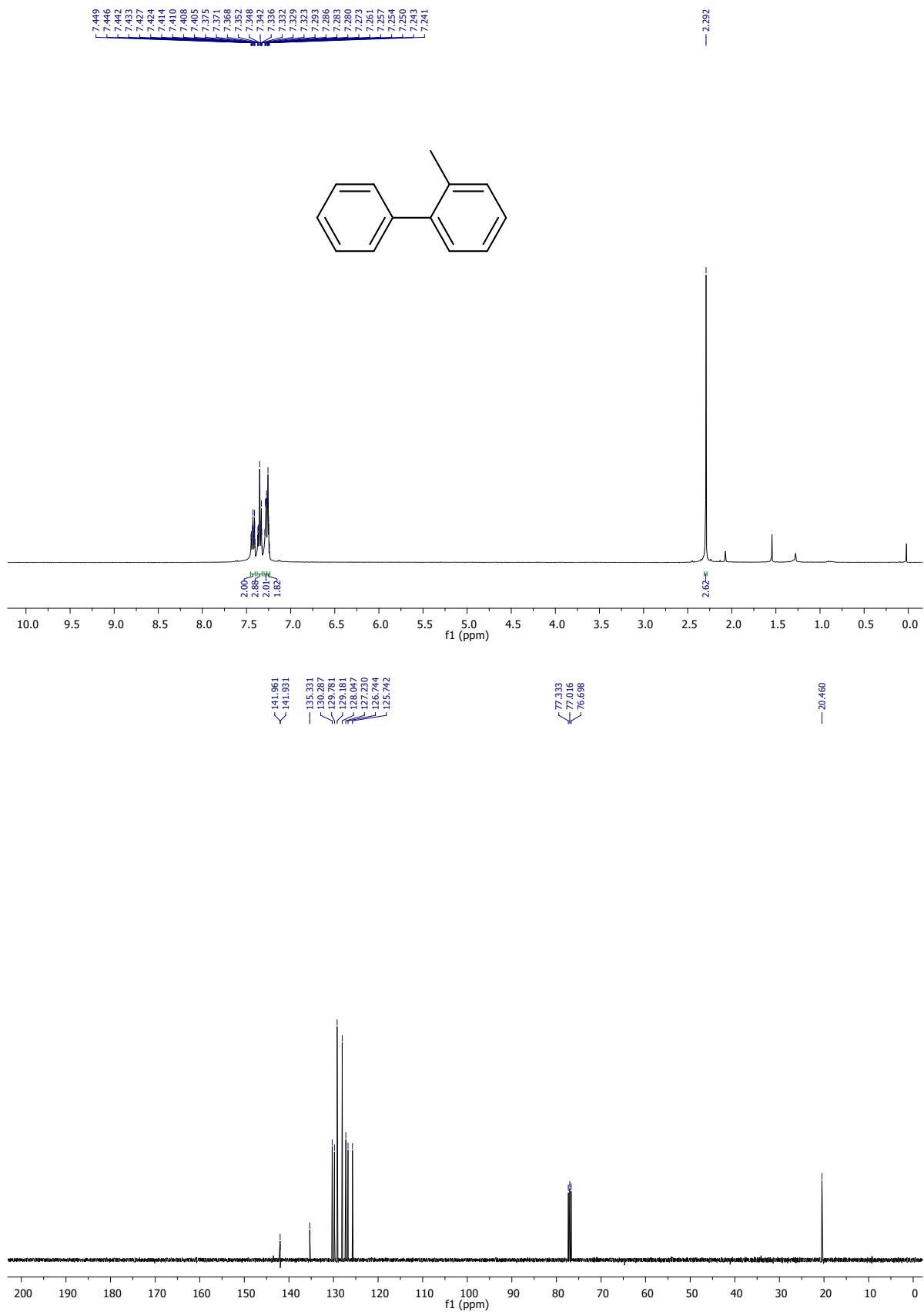
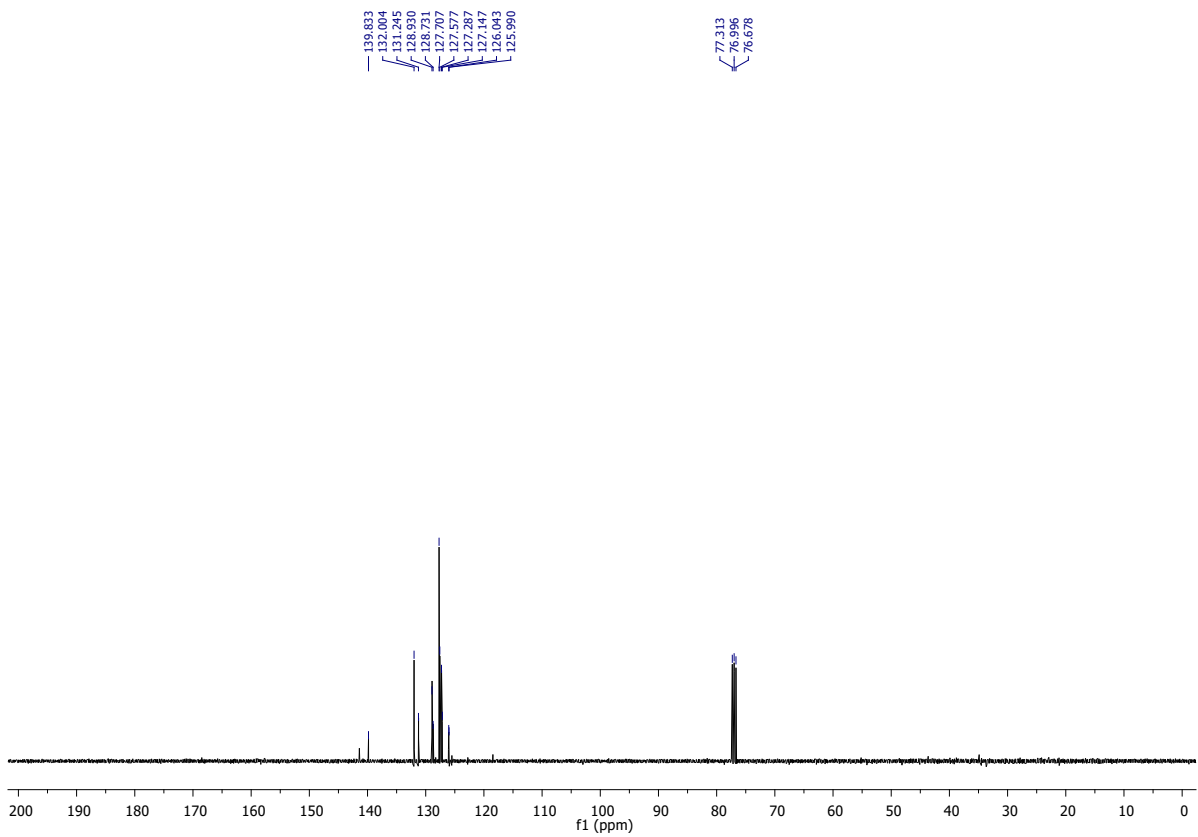
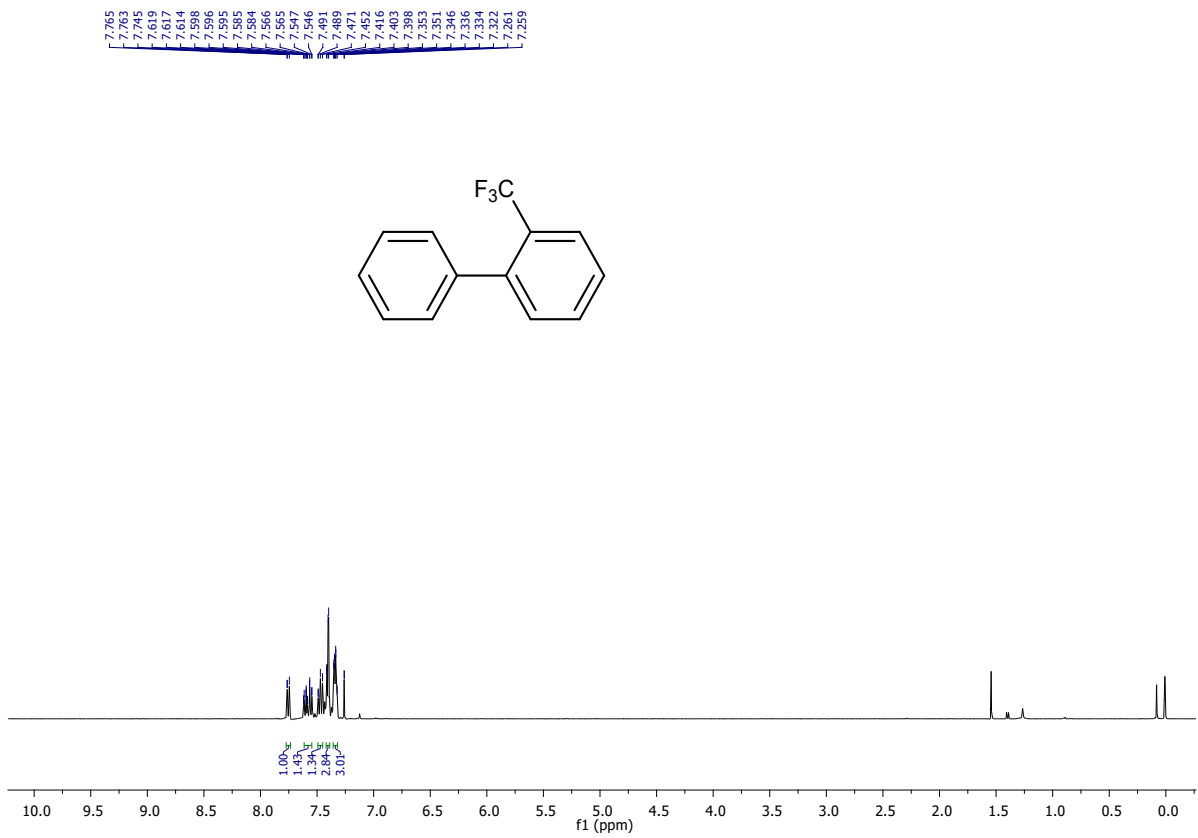


Figure S37. ¹H and ¹³C NMR spectra of 2-Methylbiphenyl (CDCl₃).



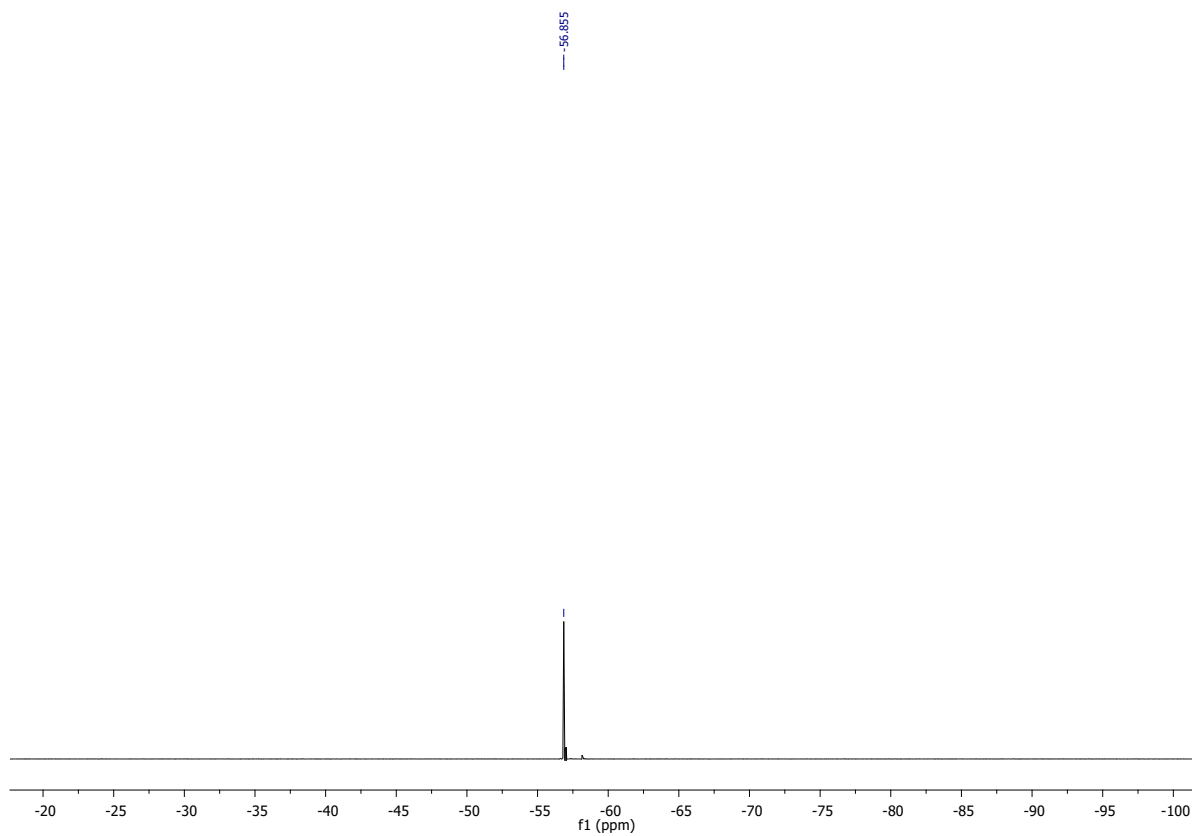


Figure S38. ^1H , ^{13}C and ^{19}F NMR spectrums of 2-(Trifluoromethyl)biphenyl (CDCl_3).

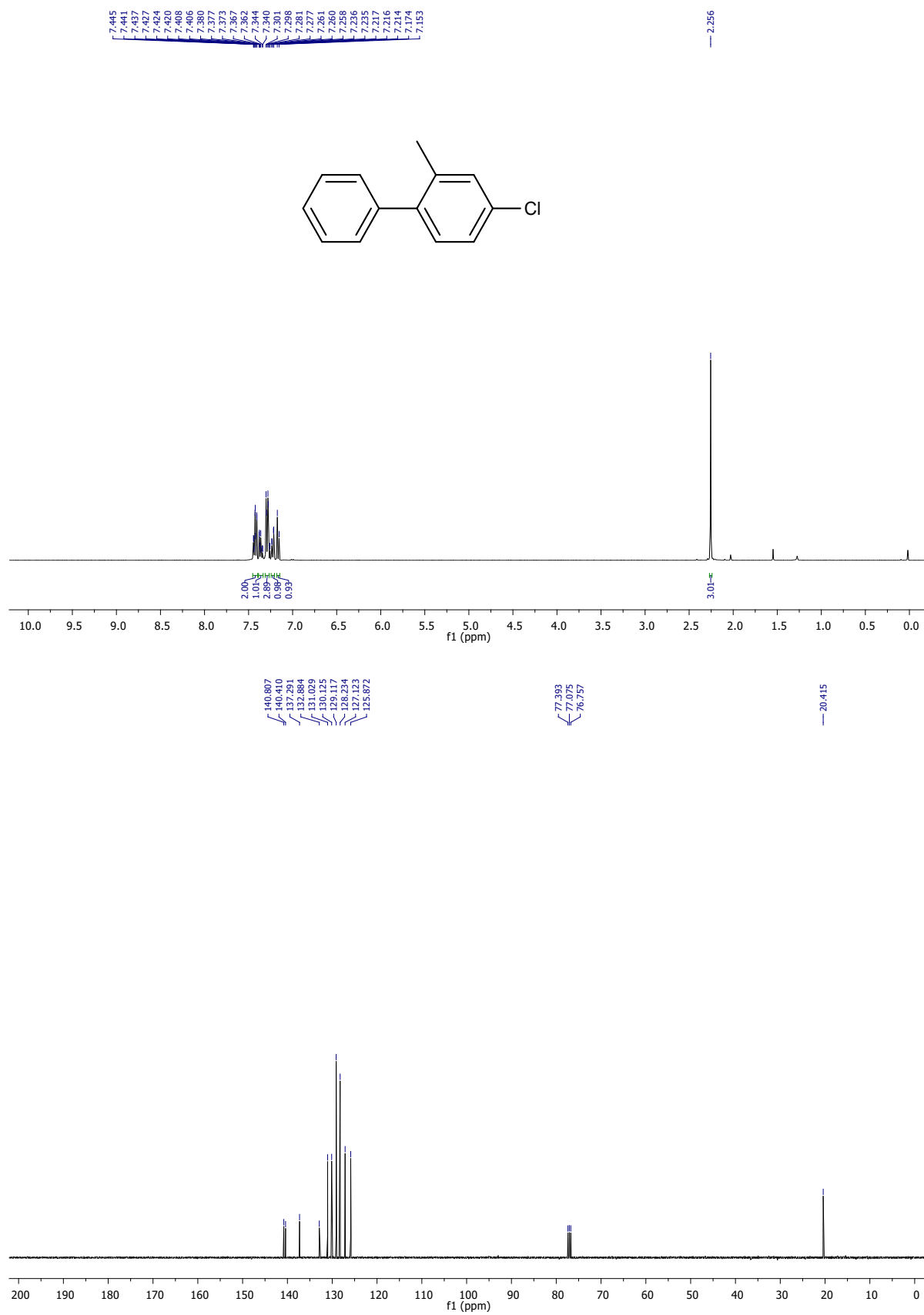


Figure S39. ¹H and ¹³C NMR spectra of 4-Chloro-2-methylbiphenyl (CDCl₃).

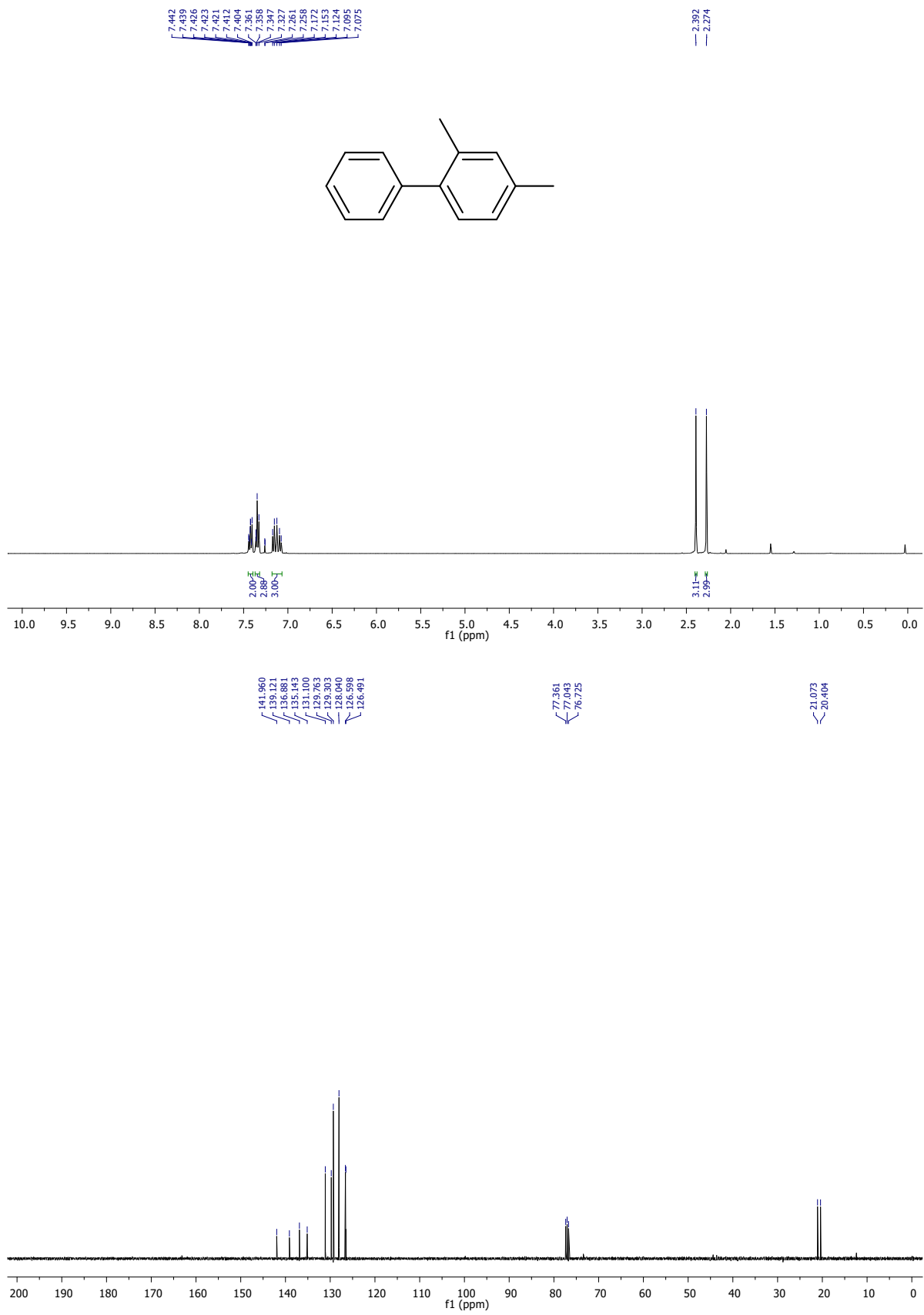
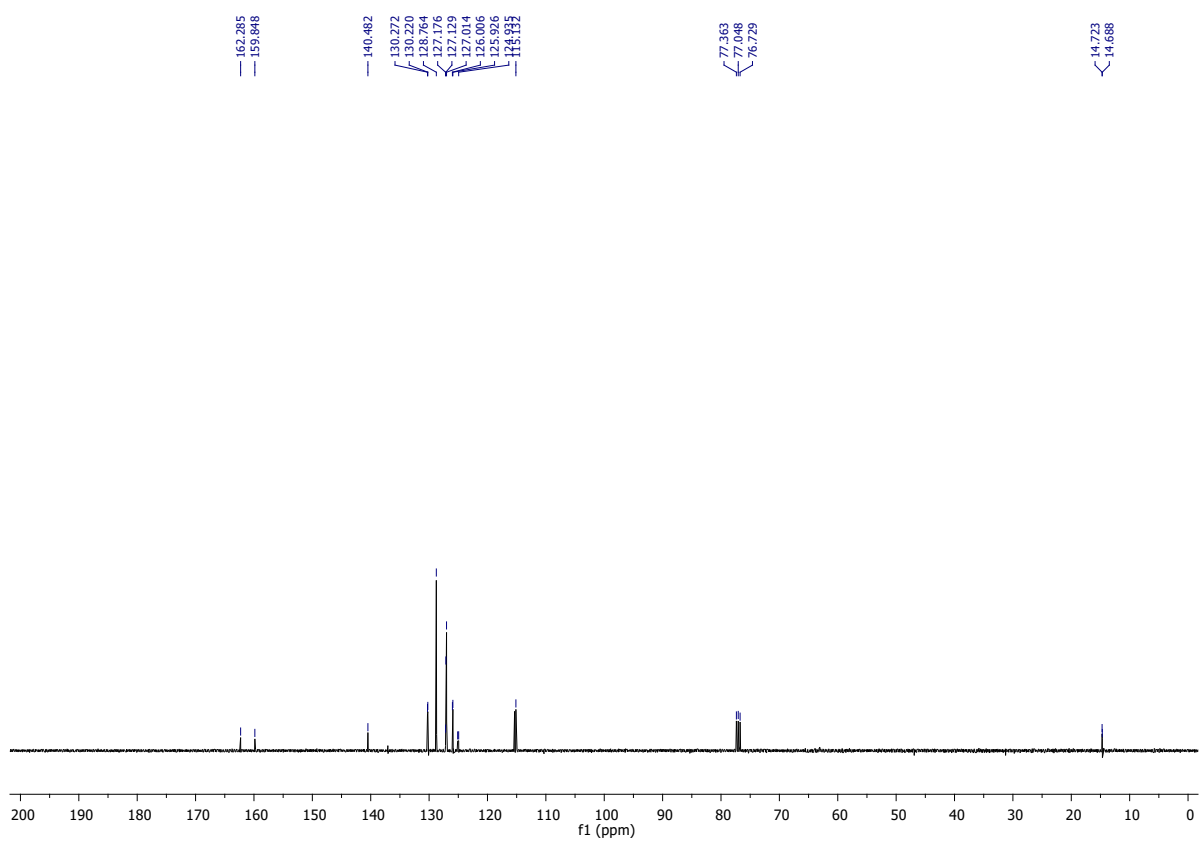
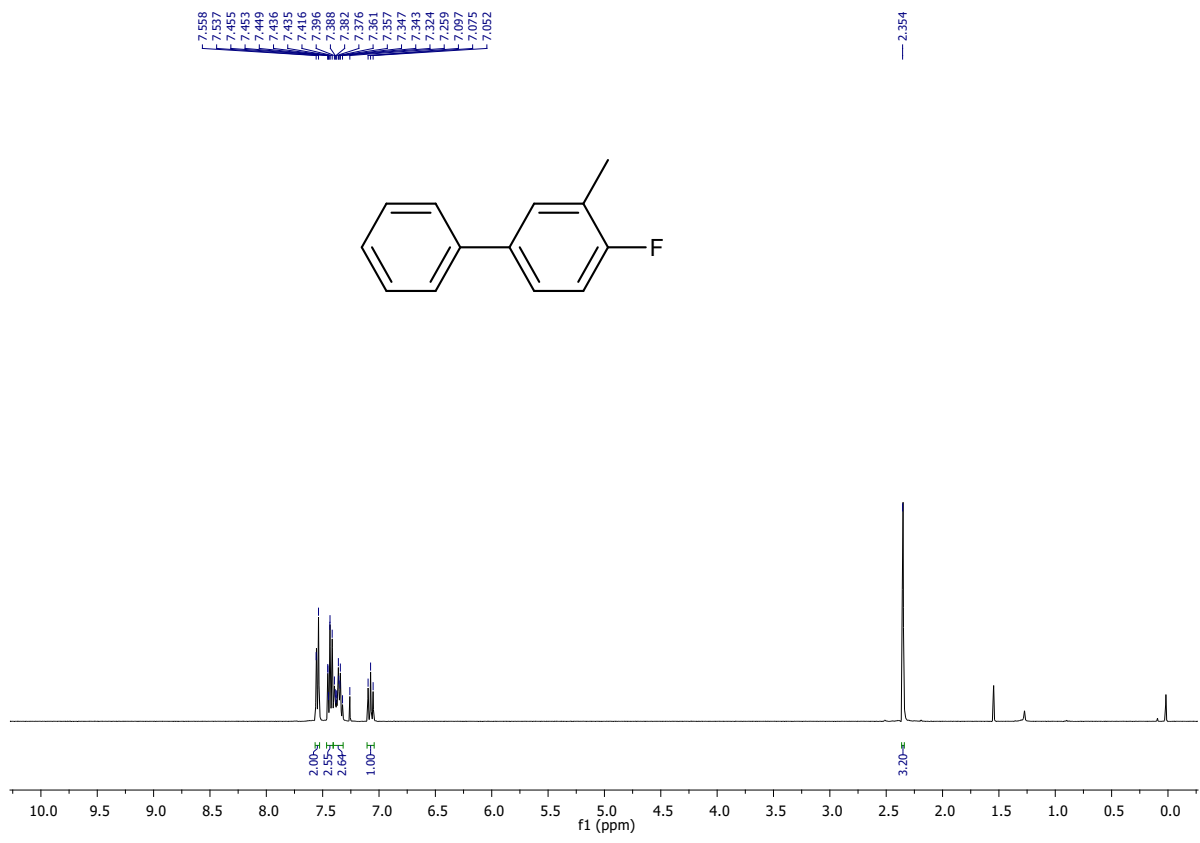


Figure S40. ¹H and ¹³C NMR spectra of 2,4-Methylbiphenyl (CDCl₃).



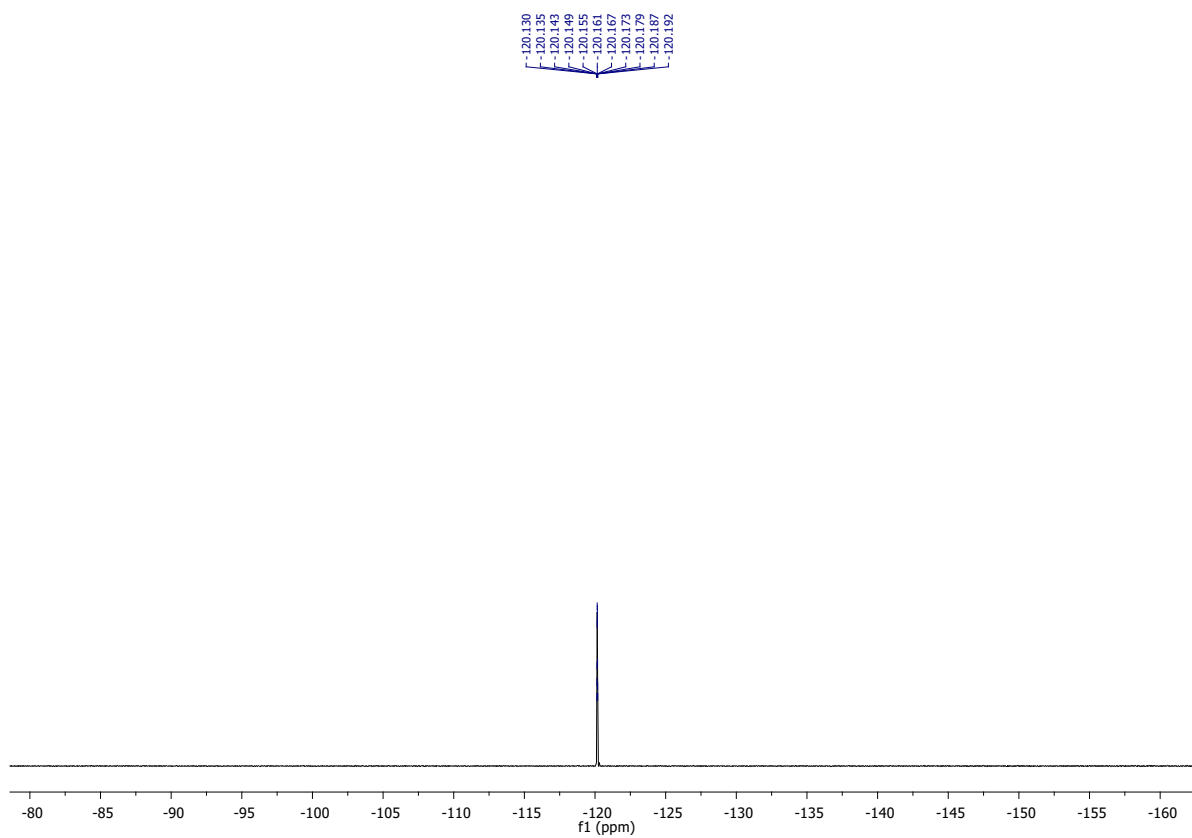
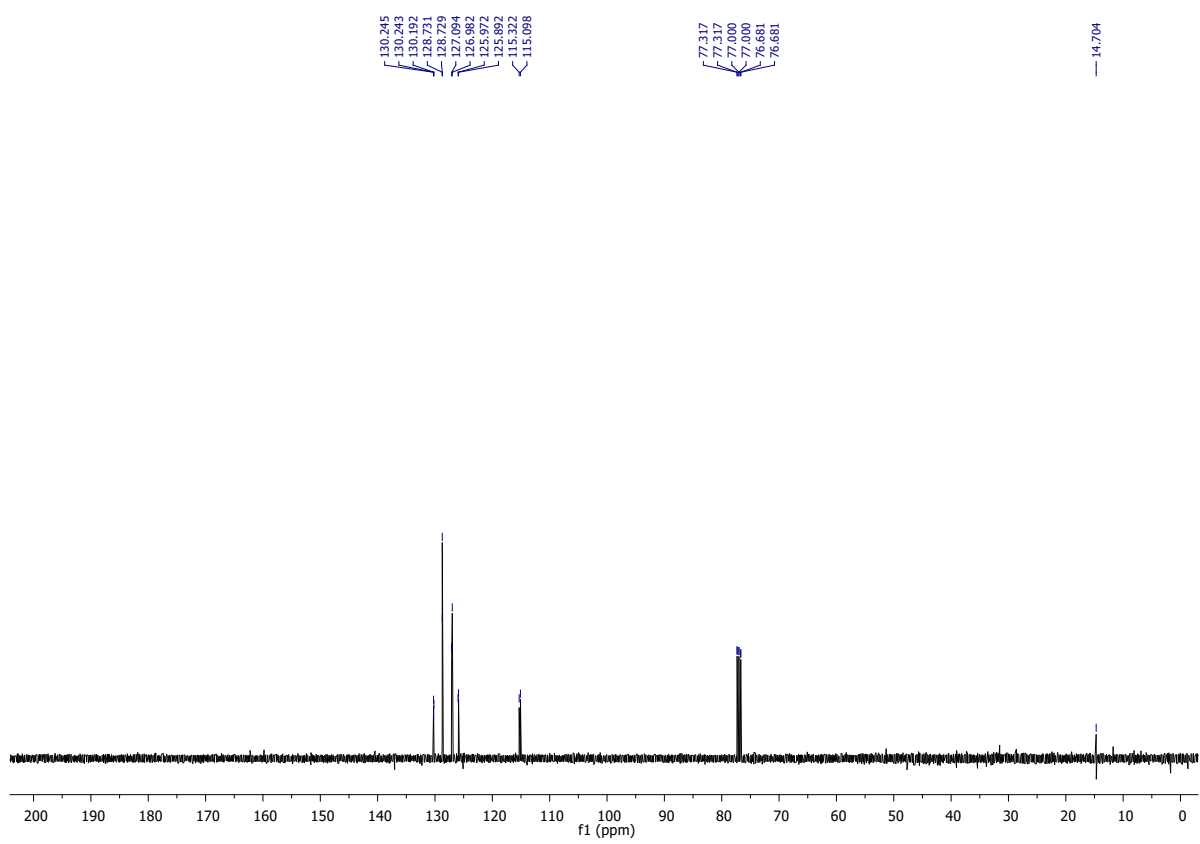
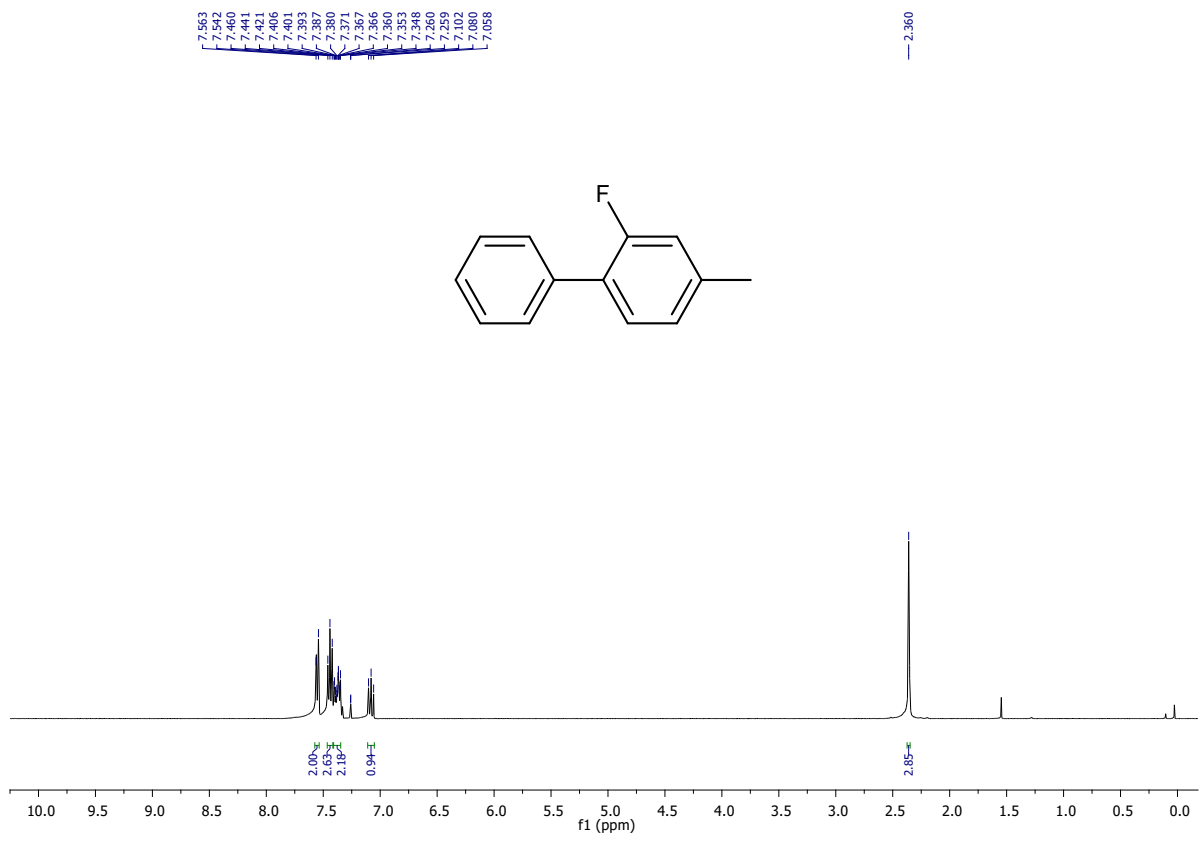


Figure S41. ^1H , ^{13}C and ^{19}F NMR spectrums of 4-Fluoro-3-methylbiphenyl (CDCl_3).



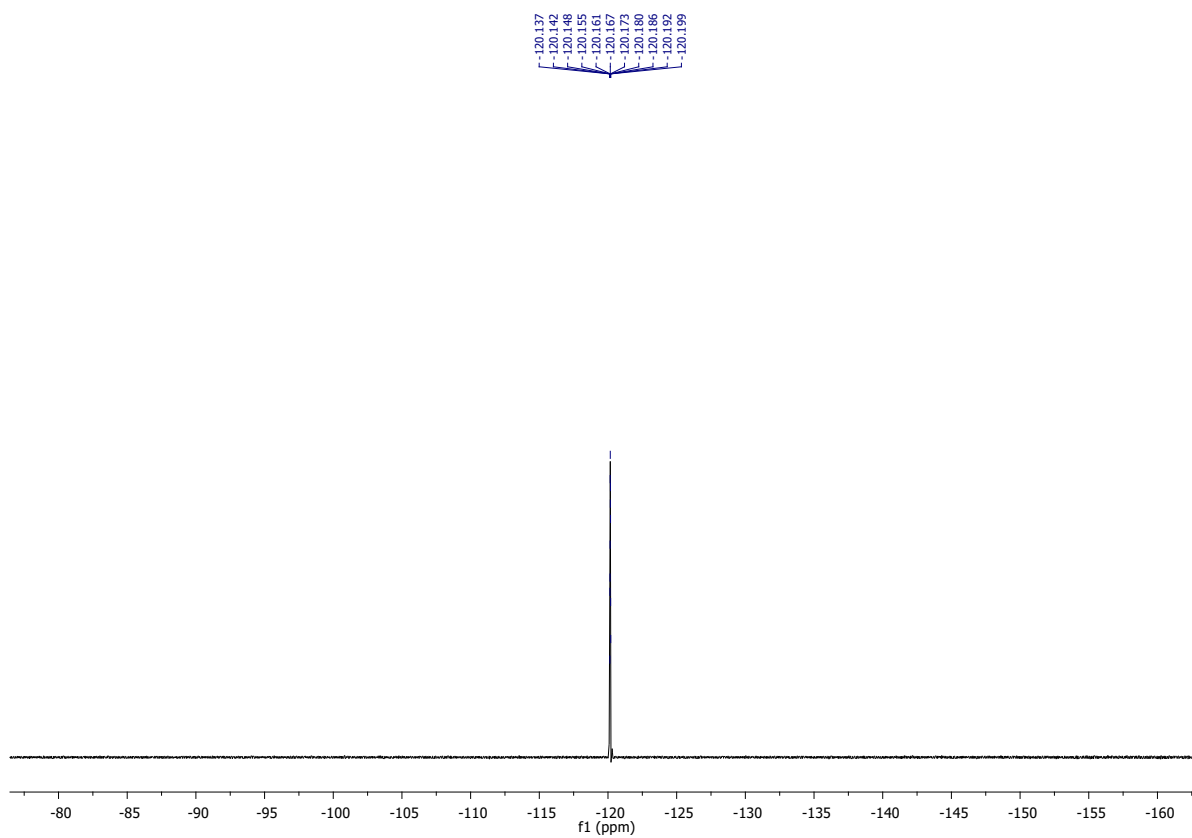


Figure S42. ^1H , ^{13}C and ^{19}F NMR spectrums of 2-Fluoro-4-methylbiphenyl (CDCl_3).

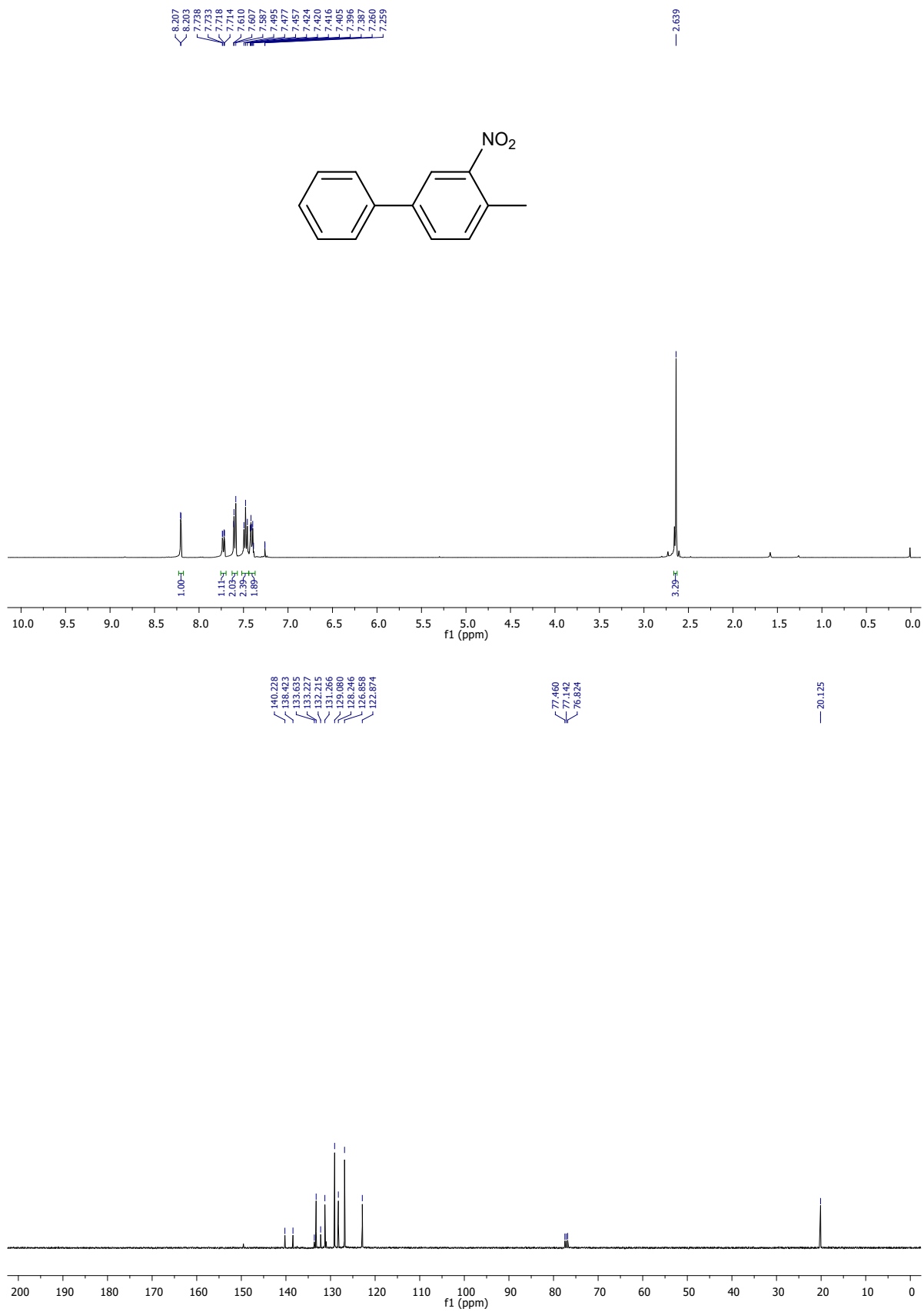


Figure S43. ¹H and ¹³C NMR spectra of 4-Methyl-3-nitrophenyl (CDCl₃).

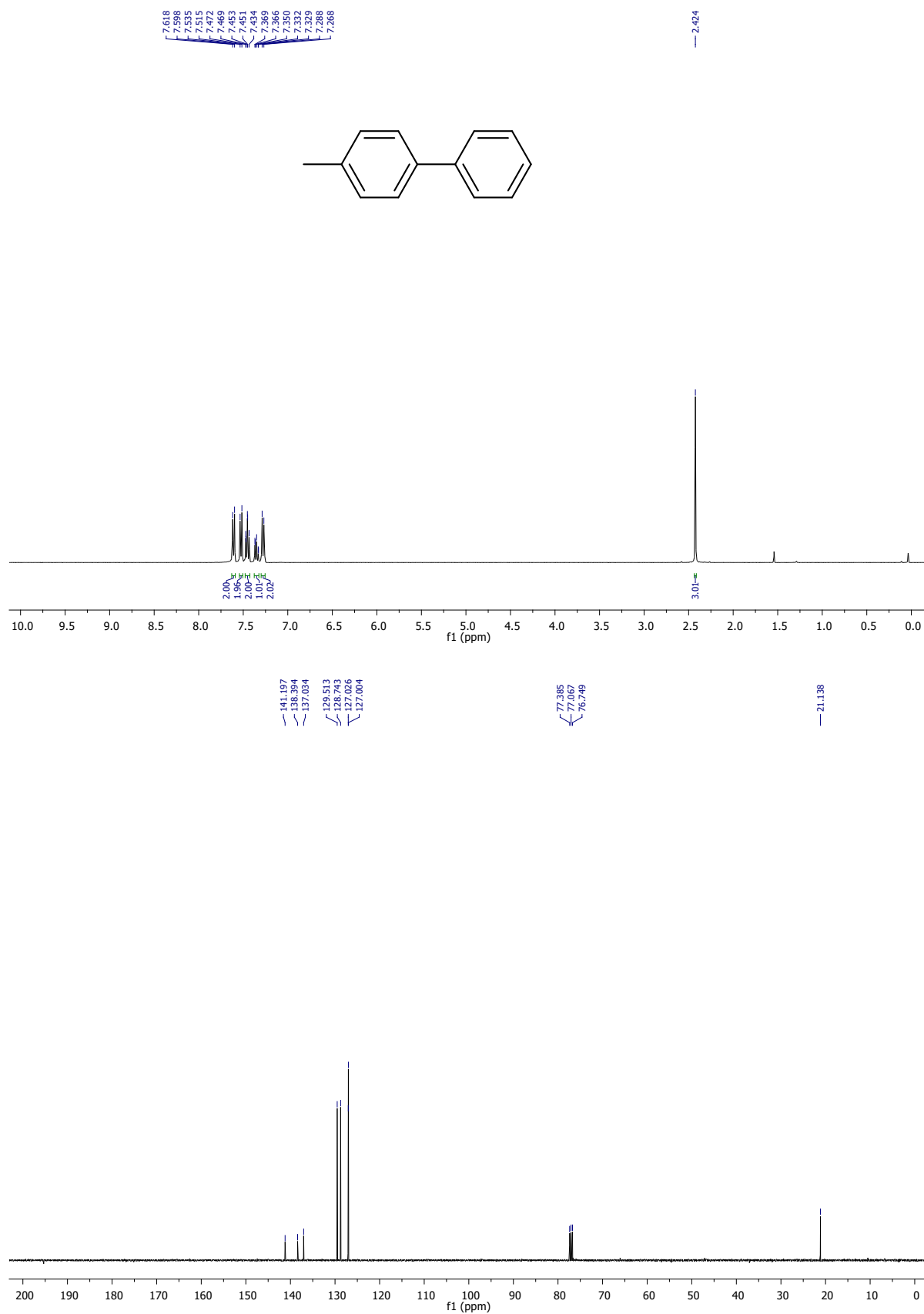


Figure S44. ¹H and ¹³C NMR spectra of 4'-Methylbiphenyl (CDCl₃).

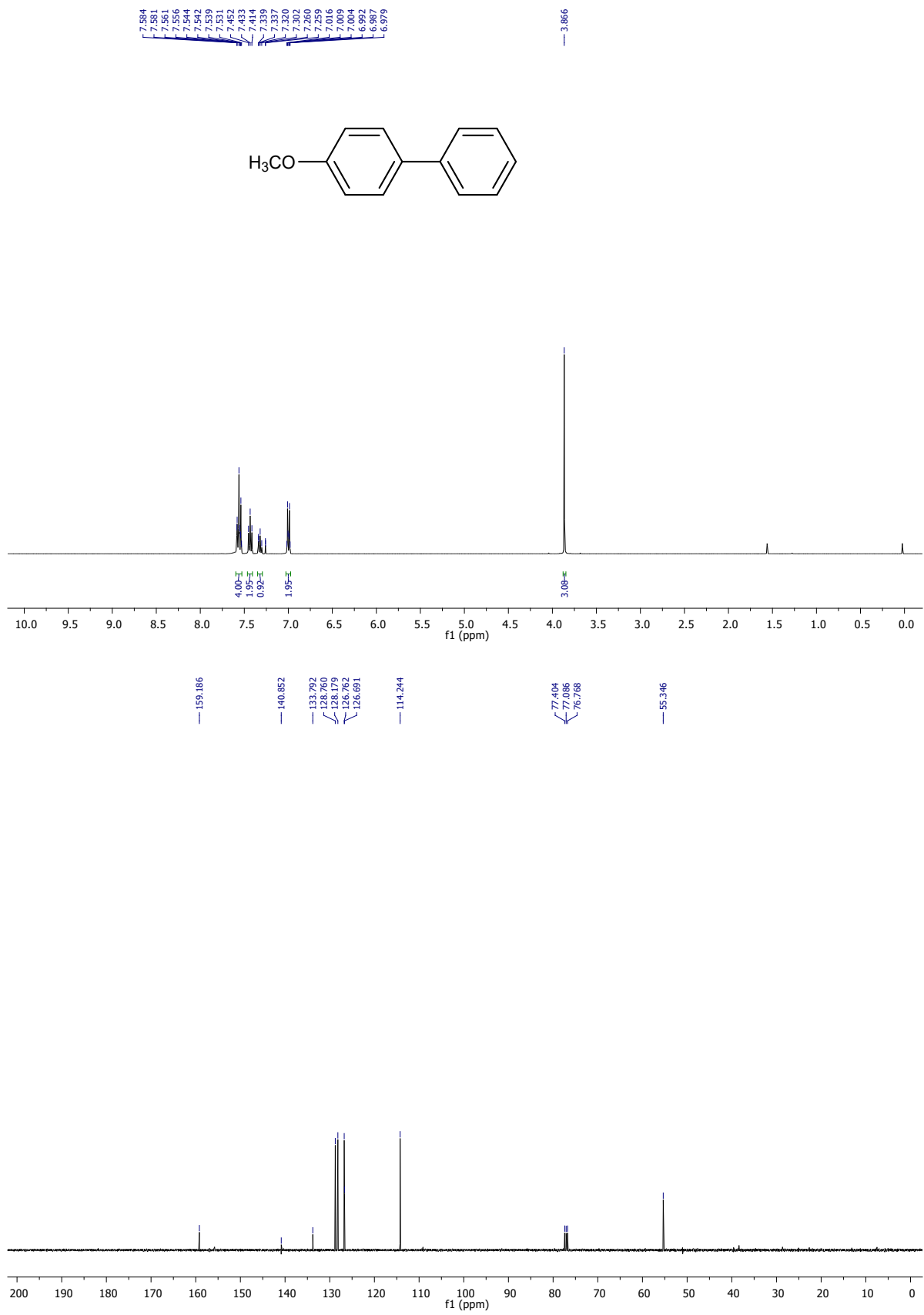


Figure S45. ¹H and ¹³C NMR spectra of 4'-Methoxybiphenyl (CDCl₃).

FTIR Spectrums

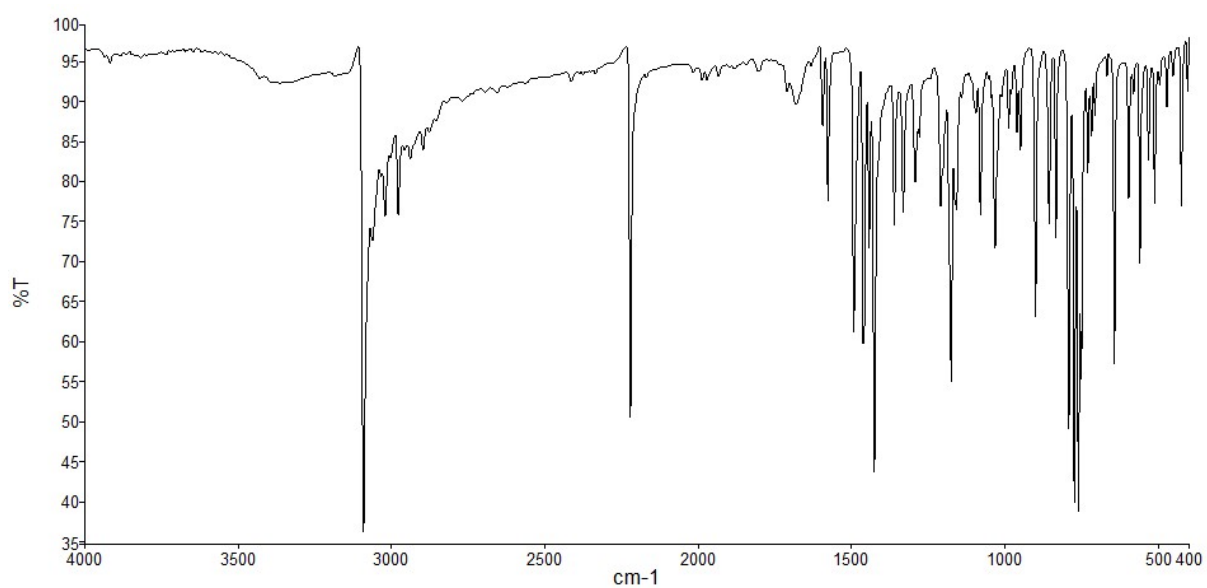


Figure S46. IR spectrum of **1a**.

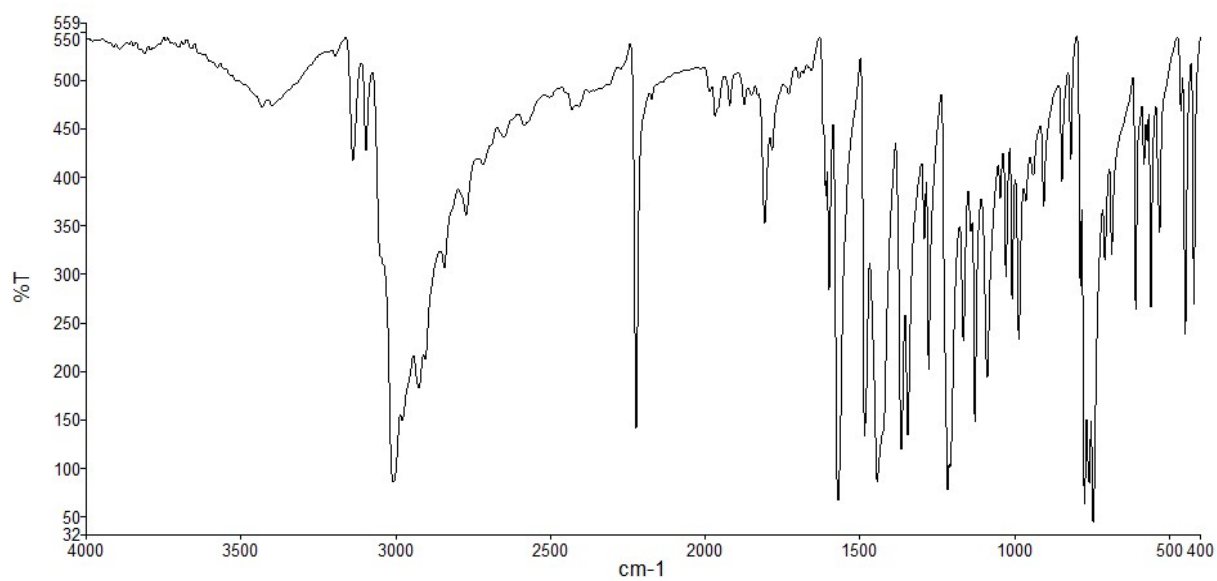


Figure S47. IR spectrum of **1b**.

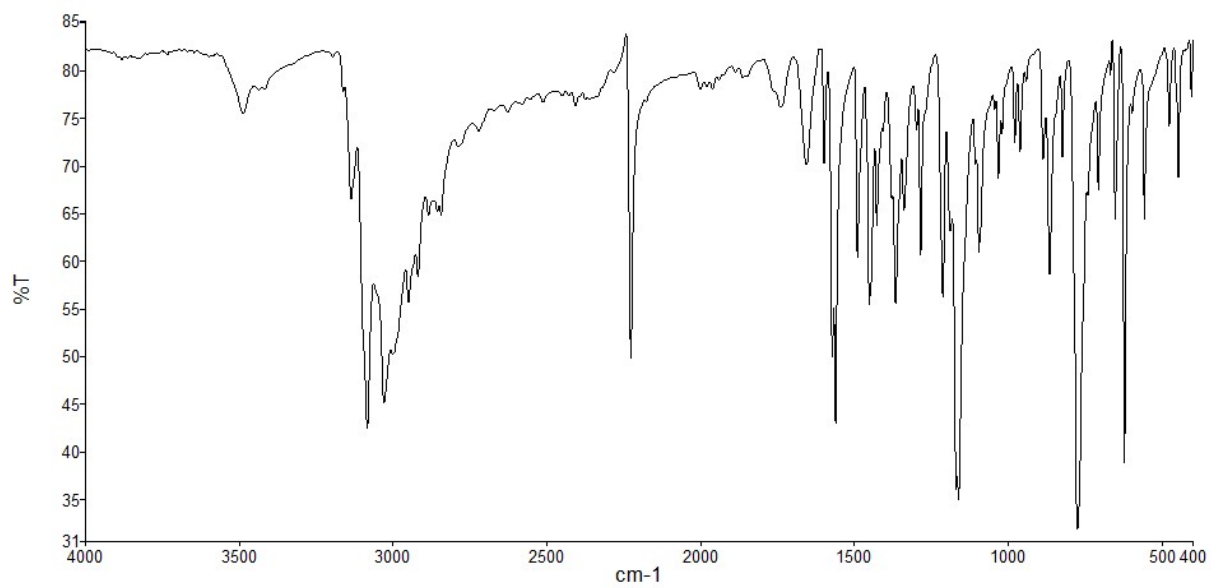


Figure S48. IR spectrum of **1c**.

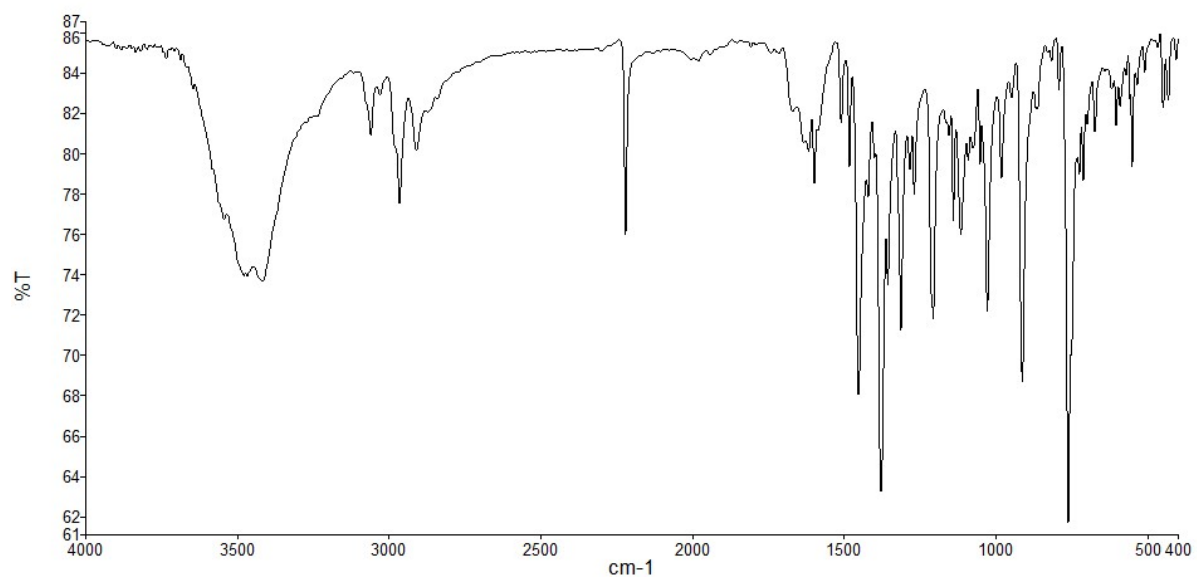


Figure S49. IR spectrum of **1d**.

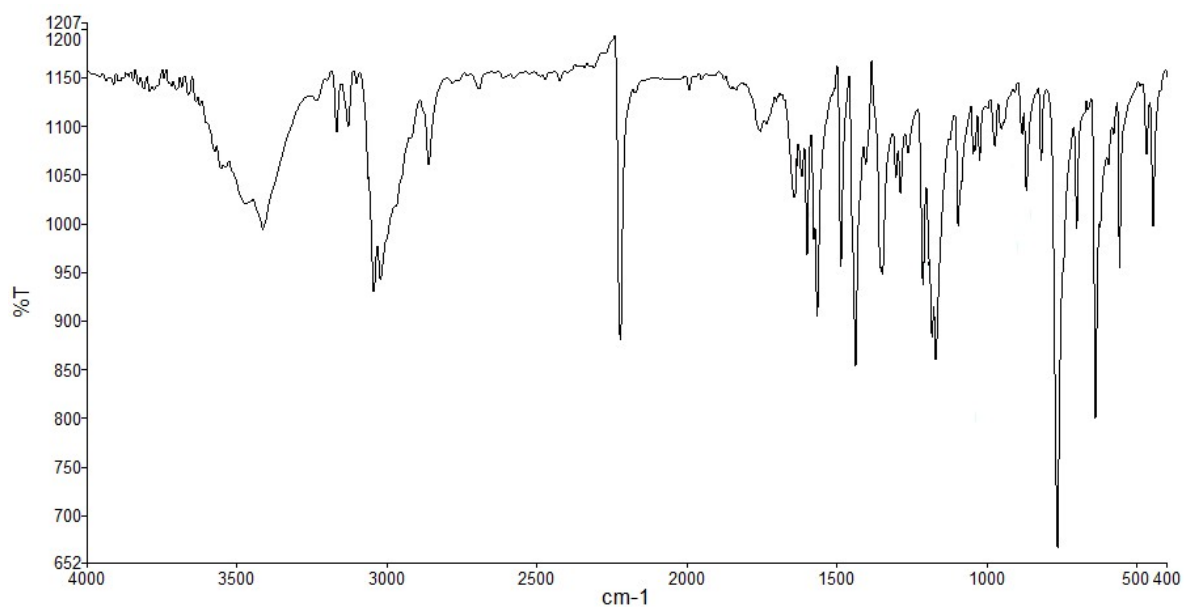


Figure S50. IR spectrum of **1e**.

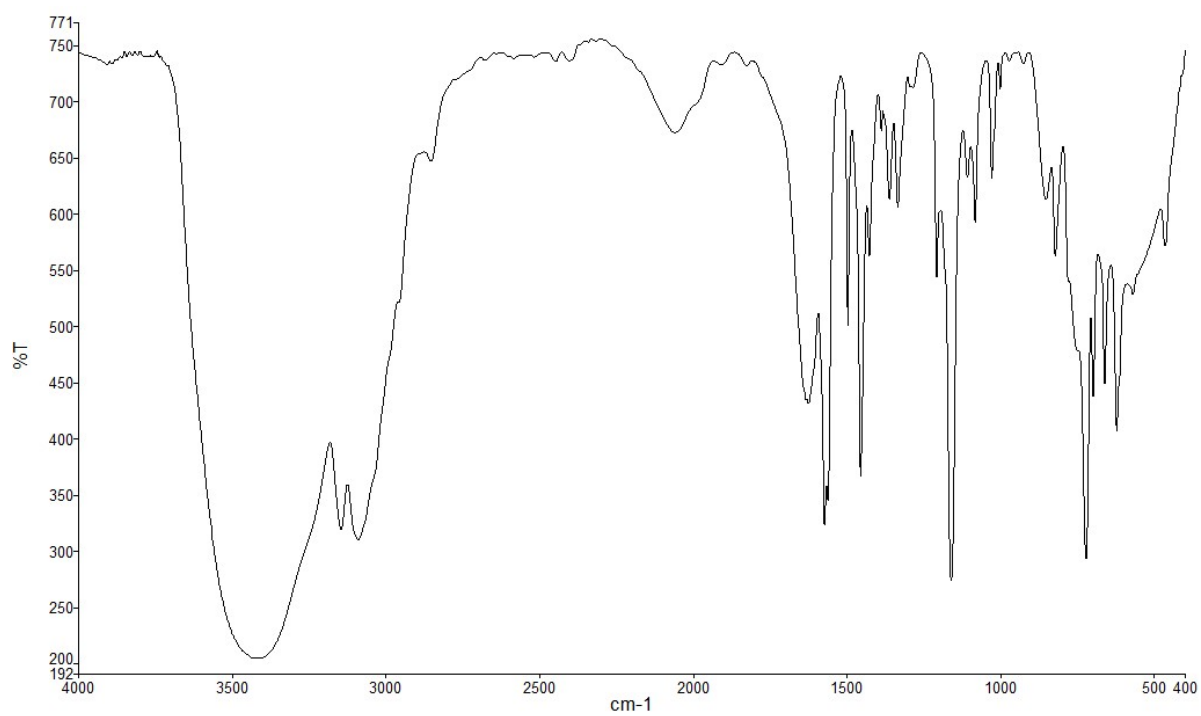


Figure S51. IR spectrum of **1f**.

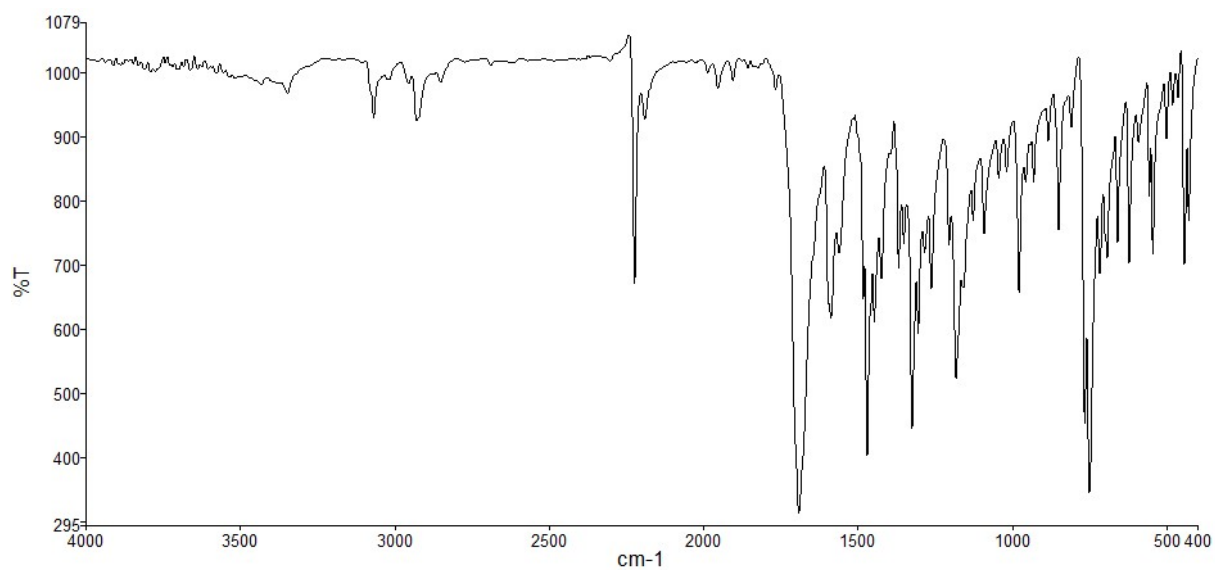


Figure S52. IR spectrum of **2a**.

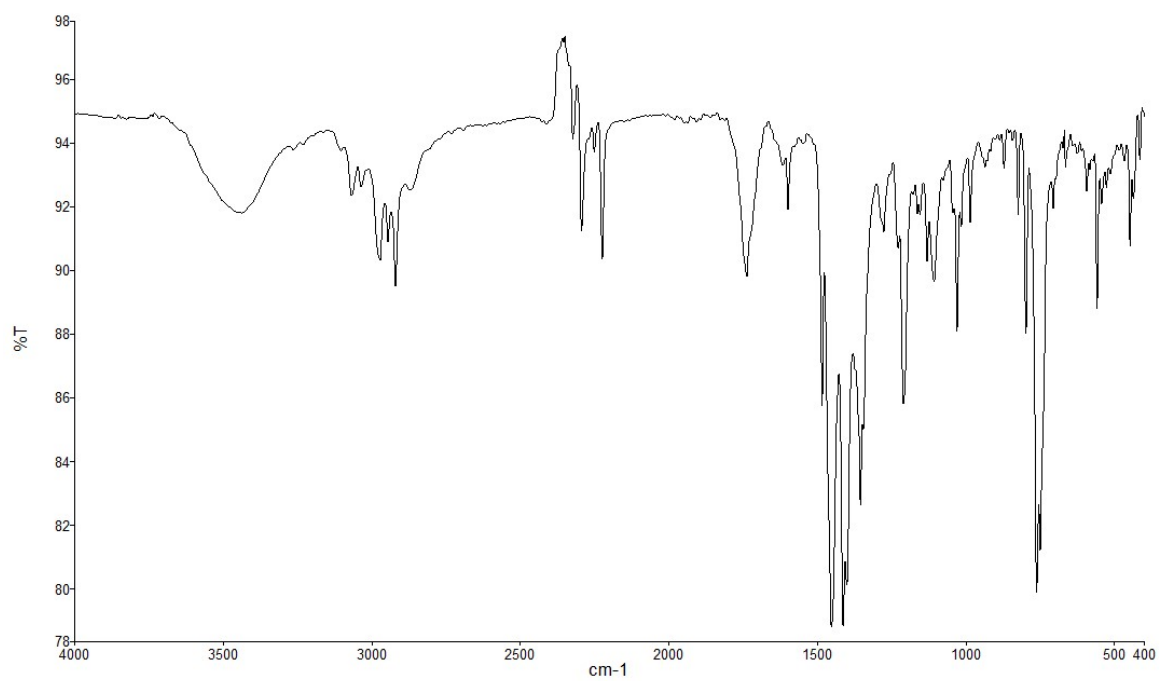


Figure S53. IR spectrum of **2b**.

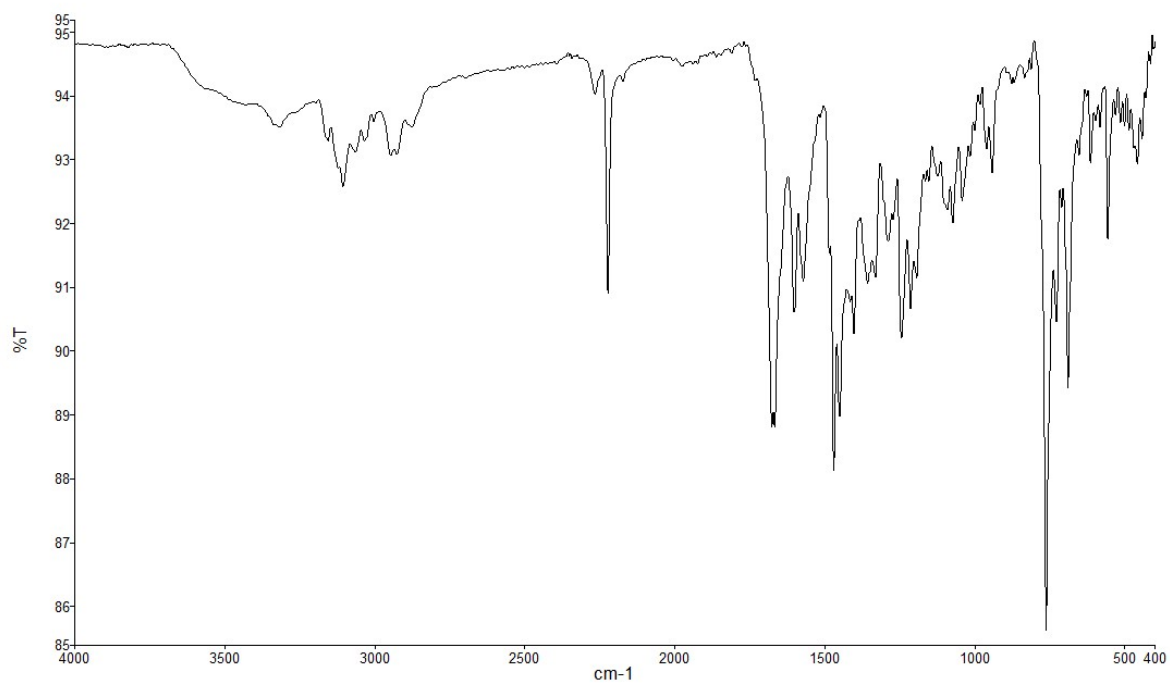


Figure S54. IR spectrum of **2c**.

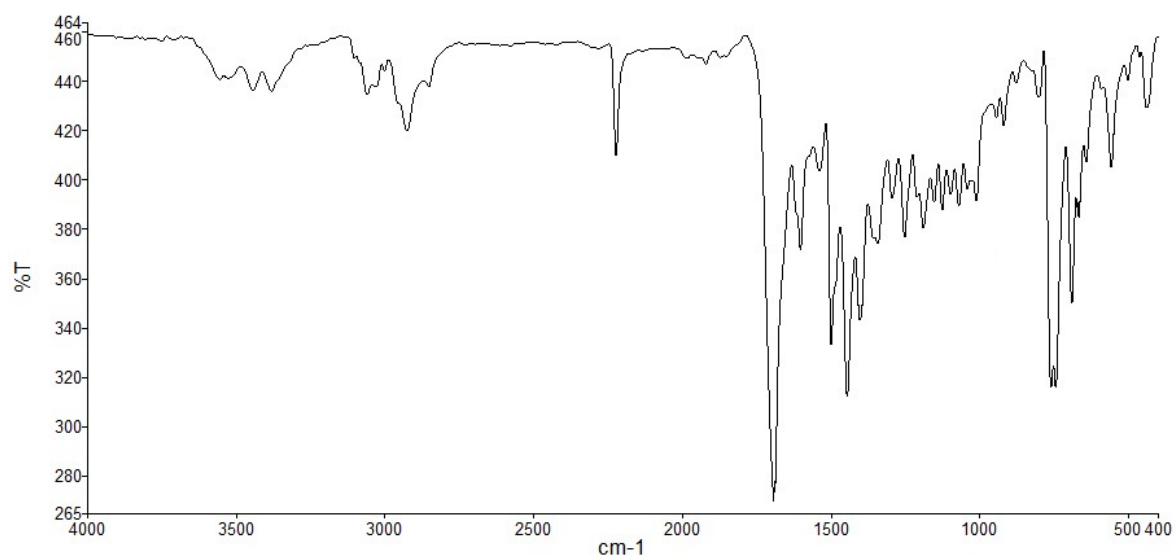


Figure S55. IR spectrum of **3b**.

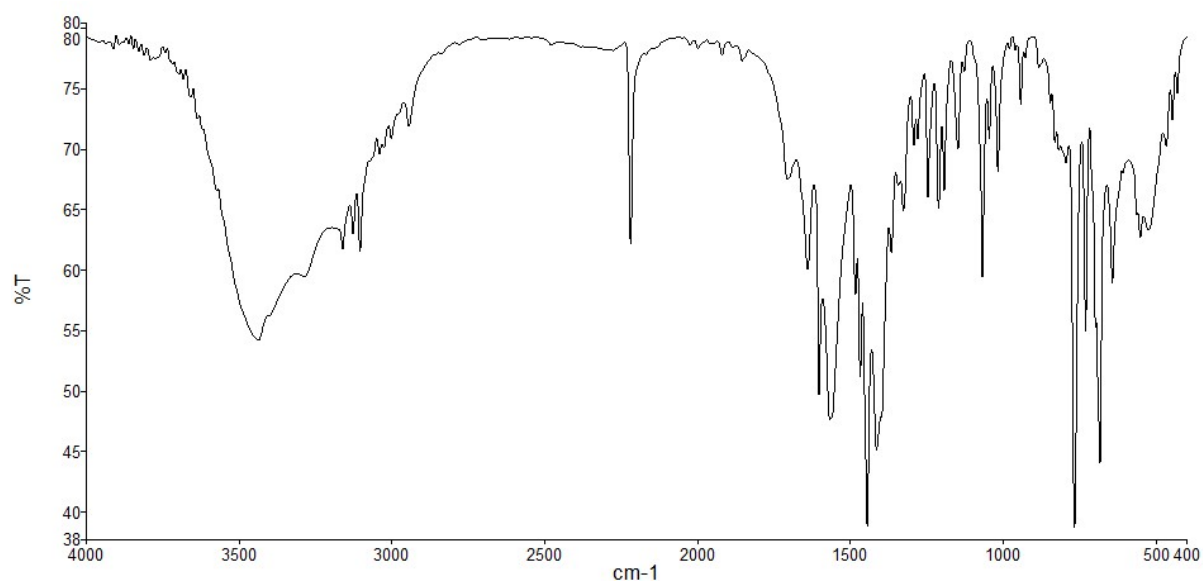


Figure S56. IR spectrum of **3c**.

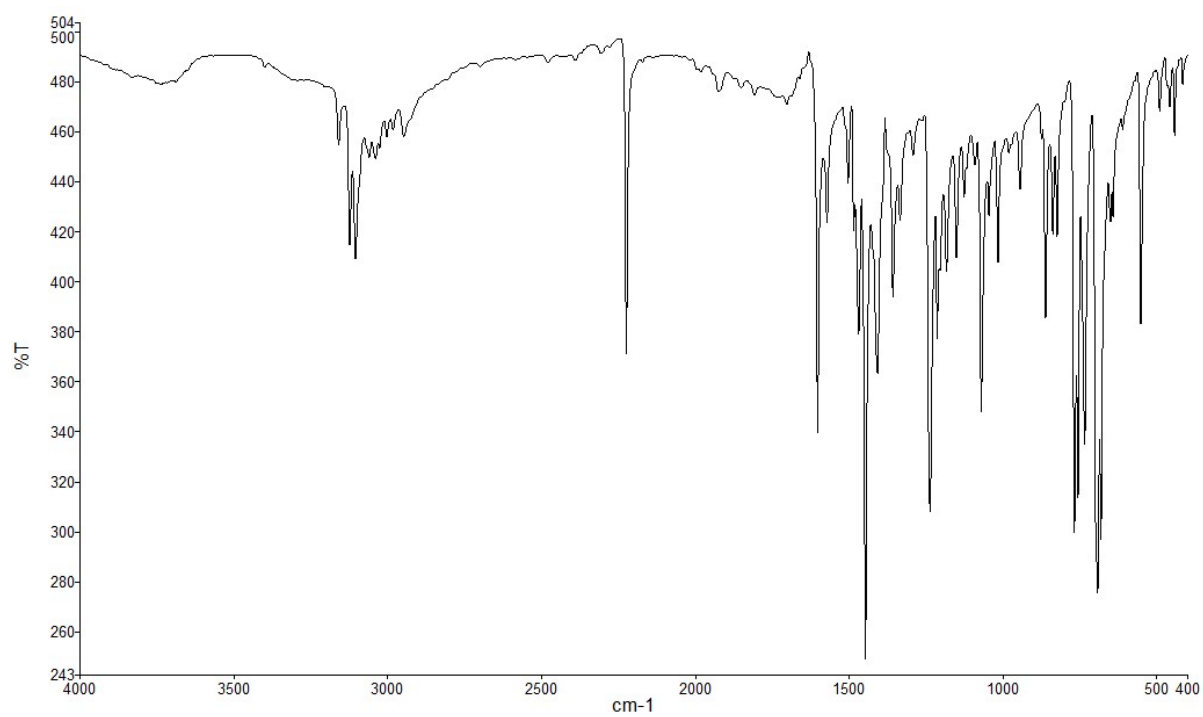


Figure S57. IR spectrum of **3d**.

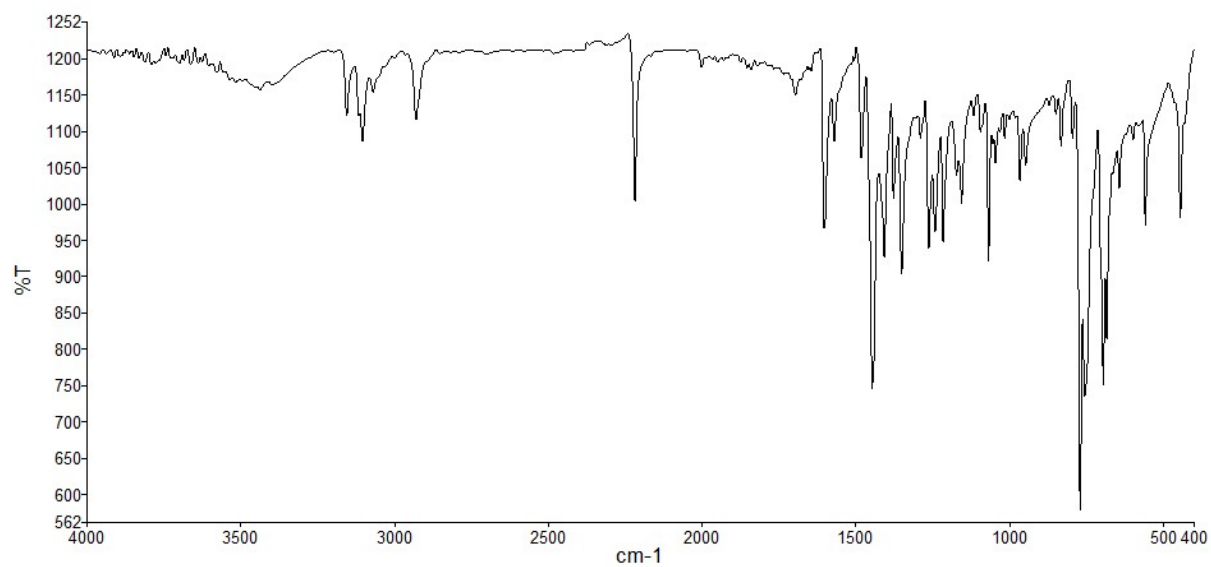


Figure S58. IR spectrum of **3e**.

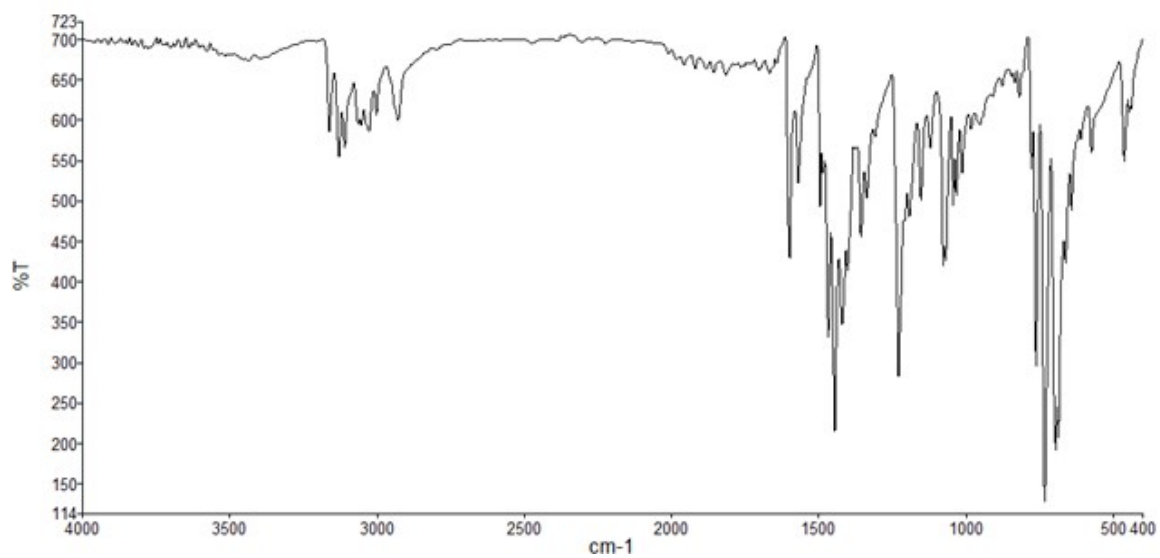


Figure S59. IR spectrum of **3f**.

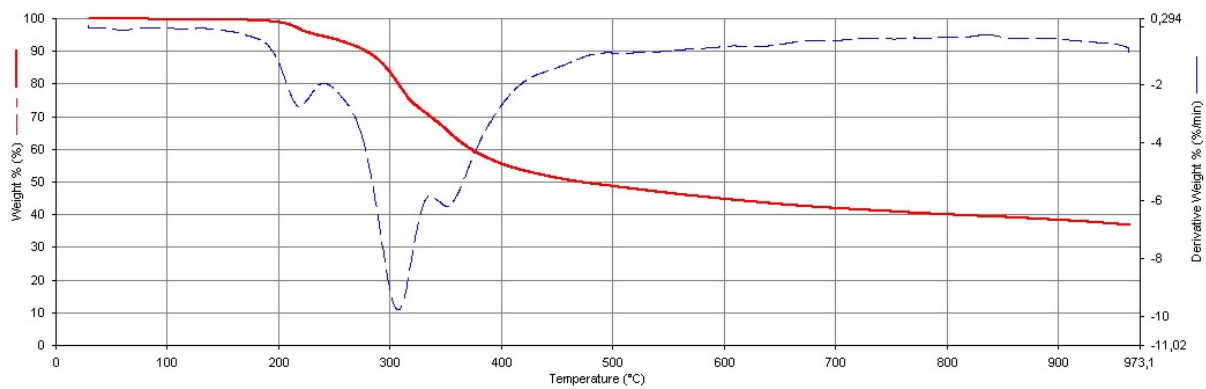


Figure S60. TGA spectrum of **3c**.

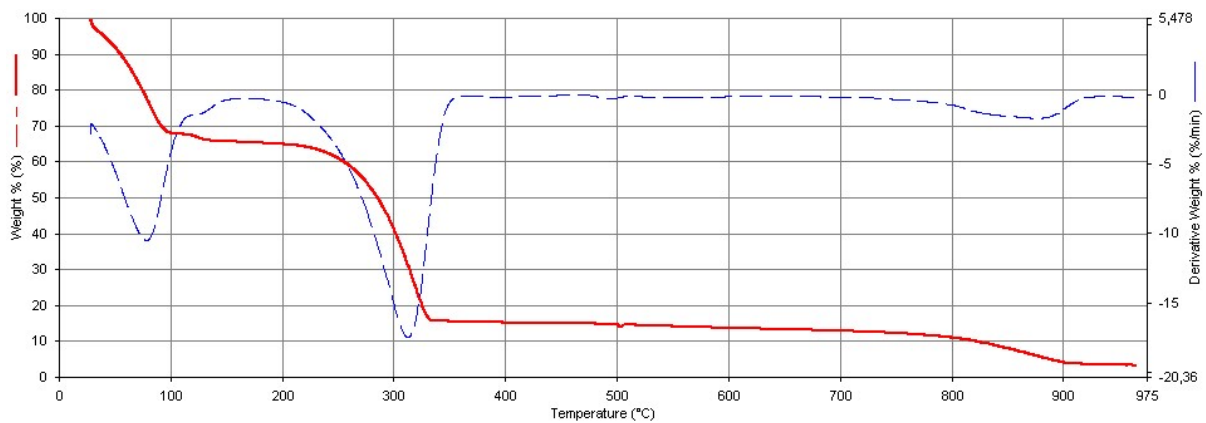


Figure S61. TGA spectrum of Pd nanoparticles of **3c**.



Figure S62. FT-IR spectrum of Pd nanoparticles of **3c**.

Table S1. Crystal data and structure refinement parameters for **3c**, **3e** and **3f**

Complex	3c	3e	3f
Formula	C ₁₇ H ₁₆ Br ₂ N ₄ Pd	C ₂₄ H ₁₉ Br ₂ N ₅ Pd	C ₁₆ H ₁₇ Br ₂ N ₃ Pd
Formula weight	542.56	643.66	517.54
Crystal shape/colour	Prism/orange	Prism/orange	Prism/orange
Crystal size (mm)	0.39×0.29×0.13	0.24×0.18×0.14	0.34×0.28×0.16
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	<i>P</i> -1	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
a (Å)	7.4786(9)	18.6682(12)	10.0563(5)
b (Å)	11.0996(11)	15.9603(13)	14.1910(9)
c (Å)	11.7959(16)	8.1346(5)	14.2442(9)
α (°)	90.731(10)	90	72.709(5)
β (°)	100.478(10)	94.651(6)	72.523(5)
γ (°)	106.482(10)	90	72.840(5)
V (Å ³)	921.1(2)	2415.7(3)	1803.4(2)
Z	2	4	4
Z'	1	0.5	2
D _x (g cm ⁻³)	1.956	1.770	1.906
μ (mm ⁻¹)	5.35	4.097	5.459
T _{min} , T _{max}	0.305, 0.574	0.541, 0.634	0.537, 0.731
F(000)	524	1256	1000
θ (°)	2.89-25.65	3.52-23.57	3.14-25.02
R _{int}	-	0.0298	0.0422
Data/restrain/parameter	3823/3/ 219	2274/0/147	6760/42/409
Goodness of fit (<i>F</i> ²)	1.065	1.012	1.002
R ₁ , wR ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0637, 0.2259	0.0416, 0.0579	0.0488, 0.0639
R ₁ , wR ₂ (all data)	0.1117, 0.2556	0.0889, 0.0705	0.1052, 0.0793
Δρ _{min} / Δρ _{max} (e/Å ³)	-1.799, 1.474	-0.549, 0.349	-0.881, 0.917