Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

C-C Coupling with Nitron NHC Complexes

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Contents

^{1}H-NMR spectra of Nitron

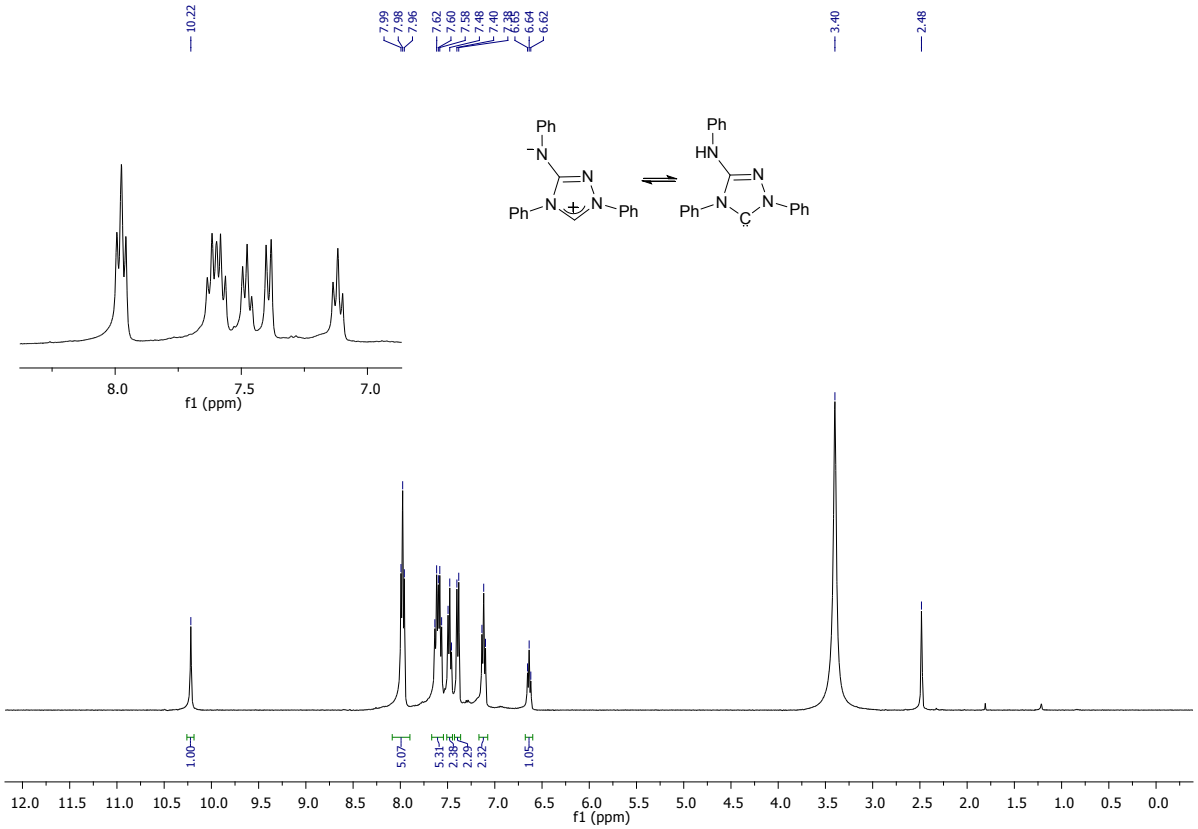


Figure S1. ^{1}H NMR spectrum of Nitron ($CDCl_3$).

^{1}H- and ^{13}C- NMR spectras of the complexes **1**-**9**

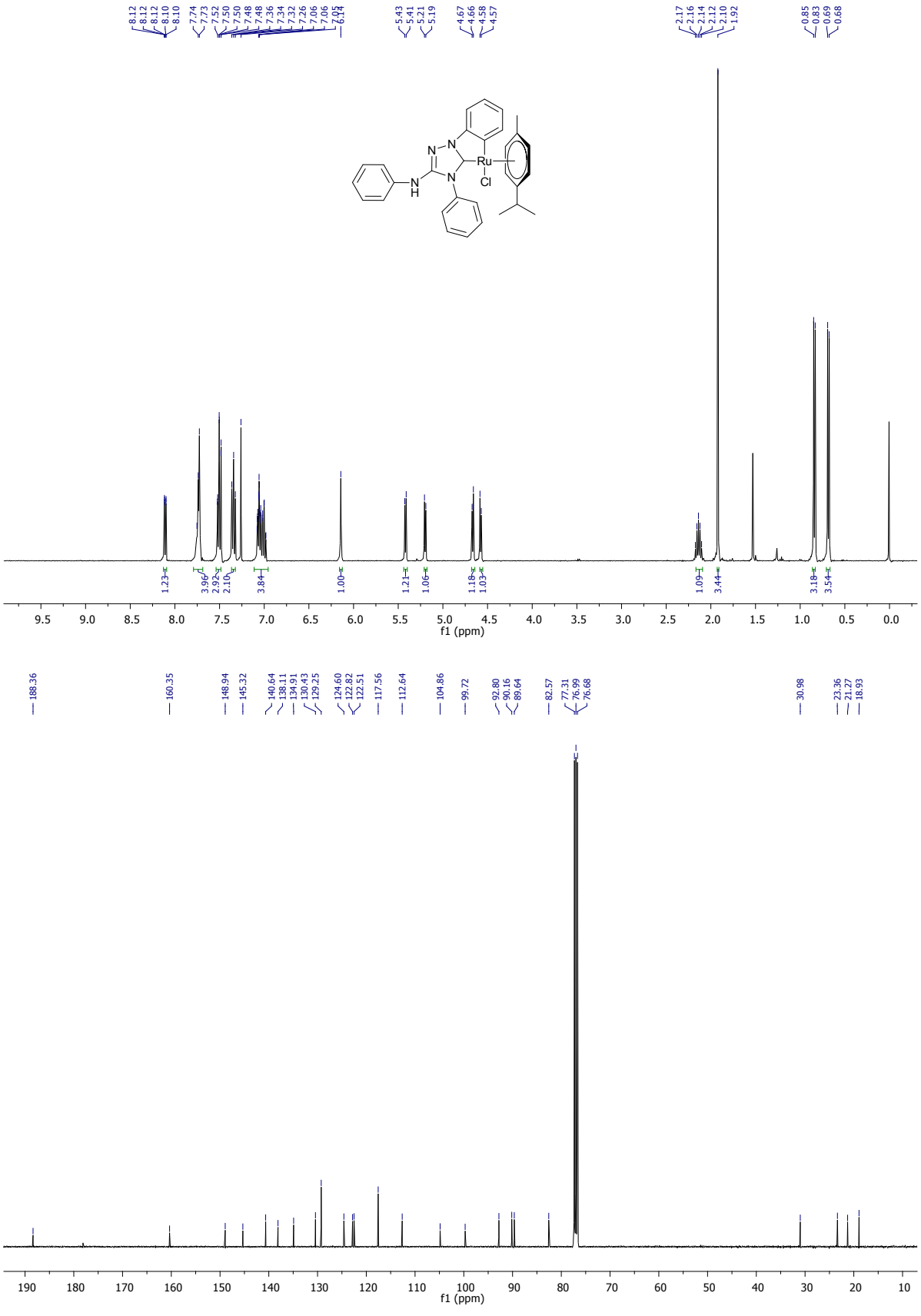


Figure S2. ^{1}H and ^{13}C NMR spectrums of complex **1** ($CDCl_3$).

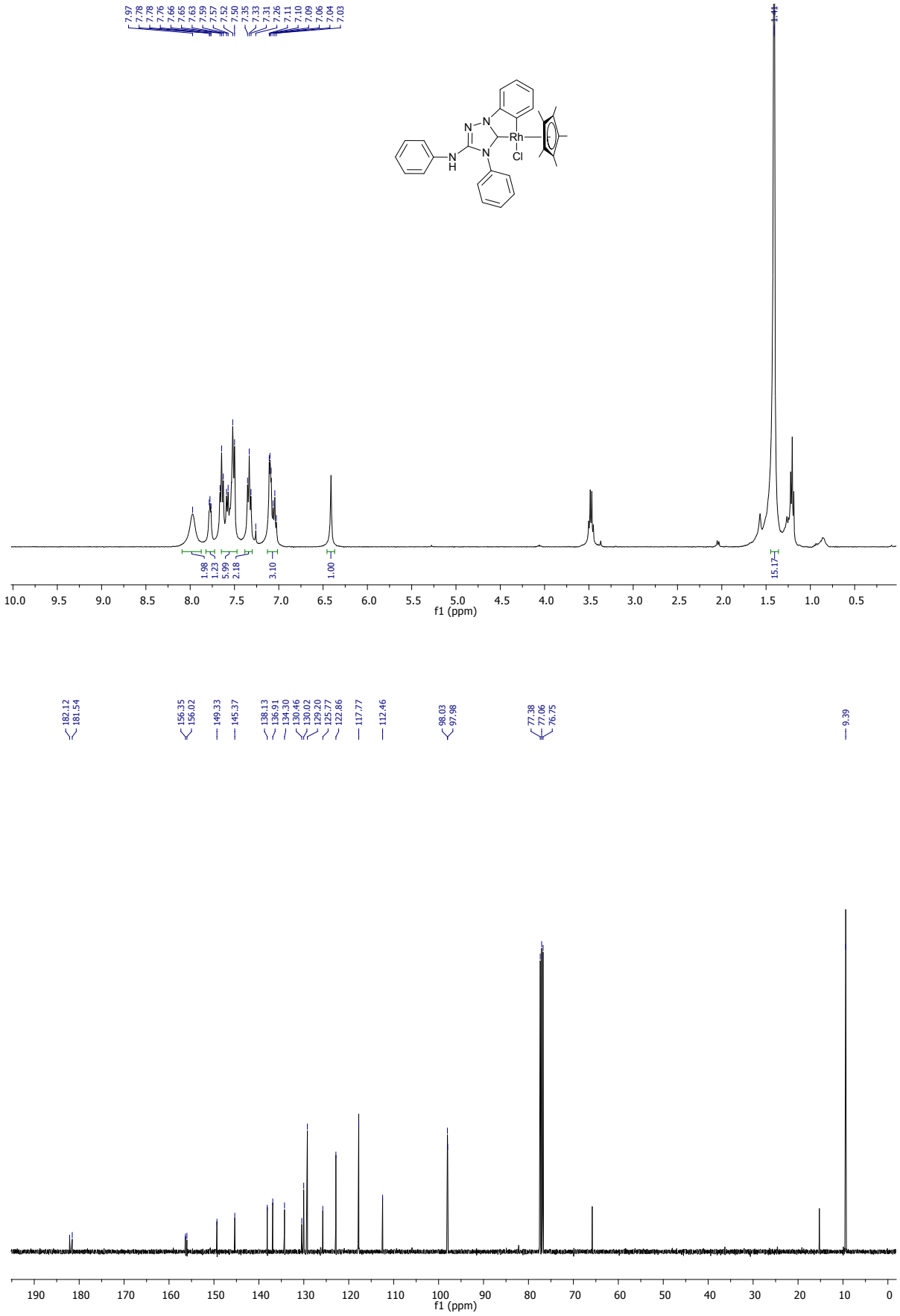


Figure S3. ^{1}H and ^{13}C NMR spectrums of complex **2** ($CDCl_3$).

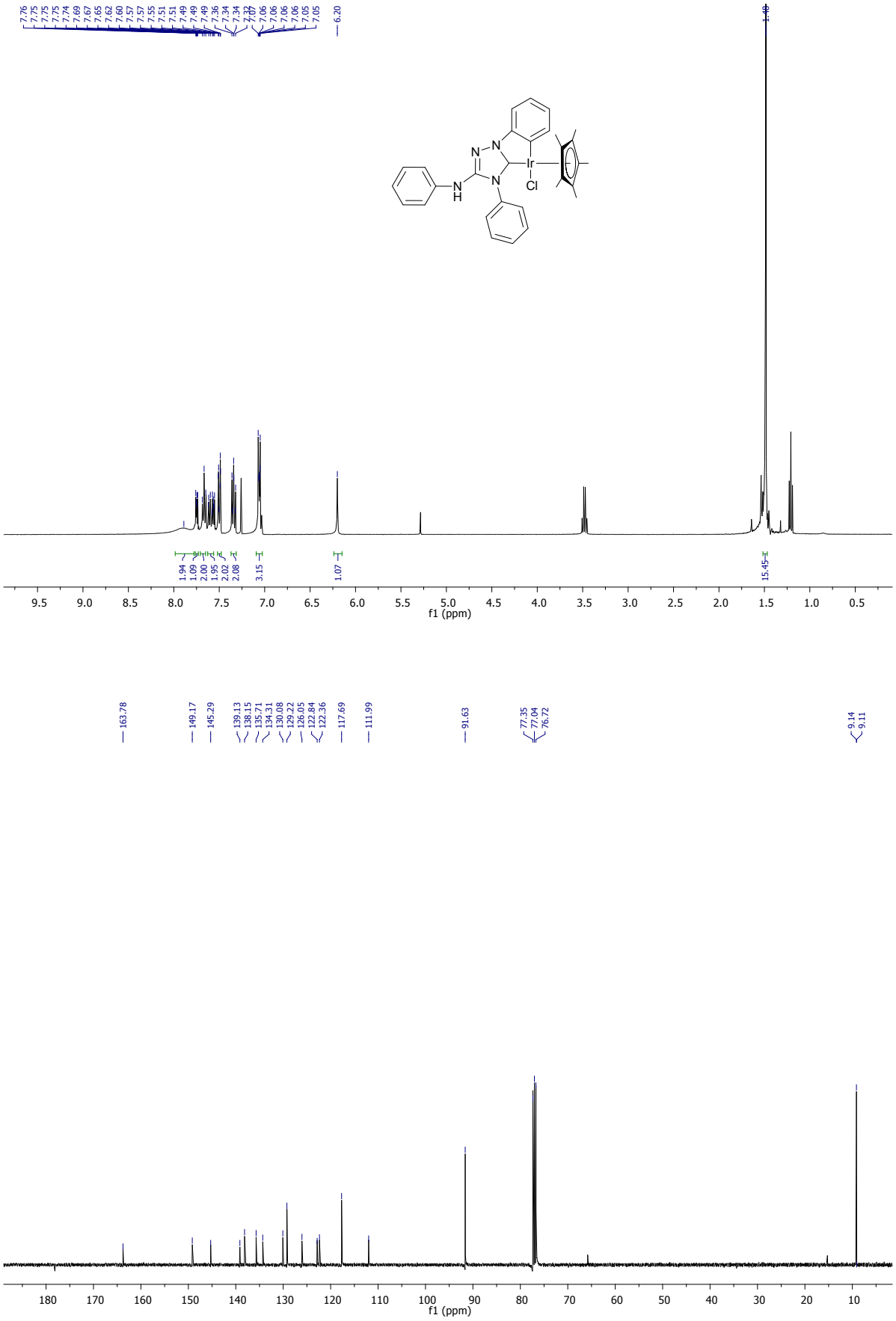


Figure S4. ^{1}H and ^{13}C NMR spectrums of complex **3** ($CDCl_3$).

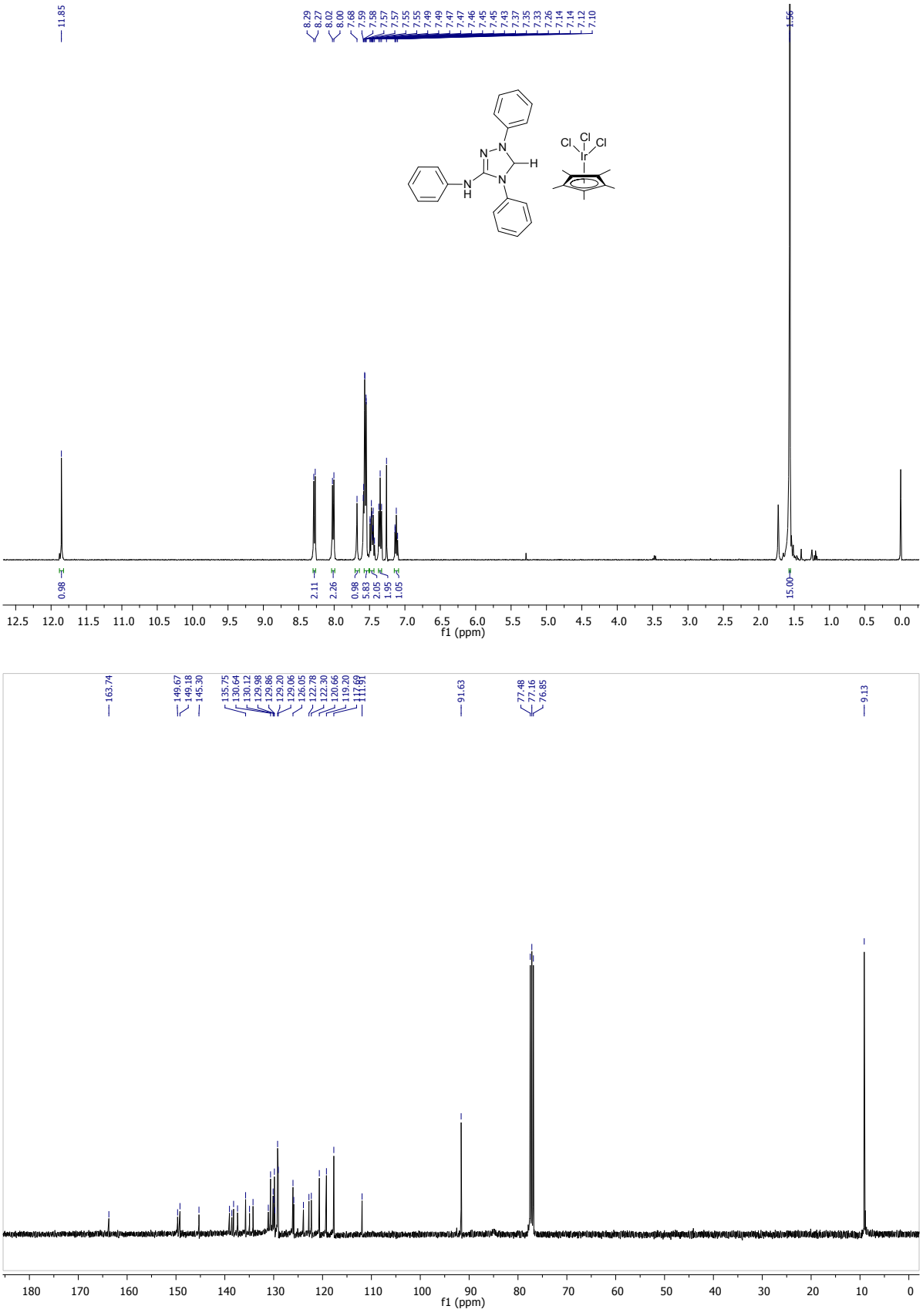


Figure S5. ^{1}H and ^{13}C NMR spectrums of complex **4** ($CDCl_3$)

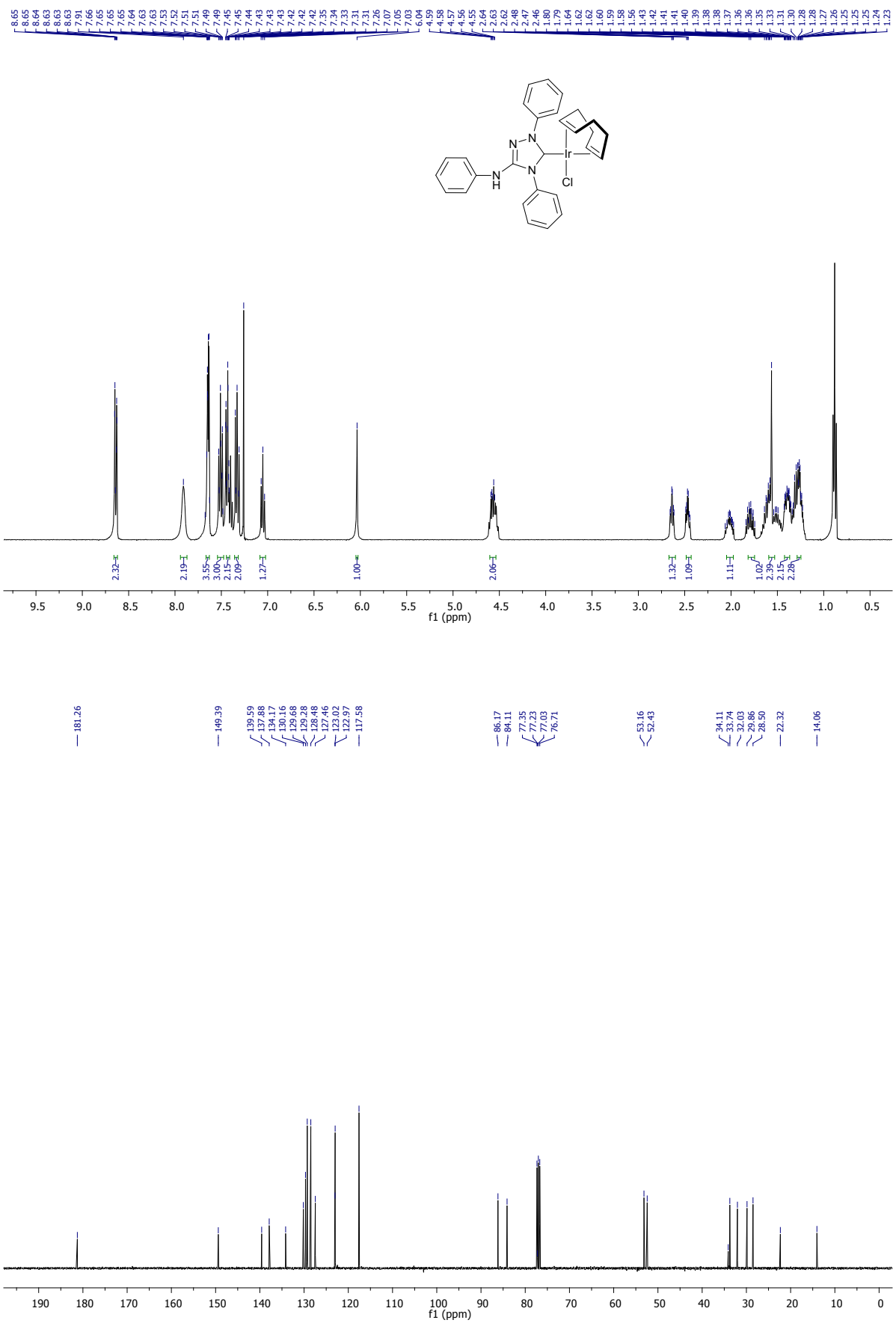


Figure S6. ^{1}H and ^{13}C NMR spectrums of complex **5** ($CDCl_3$).

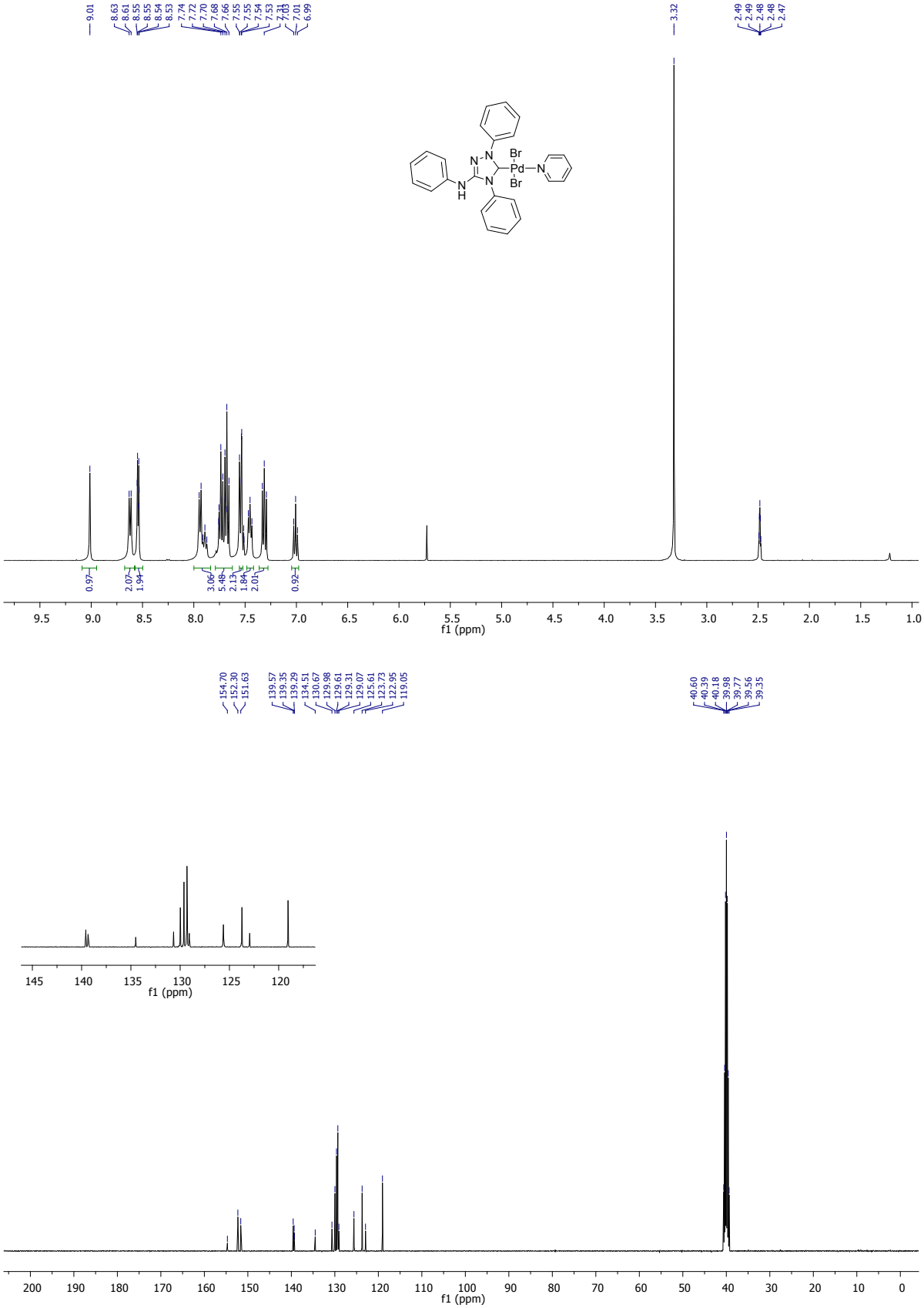


Figure S7. ^{1}H and ^{13}C NMR spectrums of complex **6** (DMSO-d_6).

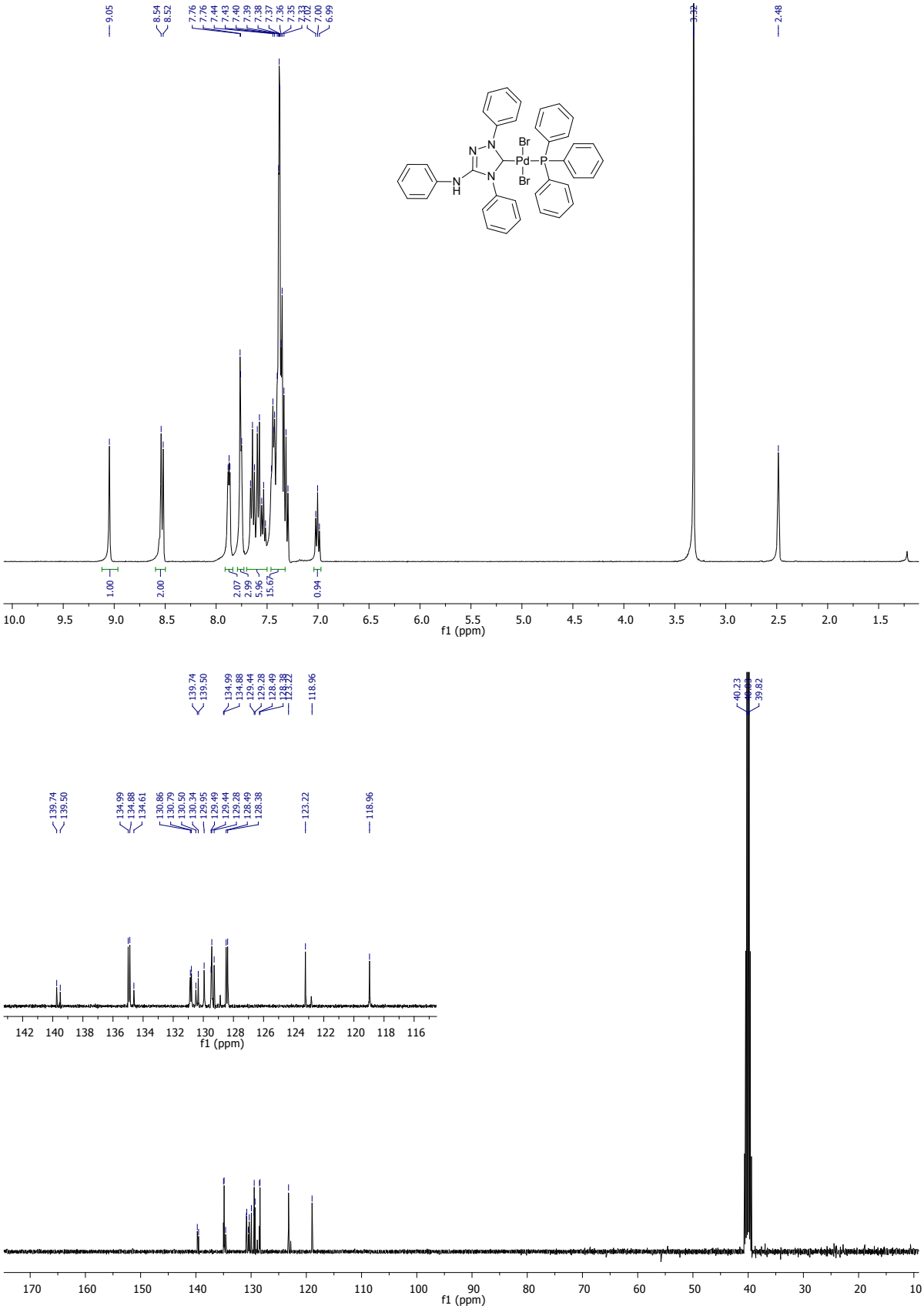


Figure S8. ^{1}H and ^{13}C NMR spectrums of complex **7** (DMSO-d_6).

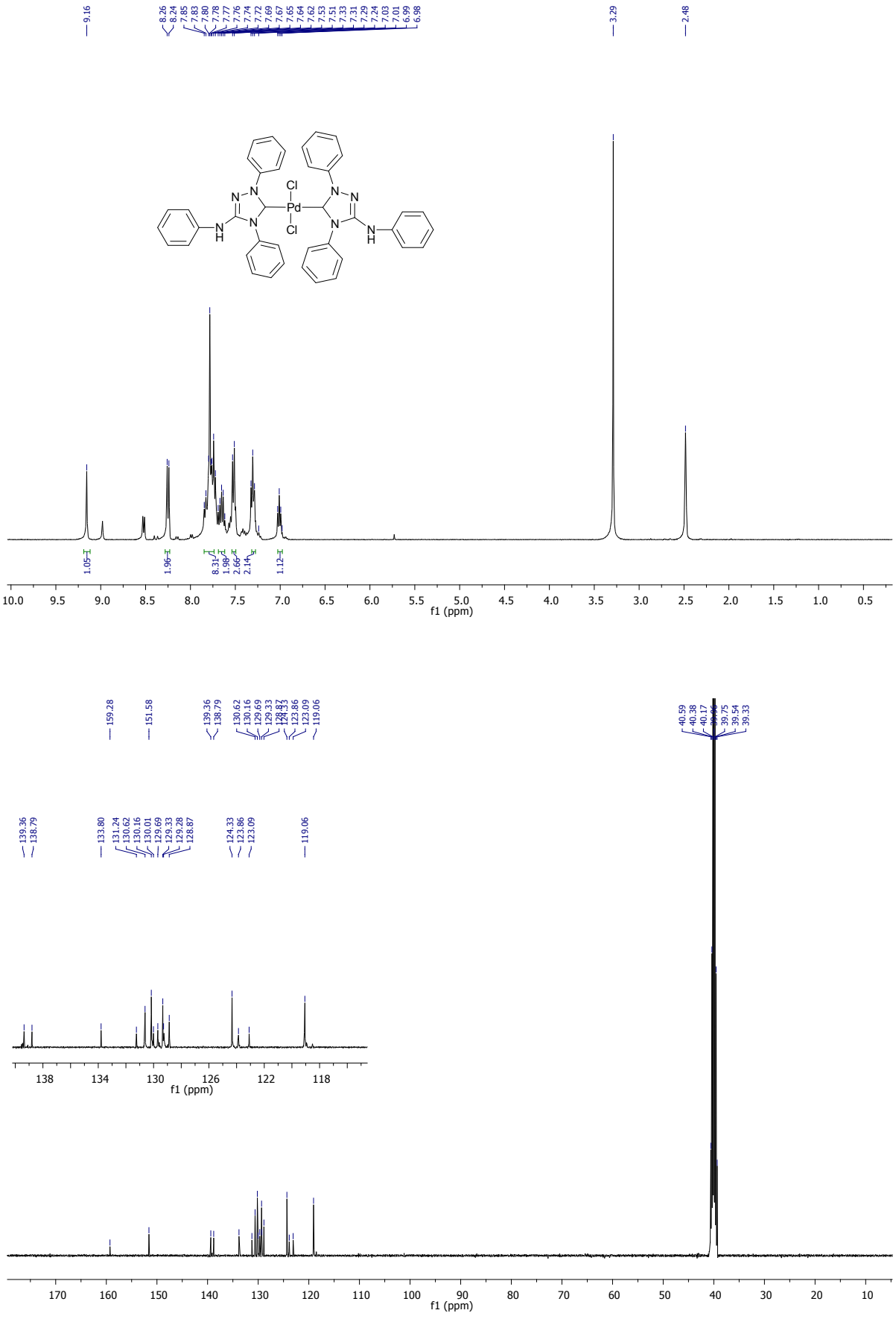


Figure S9. ^{1}H and ^{13}C NMR spectrums of complex **8** (DMSO-d_6).

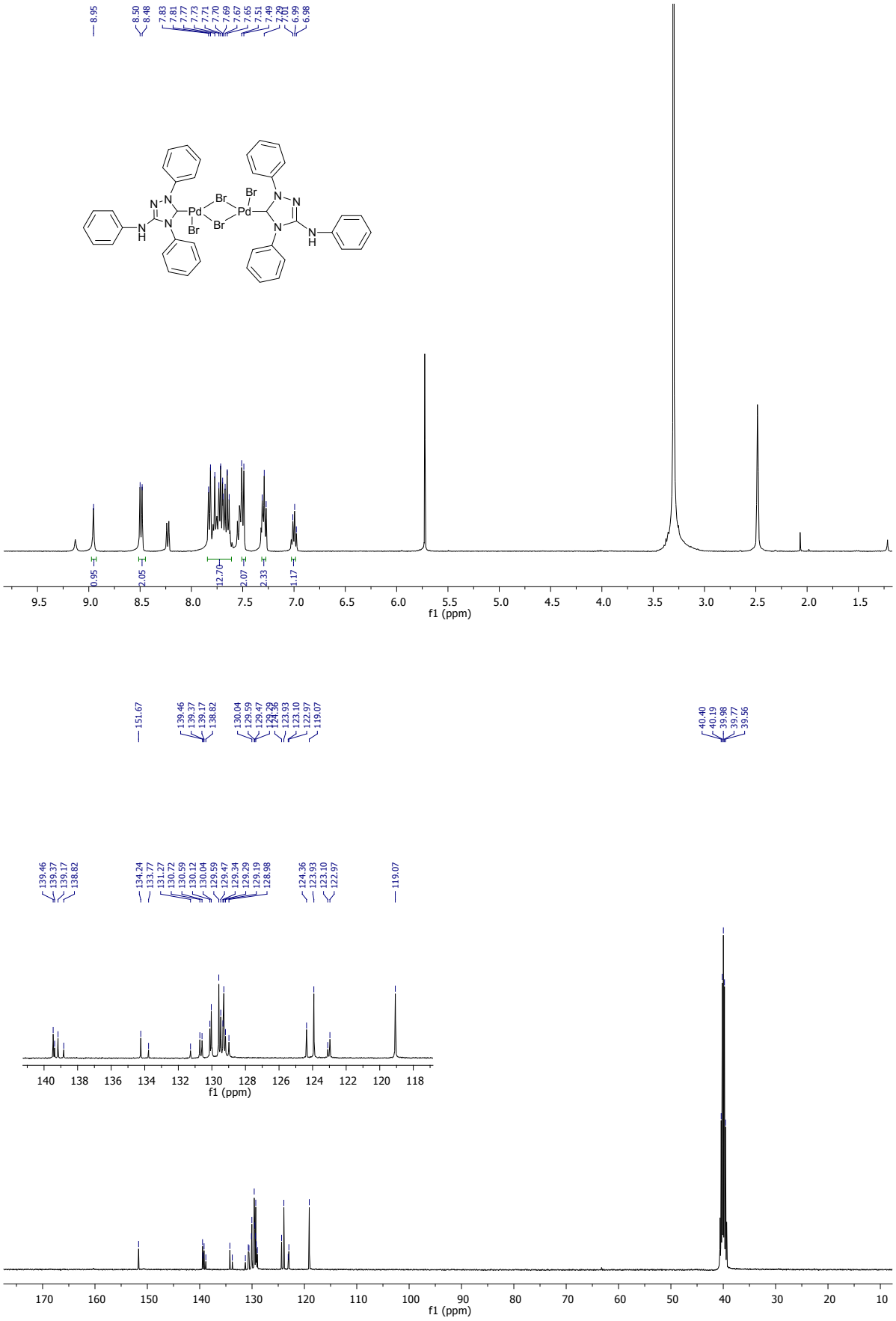


Figure S10. ^{1}H and ^{13}C NMR spectrums of complex **9** (DMSO-d_6).

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

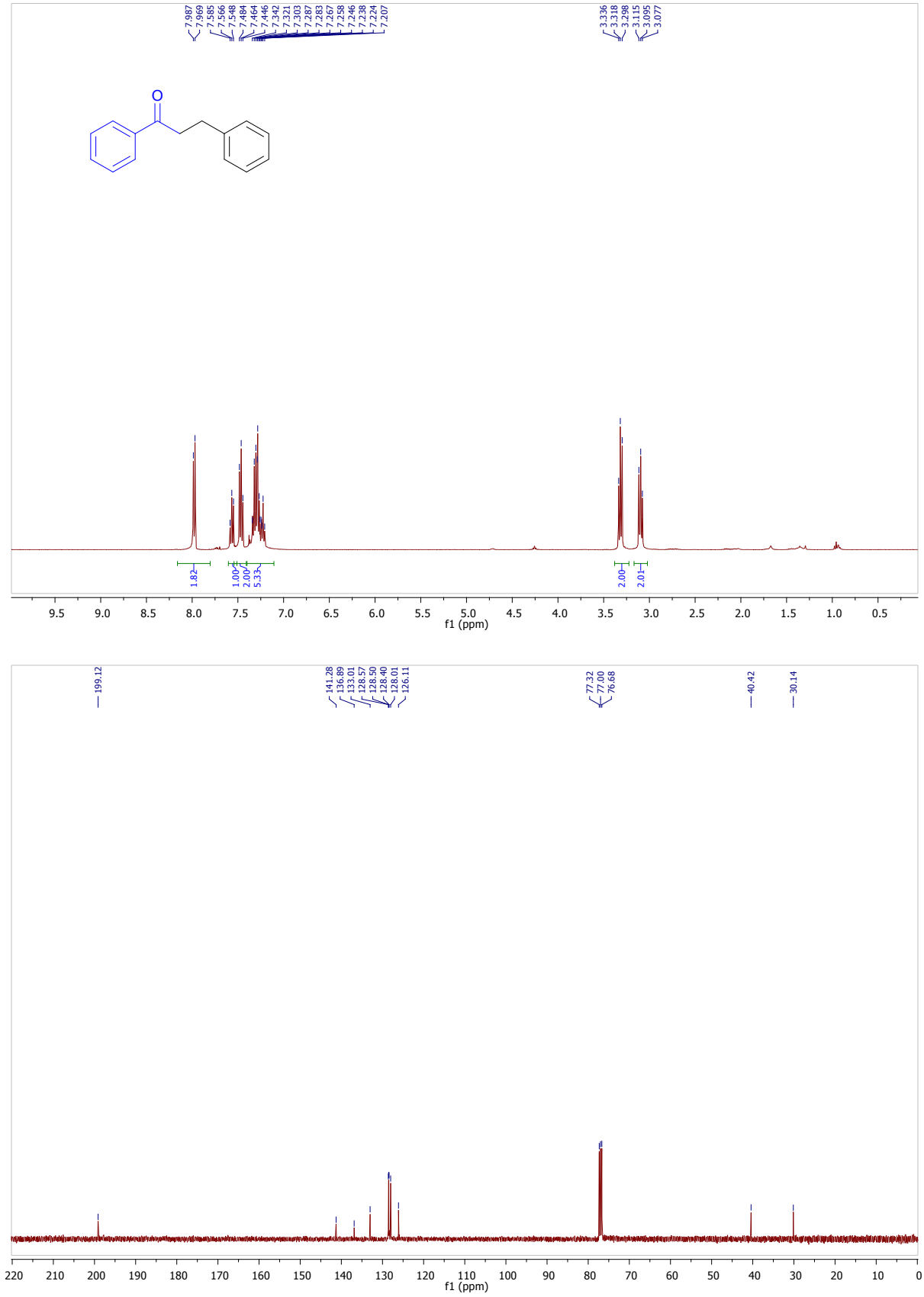


Figure S11. ^{1}H- and ^{13}C-NMR spectrums of 1,3-diphenylpropan-1-one (**22aa**).

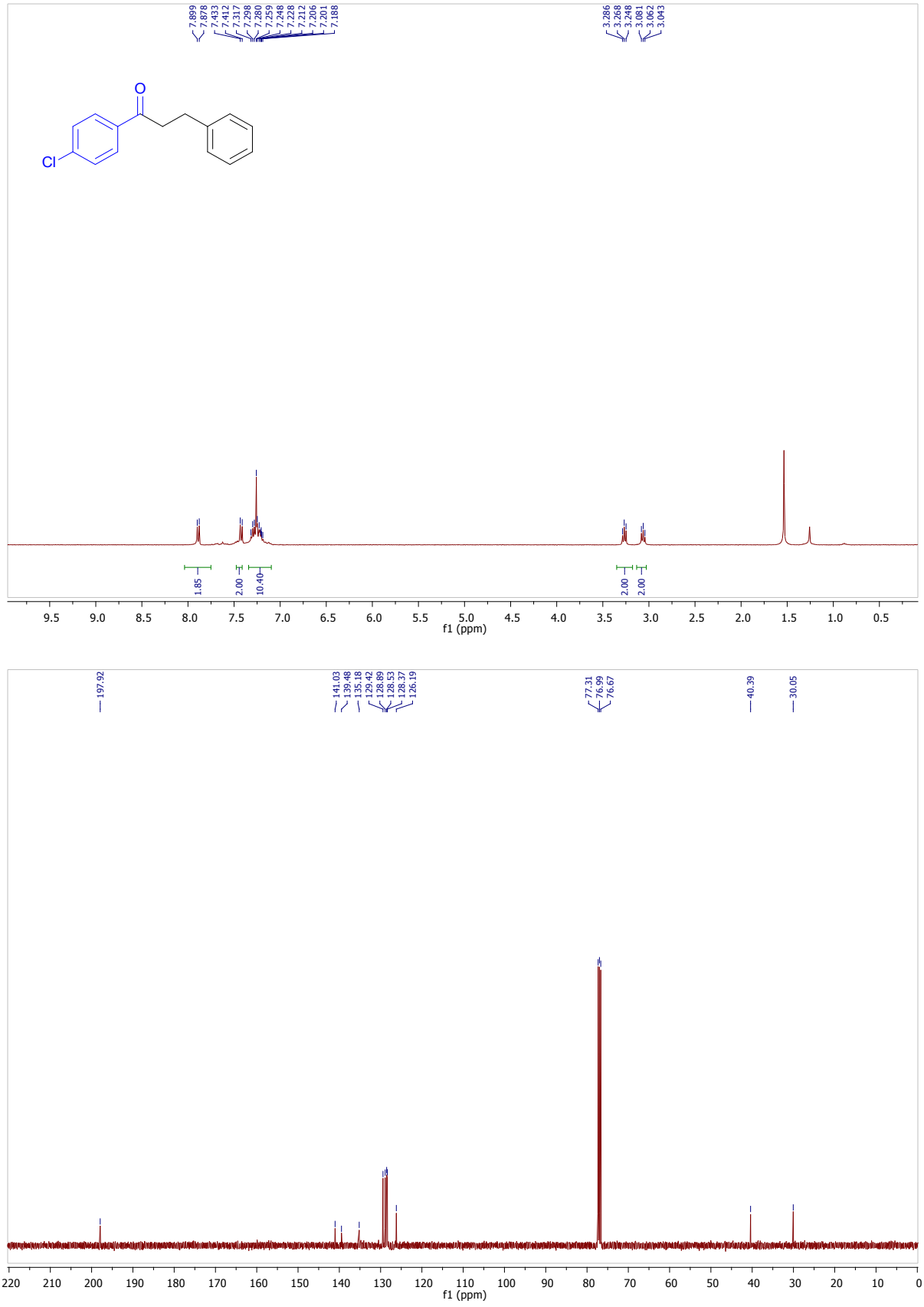
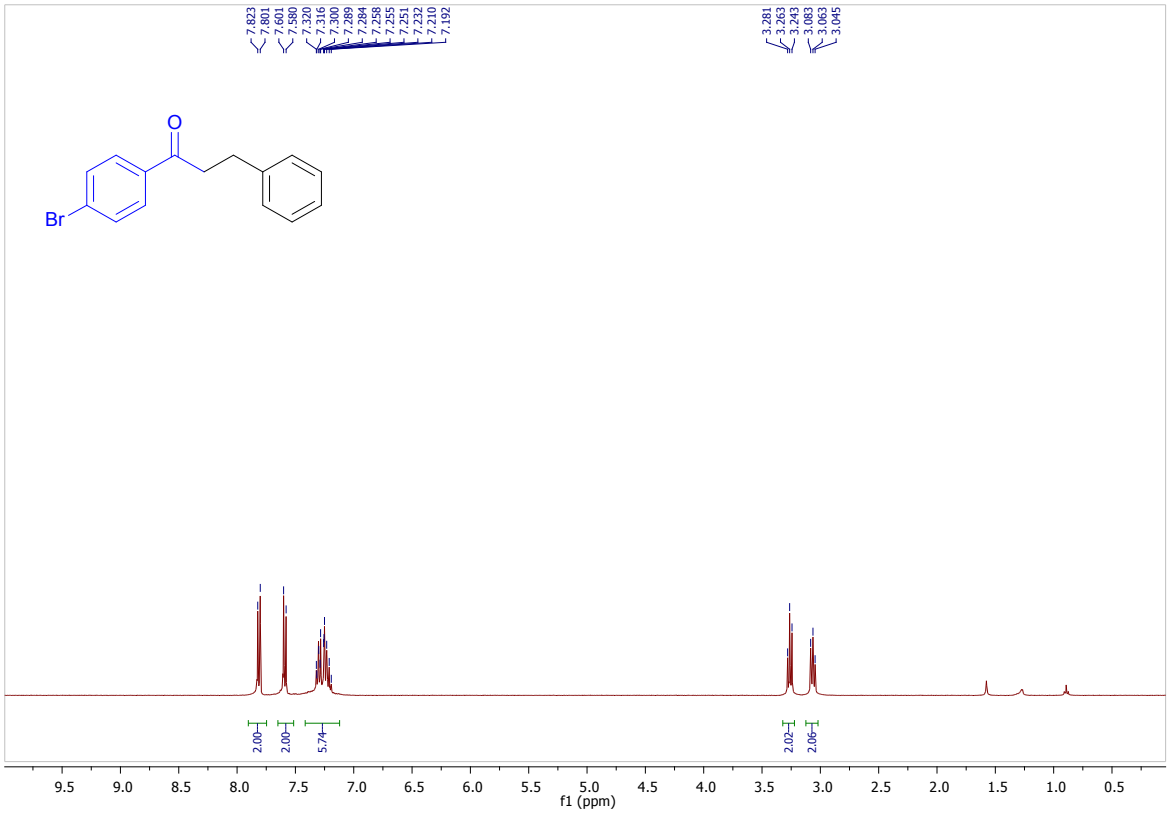


Figure S12. ^{1}H- and ^{13}C-NMR spectrums of 1-(4-chlorophenyl)-3-phenylpropan-1-one (**22ba**).



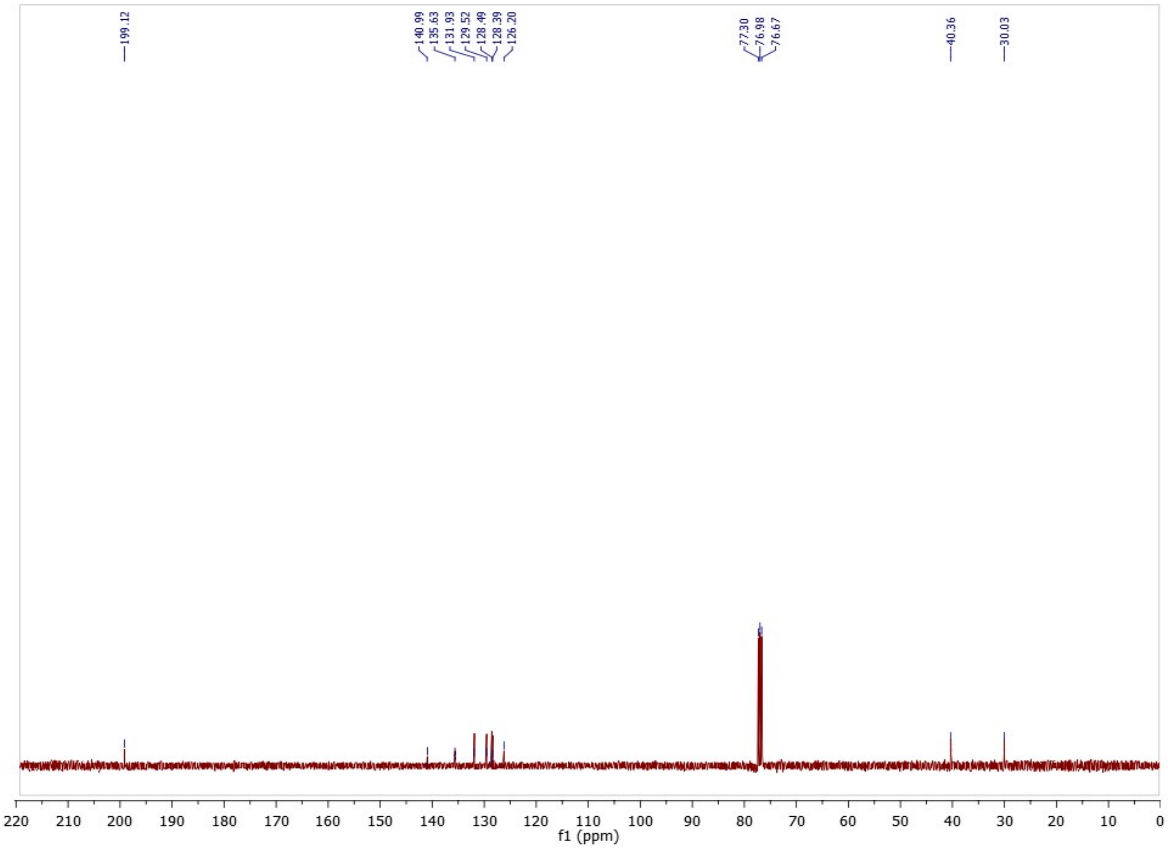


Figure S13. ^{1}H- and ^{13}C-NMR spectrums of 1-(4-bromophenyl)-3-phenylpropan-1-one (**22da**).

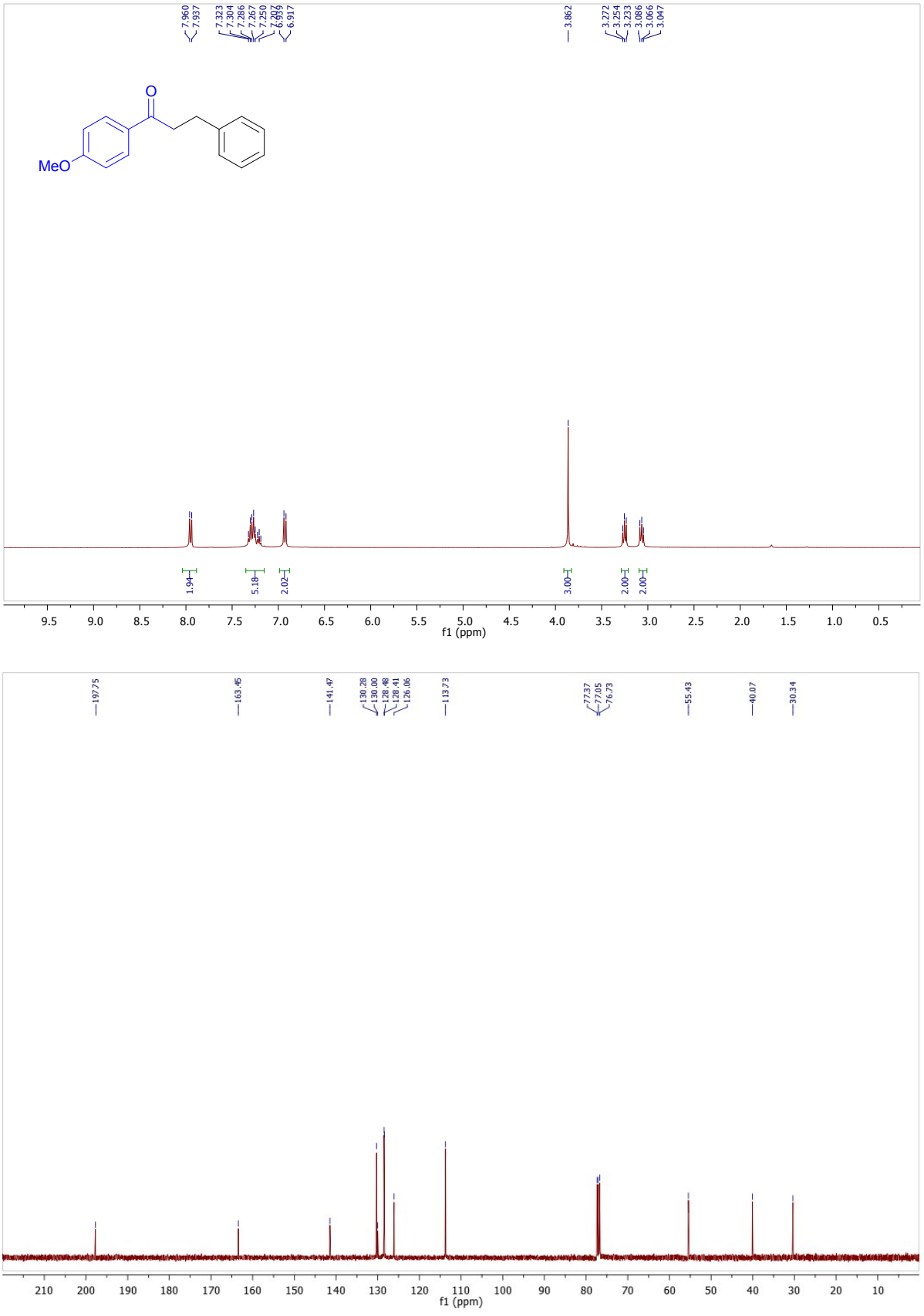


Figure S14. ^{1}H- and ^{13}C-NMR spectrums of 1-(4-methoxyphenyl)-3-phenylpropan-1-one (**22ea**).

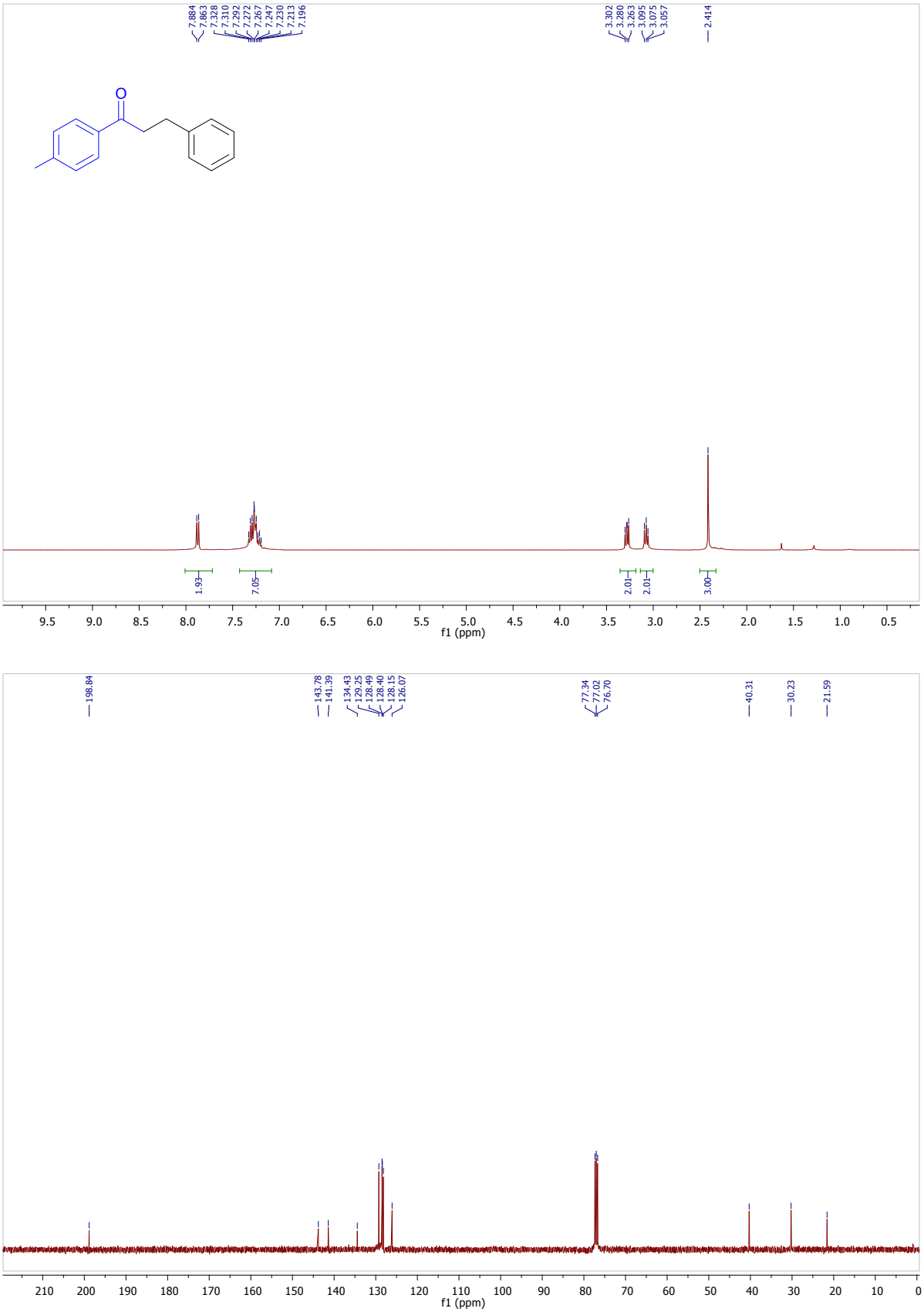


Figure S15. ^{1}H- and ^{13}C-NMR spectrums of 1-(4-methylphenyl)-3-phenylpropan-1-one (**22fa**).

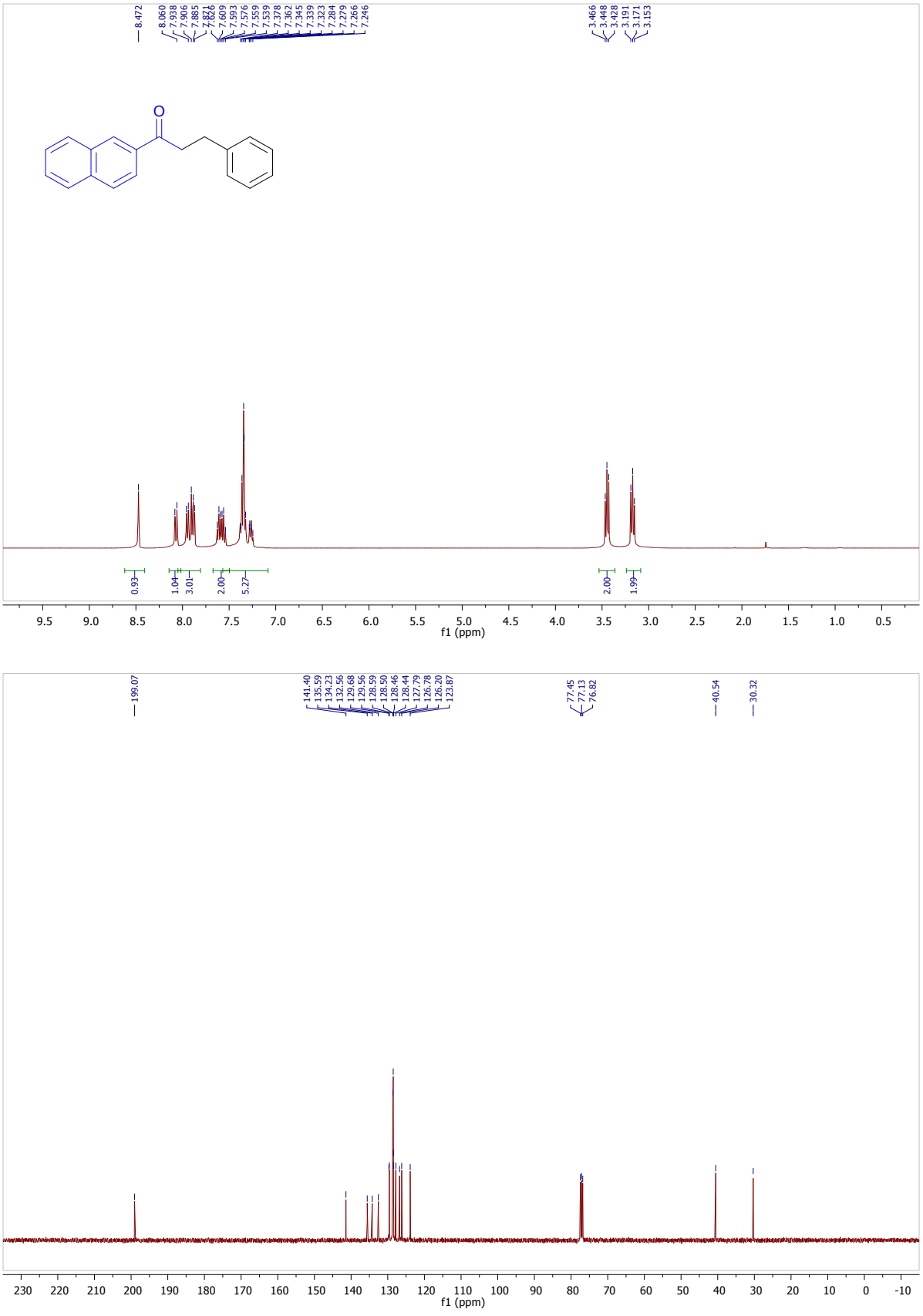


Figure S16. ^{1}H- and ^{13}C-NMR spectrums of 1-(naphthalen-2-yl)-3-phenylpropan-1-one (**22ia**).

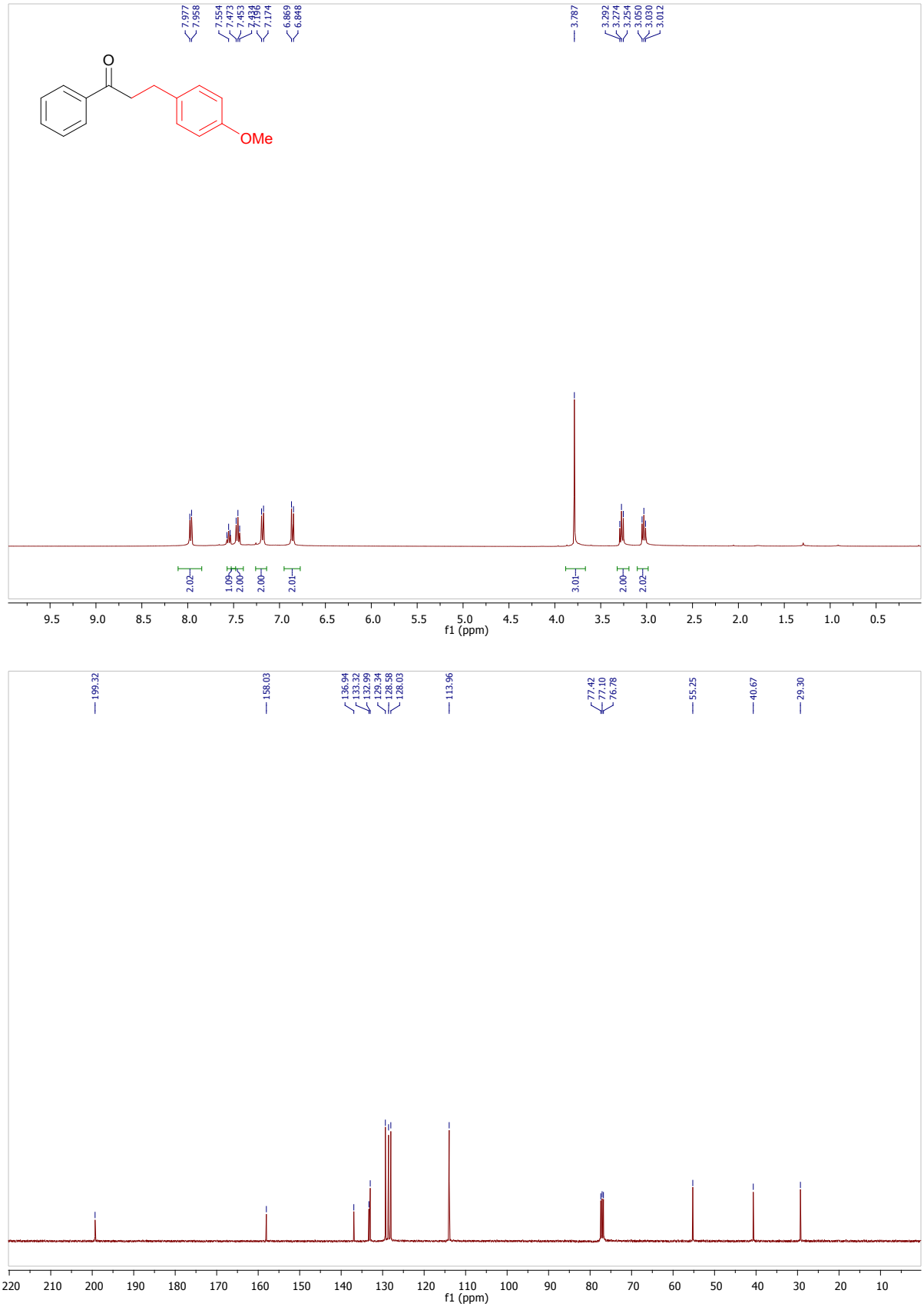


Figure S17. ^{1}H- and ^{13}C-NMR spectrums of 3-(4-methoxyphenyl)-1-phenylpropan-1-one (**22ab**).

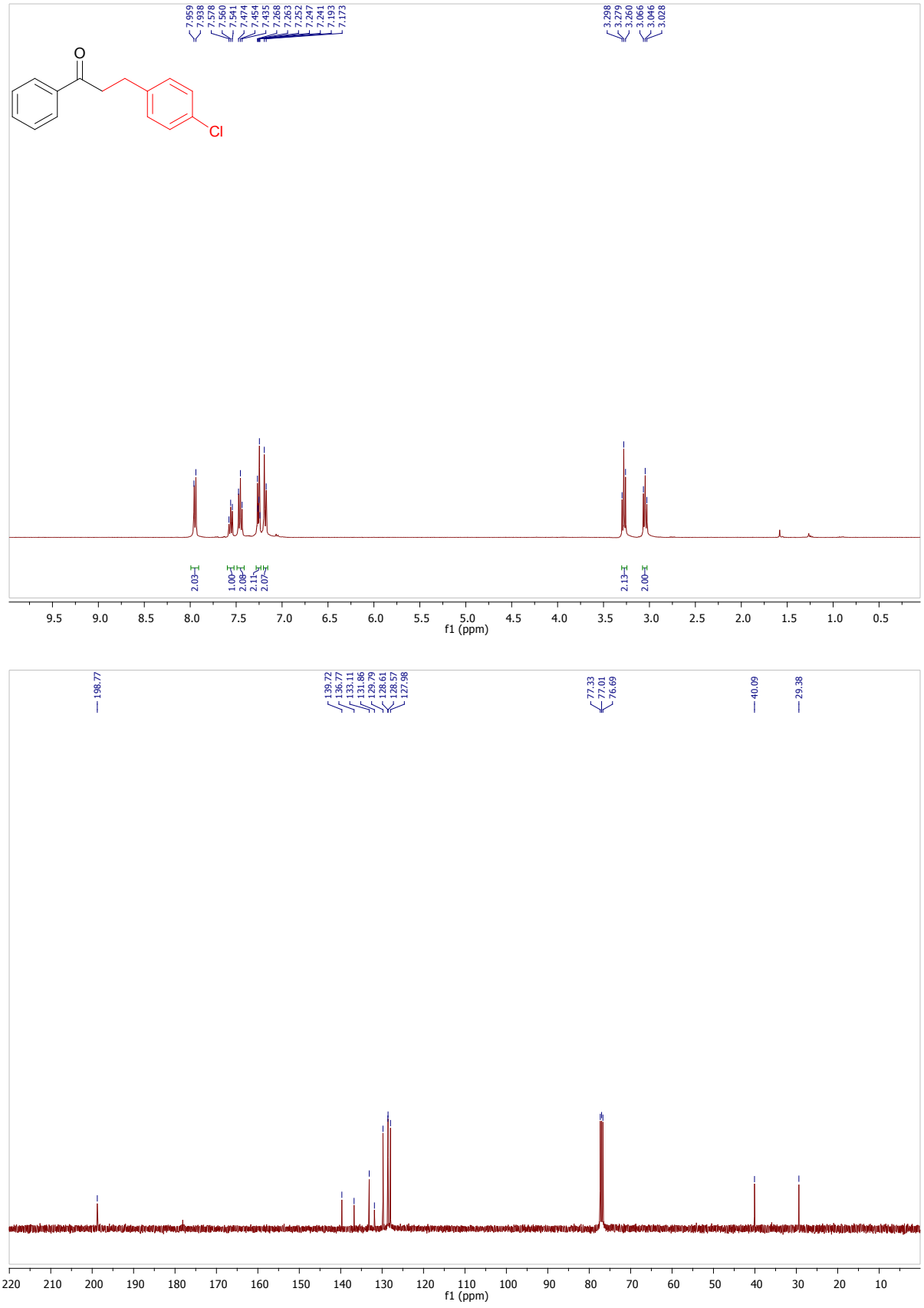


Figure S18. ^{1}H- and ^{13}C-NMR spectrums of 3-(4-chlorophenyl)-1-phenylpropan-1-one (**22af**).

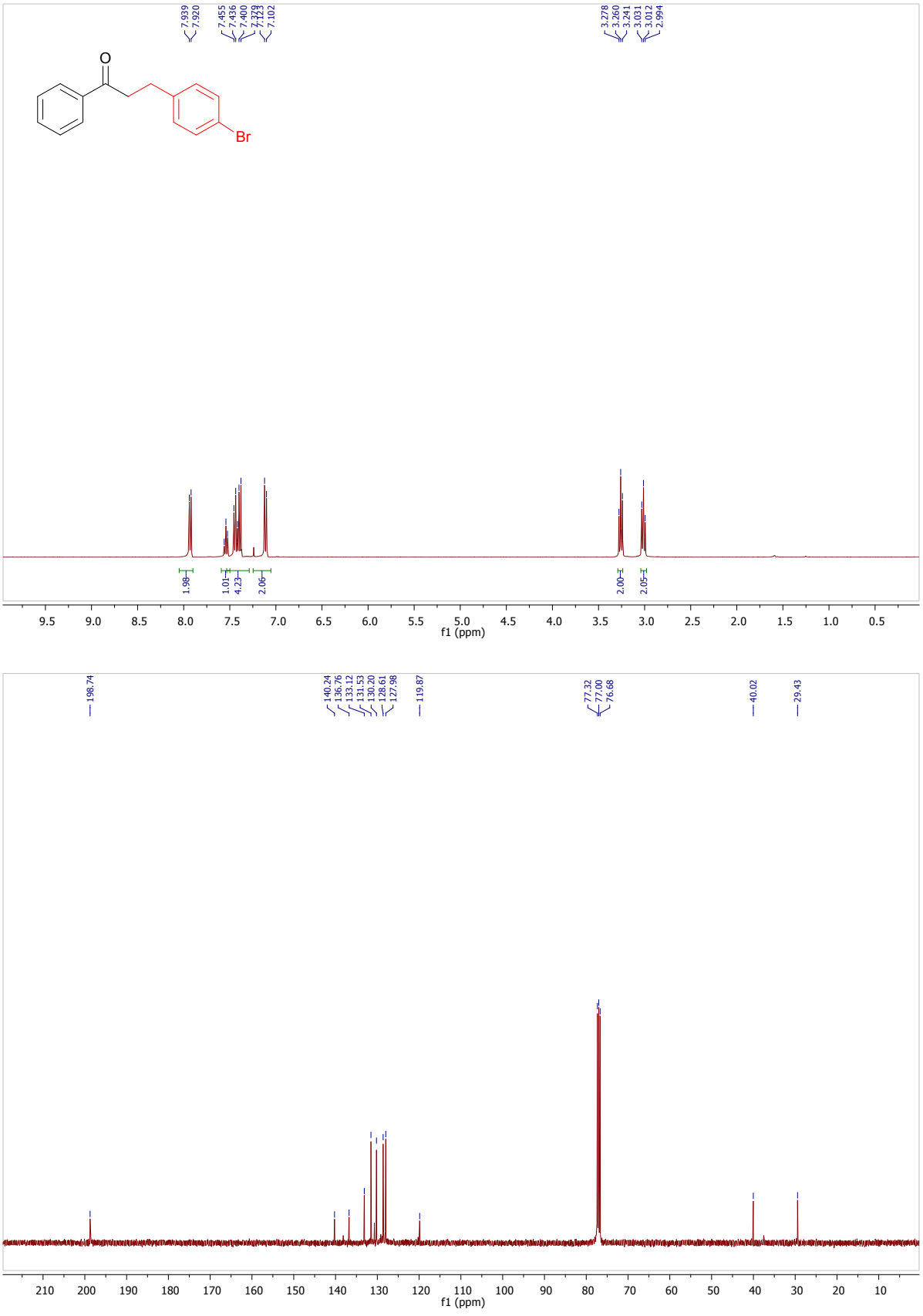


Figure S19. ^{1}H- and ^{13}C-NMR spectrums of 3-(4-bromophenyl)-1-phenylpropan-1-one (**22ah**).

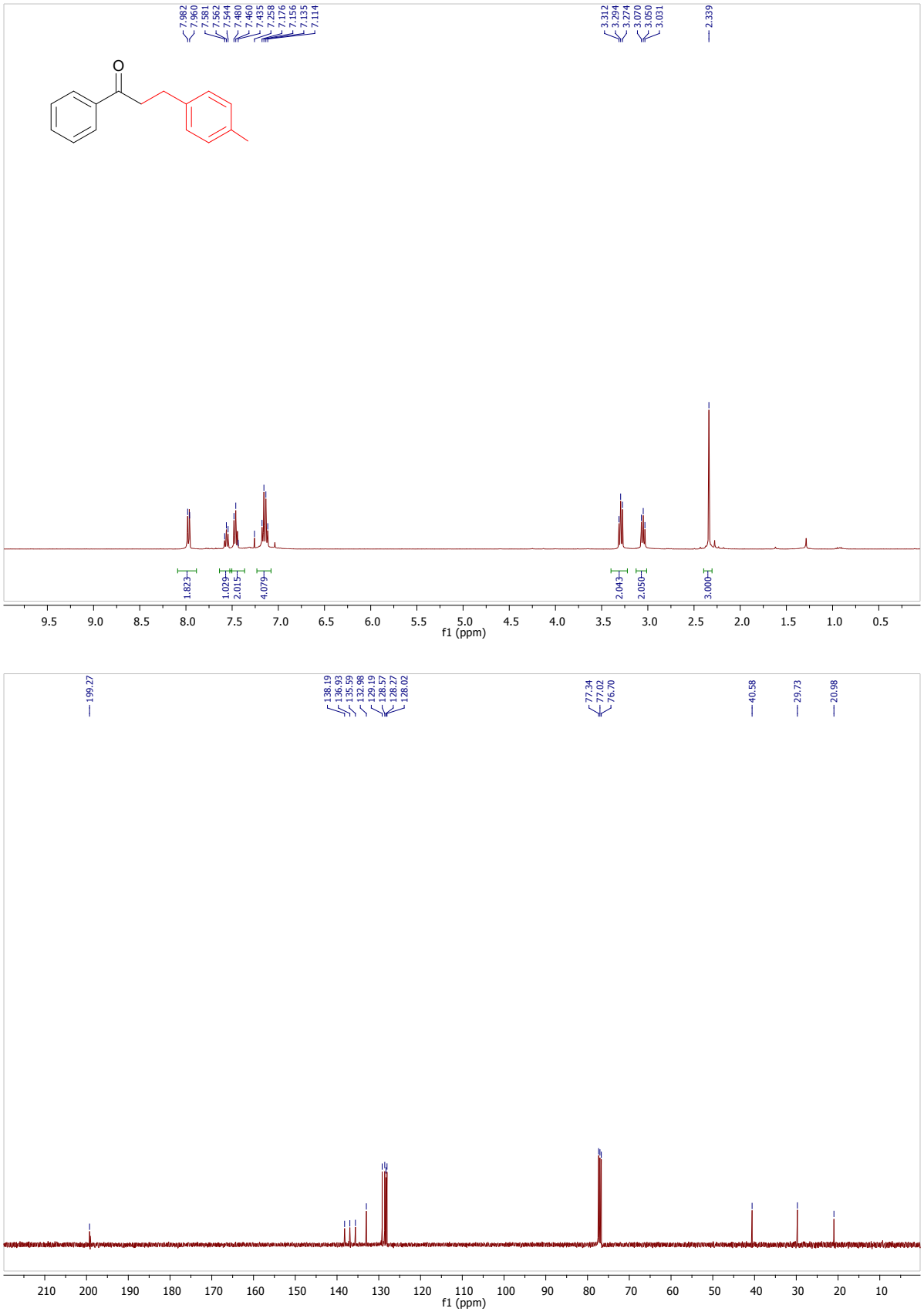


Figure S20. ^{1}H- and ^{13}C-NMR spectrums of 3-(4-methylphenyl)-1-phenylpropan-1-one (**22ad**).

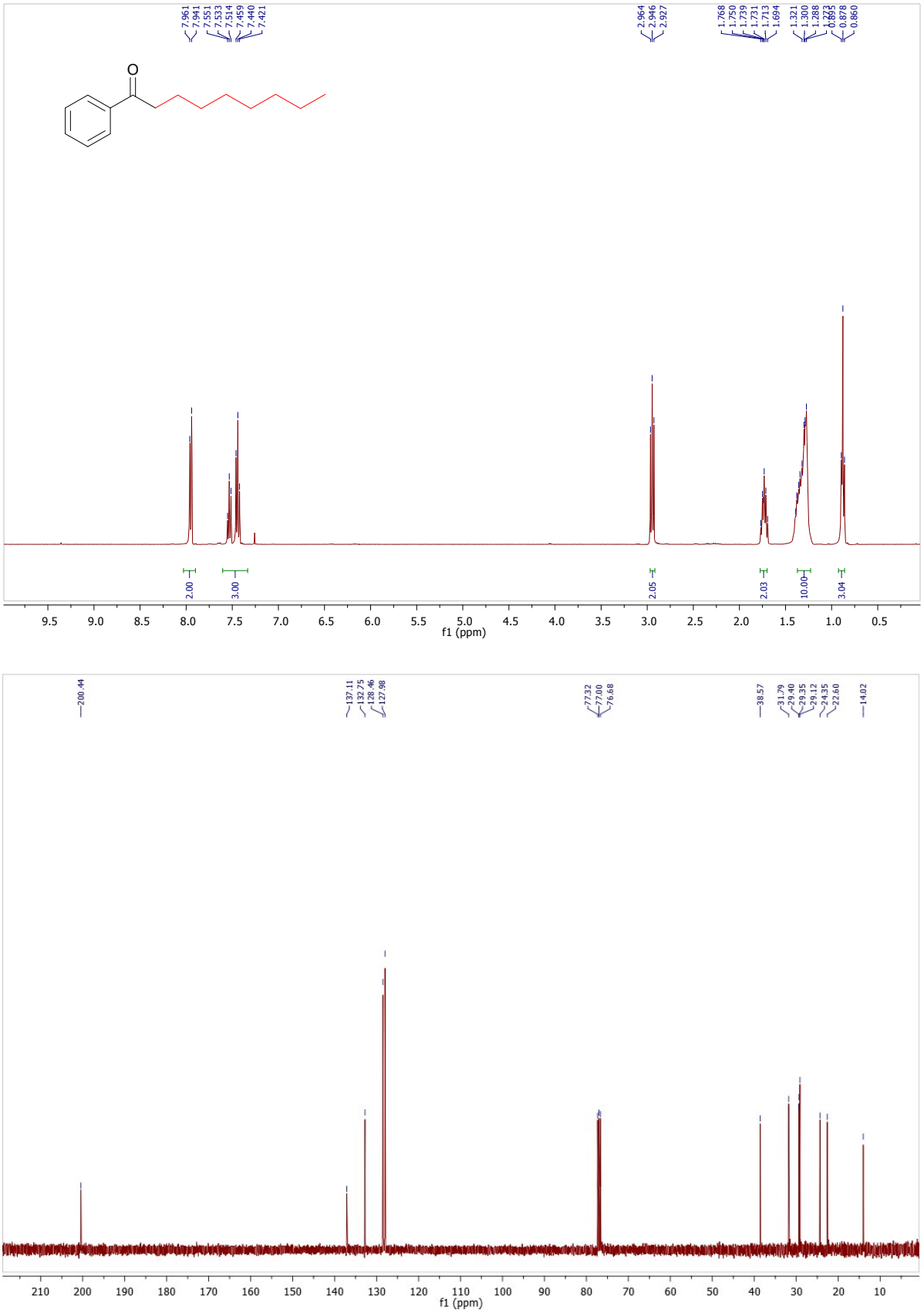


Figure S21. ^{1}H- and ^{13}C-NMR spectrums of 1-phenylnonan-1-one (**22aj**).

1,3-diphenylpropan-1-one (**22aa**). White solid, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 7.2 Hz, 2 H, Ar-*H*), 7.56 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.46 (t, *J* = 8.0 Hz, 2 H, Ar-*H*), 7.30 (m, 5 H, Ar-*H*), 3.31 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.09 (t, *J* = 8.0 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.1, 141.2, 136.8, 133.0, 128.5, 128.5, 128.4, 128.0, 126.1, 40.4, 30.1.

1-(4-chlorophenyl)-3-phenylpropan-1-one (**22ba**). White solid, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 7.42 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 7.24 (m, 5 H, Ar-*H*), 3.26 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.06 (t, *J* = 7.6 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.9, 141.0, 139.4, 135.1, 129.4, 128.8, 128.5, 128.3, 126.1, 40.3, 30.0.

1-(4-bromophenyl)-3-phenylpropan-1-one (**22da**). White solid, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.8 Hz, 2 H, Ar-*H*), 7.59 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 7.25 (m, 5 H, Ar-*H*), 3.26 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.06 (t, *J* = 8.0 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.1, 141.0, 135.5, 131.8, 129.5, 128.5, 128.3, 126.1, 40.3, 30.0.

1-(4-methoxyphenyl)-3-phenylpropan-1-one (**22ea**). White solid, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 9.2 Hz, 2 H, Ar-*H*), 7.26 (m, 5 H, Ar-*H*), 6.93 (d, *J* = 8.8 Hz, 2 H, Ar-*H*), 3.86 (s, 3 H, OCH_3), 3.25 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.06 (t, *J* = 8.4 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.7, 163.4, 141.4, 130.2, 130.0, 128.4, 128.4, 126.0, 113.7, 55.4, 40.0, 30.3.

1-(4-methylphenyl)-3-phenylpropan-1-one (**22fa**). White solid, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 7.27 (m, 7 H, Ar-*H*), 3.28 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.07 (t, *J* = 8.0 Hz, 2 H, CH_2), 2.41 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.8, 143.7, 141.3, 134.3, 129.2, 128.4, 128.4, 128.1, 126.0, 40.3, 30.2, 21.5.

1-(2-naphthyl)-3-phenylpropan-1-one (**22ia**). White solid, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1 H, Ar-*H*), 8.07 (d, *J* = 8.4 Hz, 1 H, Ar-*H*), 7.92 (m, 3 H, Ar-*H*), 7.59 (m, 2 H, Ar-*H*), 7.33 (m, 5 H, Ar-*H*), 3.44 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.17 (t, *J* = 8.0 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.0, 141.4, 135.5, 134.2, 132.5, 129.6, 129.5, 128.5, 128.5, 128.4, 128.4, 127.7, 126.7, 126.2, 123.8, 40.5, 30.3.

3-(4-methoxyphenyl)-1-phenylpropan-1-one (**22ab**). White solid; 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.6 Hz, 2 H, Ar-*H*), 7.55 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.45 (t, *J* = 8.0 Hz, 2 H, Ar-*H*), 7.18 (d, *J* = 8.8 Hz, 2 H, Ar-*H*), 6.85 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 3.78 (s, 3 H, CH_3), 3.27 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.03 (t, *J* = 8.0 Hz, 2 H, CH_2). ^{13}C NMR (100

MHz, $CDCl_3$): δ 199.3, 158.0, 136.9, 133.3, 132.9, 129.3, 128.5, 128.0, 113.3, 55.2, 40.6, 29.3.

3-(4-chlorophenyl)-1-phenylpropan-1-one (**22af**). White solid; 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 7.56 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.45 (t, *J* = 8.0 Hz, 2 H, Ar-*H*), 7.25 (m, 1 H, Ar-*H*), 7.18 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 3.28 (t, *J* = 7.2 Hz, 2 H, CH_2), 3.04 (t, *J* = 7.6 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.7, 139.7, 136.7, 133.1, 131.8, 129.7, 128.6, 128.5, 127.9, 40.0, 29.3.

3-(4-bromophenyl)-1-phenylpropan-1-one (**22ah**). Yellow oil; 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 1.2-8.0 Hz, 2 H, Ar-*H*), 7.56 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.43 (m, 4 H, Ar-*H*), 7.13 (d, *J* = 7.2 Hz, 2 H, Ar-*H*), 3.27 (t, *J* = 6.8 Hz, 2 H, CH_2), 3.03 (t, *J* = 7.6 Hz, 2 H, CH_2). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.7, 140.2, 136.7, 133.1, 131.5, 130.2, 128.6, 128.0, 119.9, 40.0, 29.4.

3-(4-methylphenyl)-1-phenylpropan-1-one (**22ad**). White solid; 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 7.2 Hz, 2 H, Ar-*H*), 7.56 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.46 (t, *J* = 7.6 Hz, 2 H, Ar-*H*), 7.15 (q, 4 H, Ar-*H*), 3.29 (t, *J* = 7.6 Hz, 2 H, CH_2), 3.05 (t, *J* = 8.0 Hz, 2 H, CH_2), 2.33 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.2, 138.1, 136.9, 135.5, 132.9, 129.1, 128.5, 128.0, 40.5, 29.7, 20.9.

1-phenyldecan-1-one (**22aj**). Yellow oil, 72% yield. ^{1}H NMR (400 MHz, 303 K, $CDCl_3$): δ 7.96 (d, *J* = 8.8 Hz, 2 H, Ar-*H*), 7.55 (t, *J* = 7.2 Hz, 1 H, Ar-*H*), 7.47 (t, *J* = 7.6 Hz, 2 H, Ar-*H*), 2.96 (d, *J* = 7.4 Hz, 2 H, CH_2), 1.75 (m, 2 H, CH_2), 1.29 (m, 12 H, CH_2), 0.89 (t, *J* = 7.0 Hz, 3 H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.5, 137.2, 132.8, 128.5, 128.0, 38.6, 31.9, 29.5, 29.4, 29.3, 24.4, 22.7, 14.1.

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

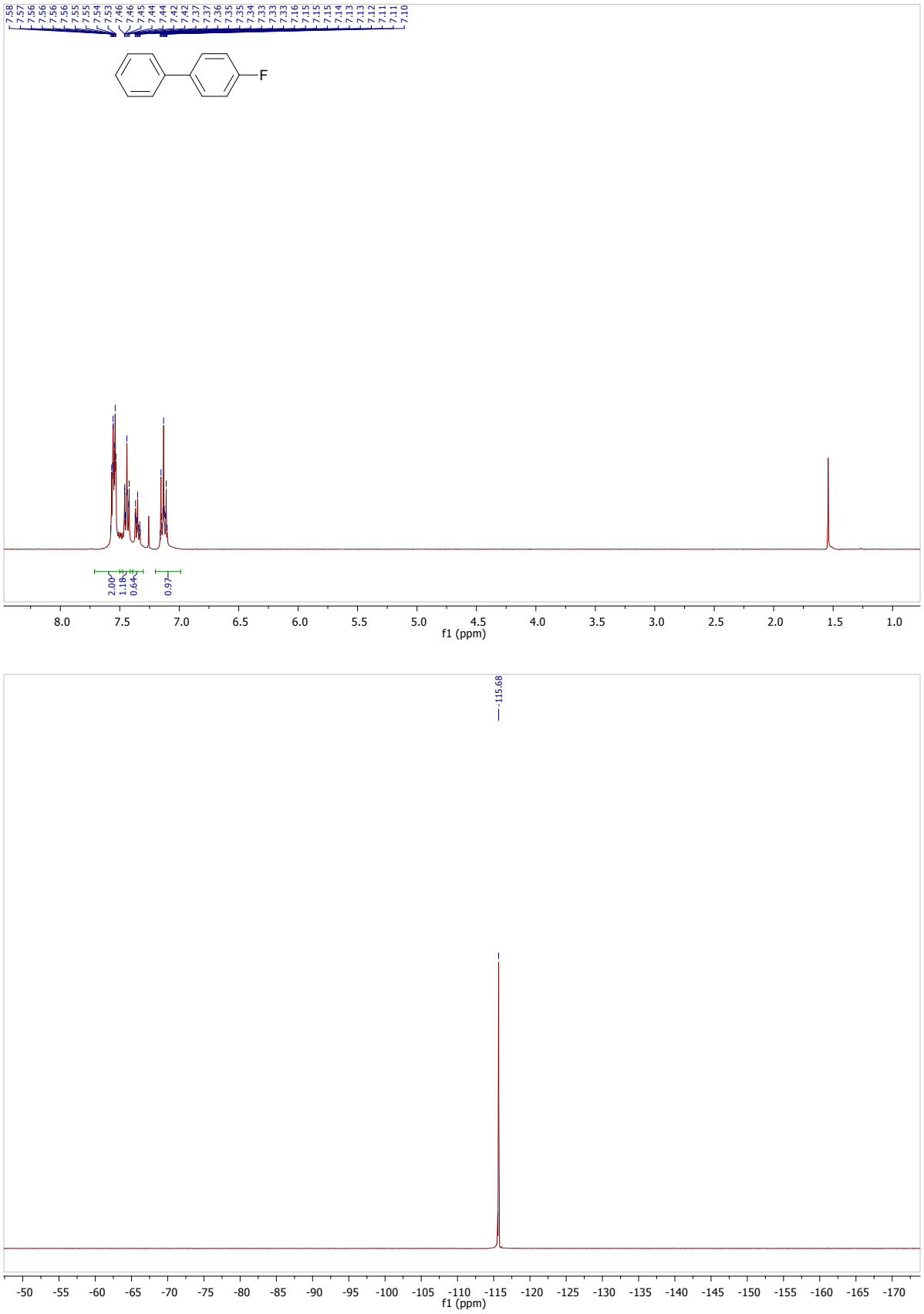


Figure S22. ^{1}H-, ^{13}C- and ^{19}F-NMR spectrums of 4-fluoro-1,1'-biphenyl (**27ad**).

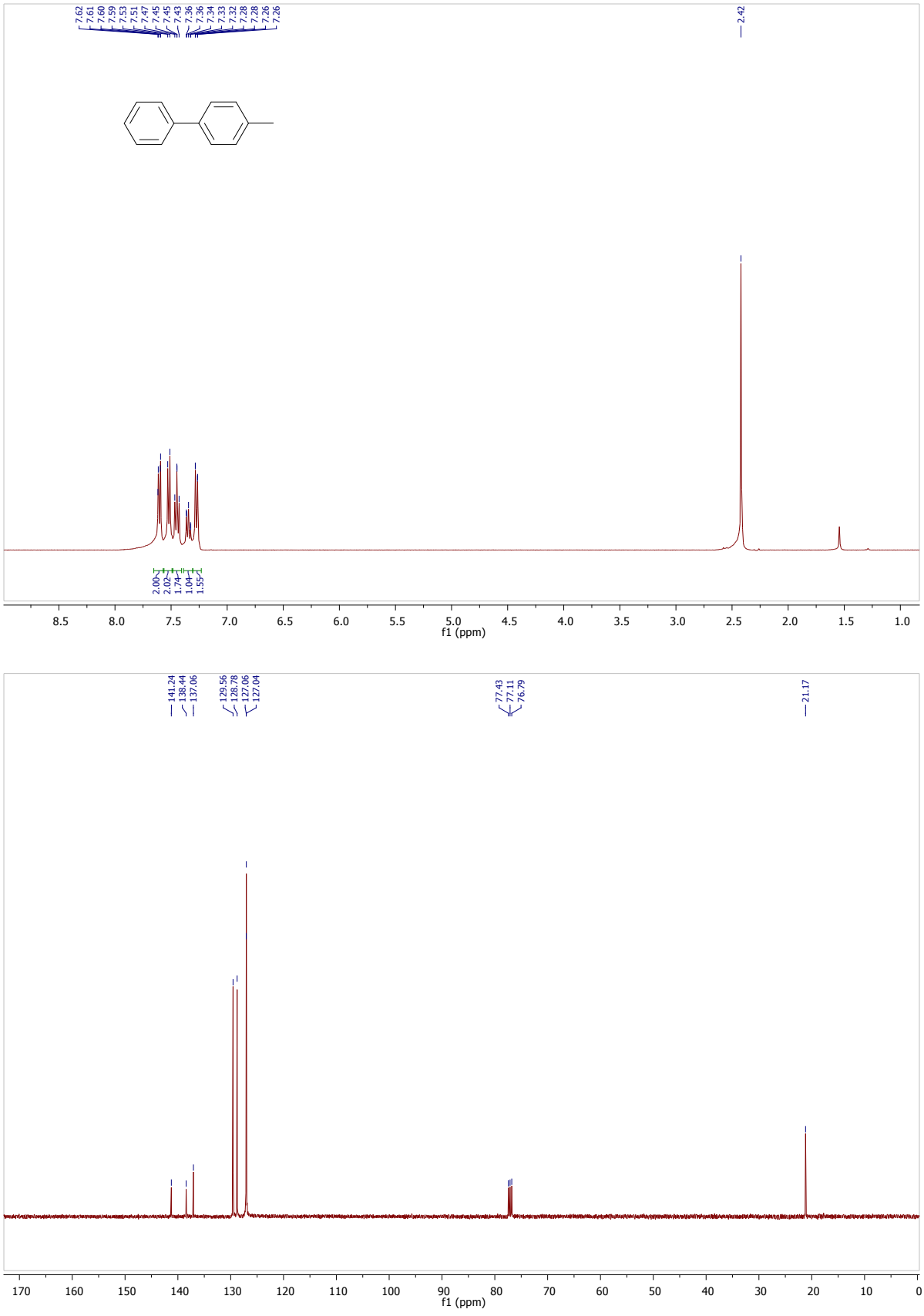
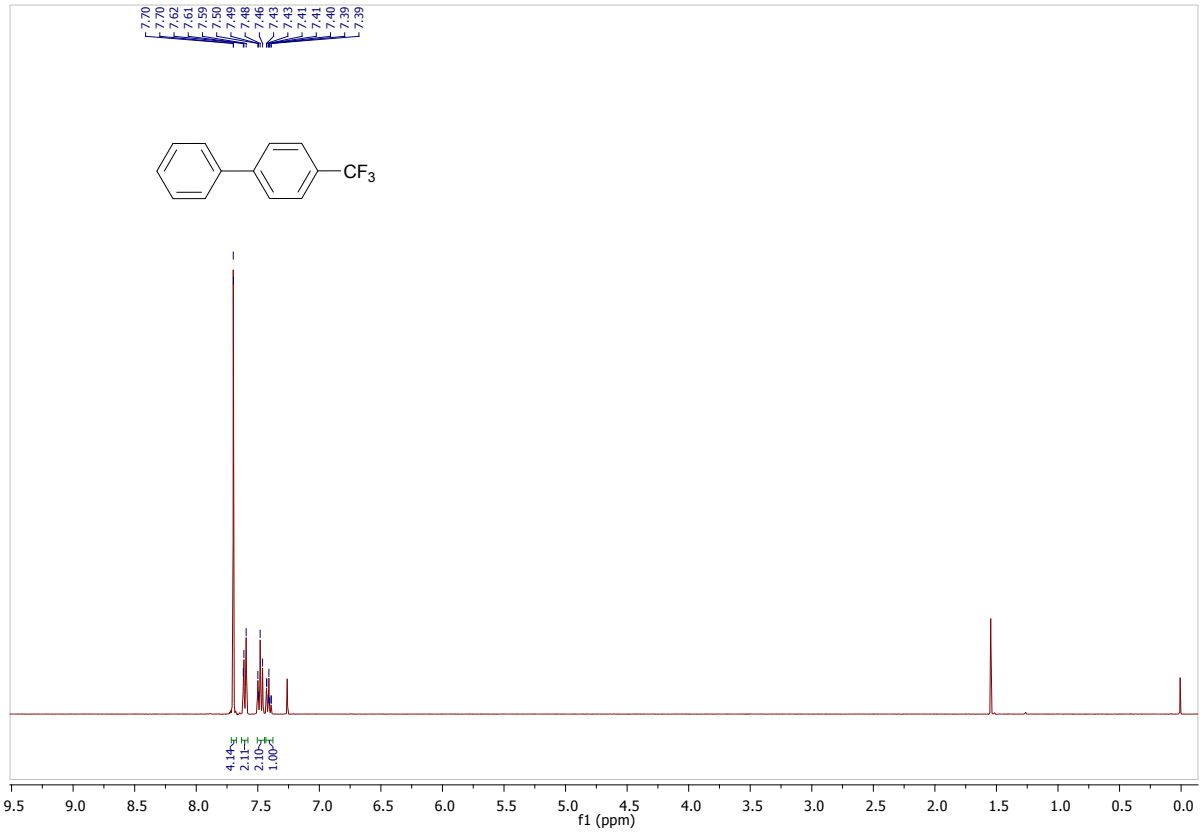
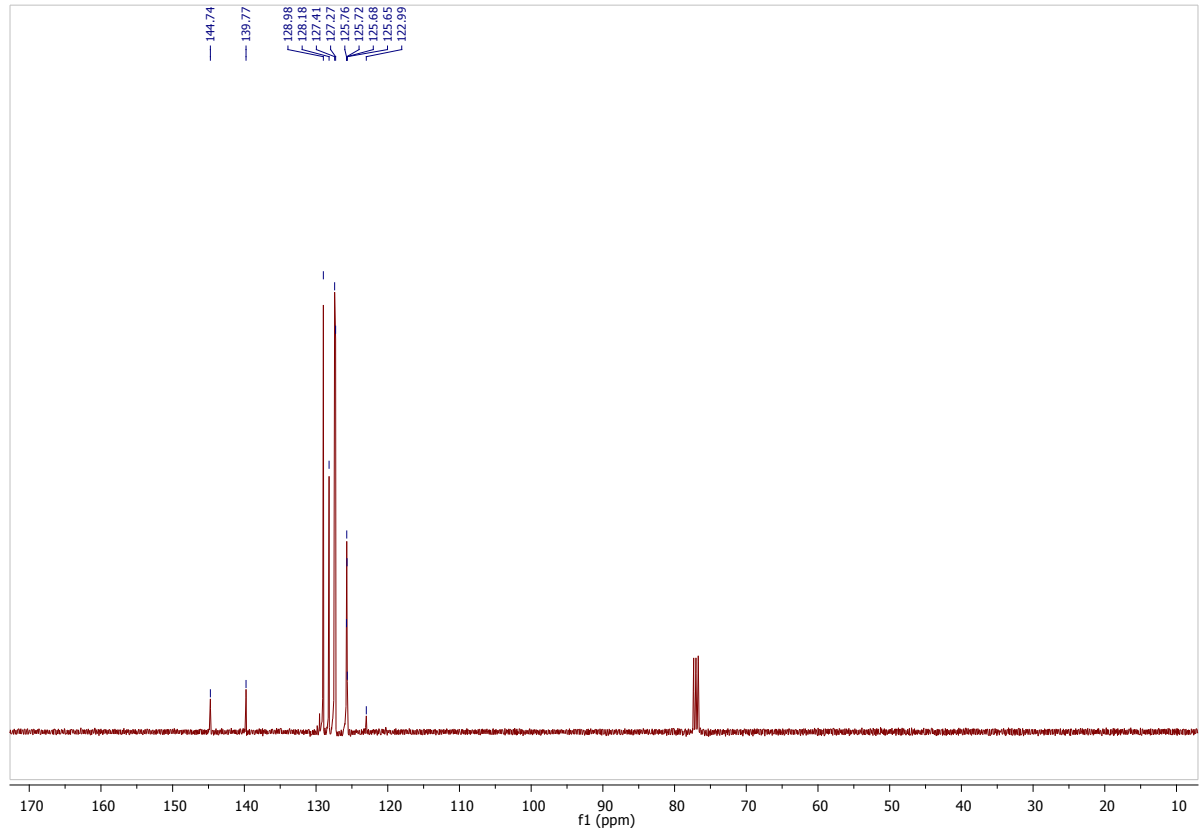


Figure S23. ^{1}H- and ^{13}C-NMR spectrums of 4-methyl-1,1'-biphenyl (**27ac**).


7.70
7.70
7.62
7.61
7.59
7.50
7.49
7.48
7.46
7.43
7.41
7.41
7.40
7.39
7.39
CF3
4.14
2.11
2.10
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


144.74
139.77
128.98
128.18
127.41
127.27
125.76
125.72
125.68
125.65
122.99
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

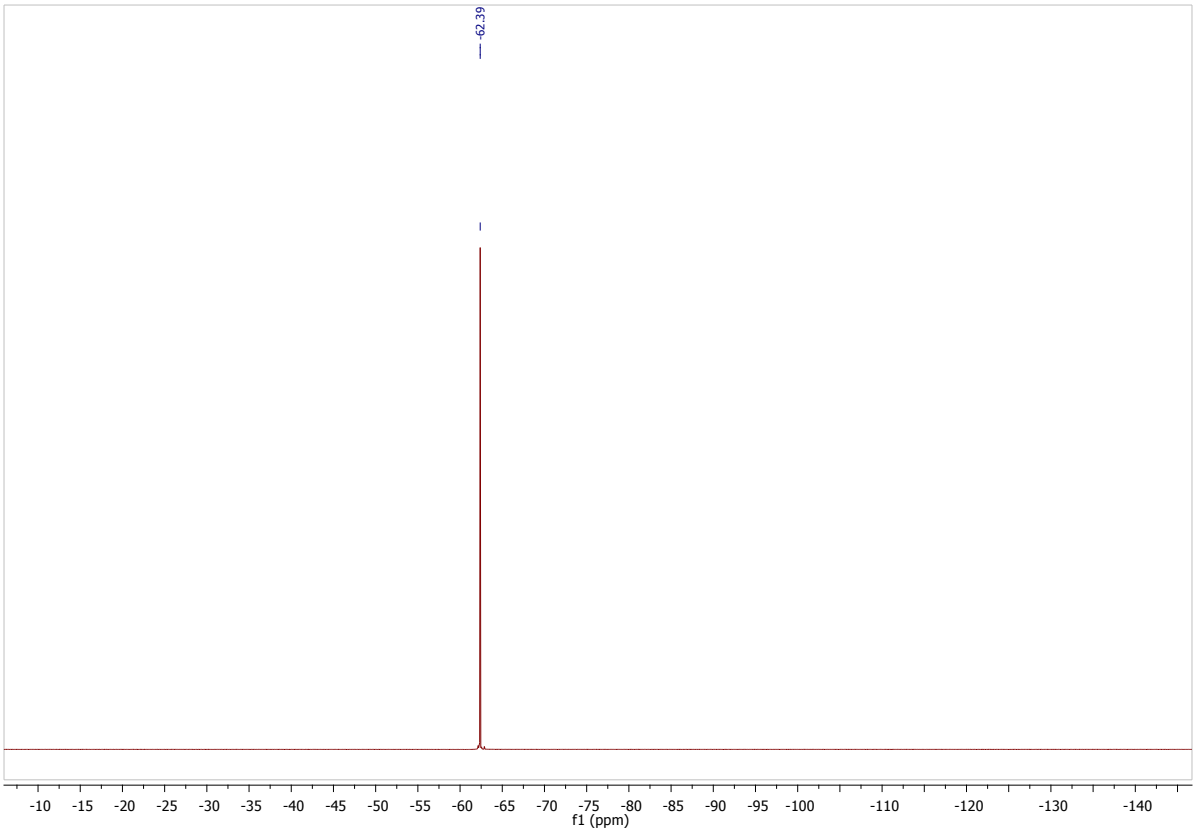


Figure S24. ^{1}H-, ^{13}C- and ^{19}F-NMR spectrums of 4-(trifluoromethyl)-1,1'-biphenyl (**27da**).

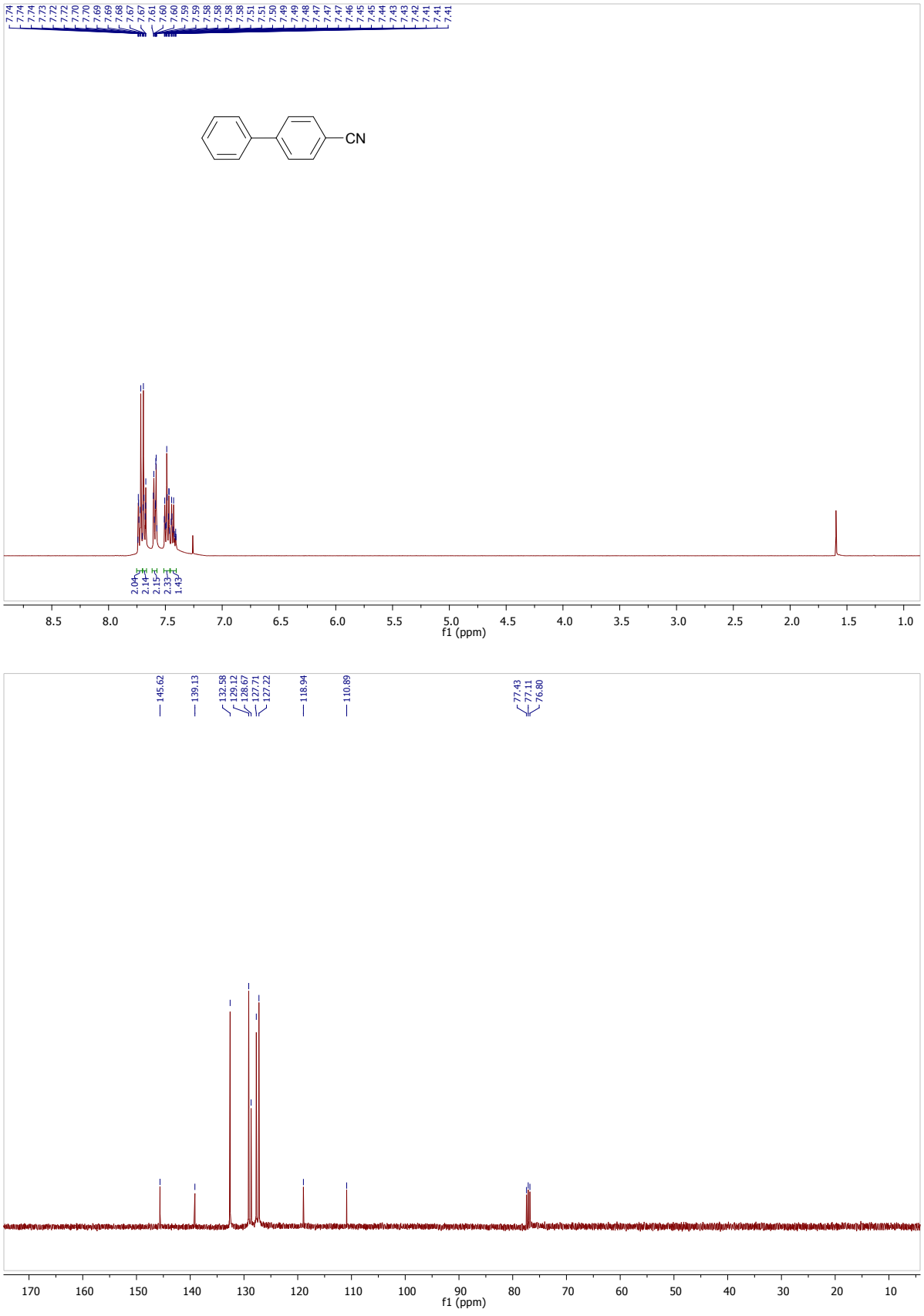


Figure S25. ^{1}H- and ^{13}C-NMR spectrums of [1,1'-biphenyl]-4-carbonitrile (**27ea**).

4-fluoro-1,1'-biphenyl (**27ad**). White solid; 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (m, 1 H, Ar-H), 7.48 (m, 1 H, Ar-H), 7.44 (m, 1 H, Ar-H), 7.35 (m, 1 H, Ar-H), 7.13 (m, 1 H, Ar-H). ^{13}C NMR (100 Hz, $CDCl_3$): δ 163.7, 161.3, 140.3, 137.4, 137.3, 128.8, 128.7, 128.7, 127.3, 127.0, 115.7, 115.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -115.68 (s, F).

4-methyl-1,1'-biphenyl (**27ac**). White solid; 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8 Hz, 2 H, Ar-H), 7.52 (d, *J* = 8 Hz, 2 H, Ar-H), 7.45 (t, *J* = 8 Hz, 2 H, Ar-H), 7.34 (t, *J* = 8 Hz, 1 H, Ar-H), 7.28 (s, 2 H, Ar-H), 2.42 (s, 3 H, Ar-CH_3). ^{13}C NMR (100 Hz, $CDCl_3$): δ 141.2, 138.4, 137.0, 129.5, 128.7, 127.0, 127.0, 21.1.

4-(trifluoromethyl)-1,1'-biphenyl (27da). White solid; 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (s, 4 H, Ar-H), 7.61 (m, 2 H, Ar-H), 7.48 (m, 2 H, Ar-H), 7.39 (m, 1 H, Ar-H). ^{13}C NMR (100 Hz, $CDCl_3$): δ 144.7, 139.7, 128.9, 128.1, 127.4, 127.2, 125.7, 125.7, 125.6, 125.6, 122.9. ^{19}F NMR (376 MHz, $CDCl_3$): δ 62.39 (s, CF_3).

[1,1'-biphenyl]-4-carbonitrile (**27ea**). White solid; 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (m, 2 H, Ar-H), 7.68 (m, 2 H, Ar-H), 7.59 (m, 2 H, Ar-H), 7.48 (m, 2 H, Ar-H), 7.42 (m, 1 H, Ar-H). ^{13}C NMR (100 Hz, $CDCl_3$): δ 145.6, 139.1, 132.5, 129.1, 128.6, 127.7, 127.2, 118.9, 110.8.

The time course of Suzuki-Miyaura Coupling reaction

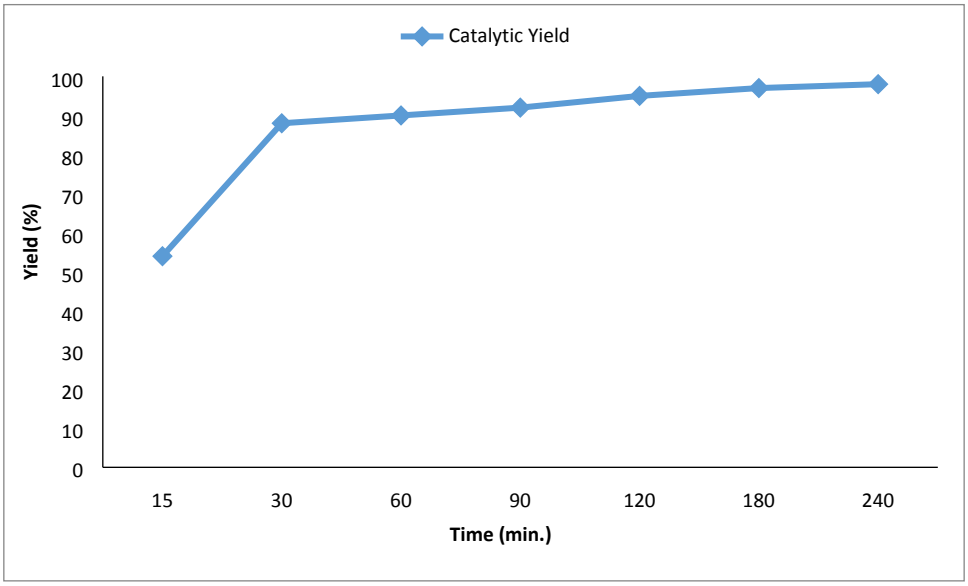


Figure S26. Time profile of the coupling reaction of bromobenzene (**25a**) and phenylboronicacid (**26a**). Reaction conditions: bromobenzene (1.0 mmol), phenylboronicacid(1.0 mmol), KOH (0.5 mmol), **6** (0.1 mol%), 0.5 mL 2-propanol + 1.5 mL H_2O, RT, 30 min., under air.

FTIR Spectrums

The IR spectra of synthesized compounds are similar. In the spectra, $\boldsymbol{\nu}_{N\text{-}H}$ stretching vibration frequencies are seen at 3250-3420 cm^{-1}. Aromatic $\boldsymbol{\nu}_{C\text{-}H}$ stretching vibration frequencies are observed between 3000-3100 cm^{-1}. Furthermore, aromatic $\boldsymbol{\nu}_{C=C}$ stretching vibration frequencies were observed between 1579-1614 cm^{-1}.

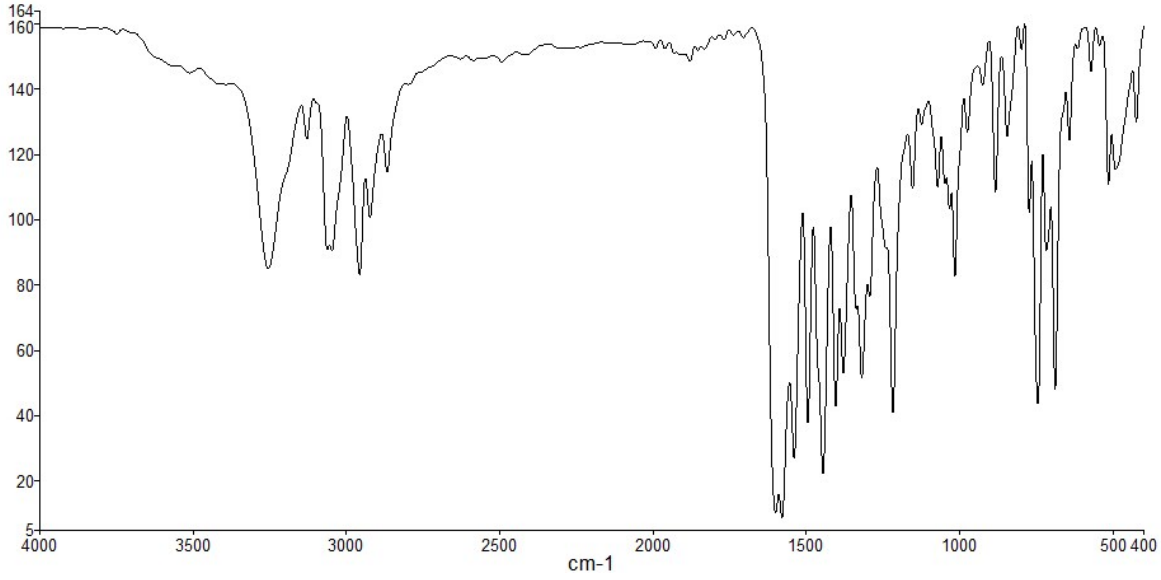


Figure S27. IR spectrum of **1**.

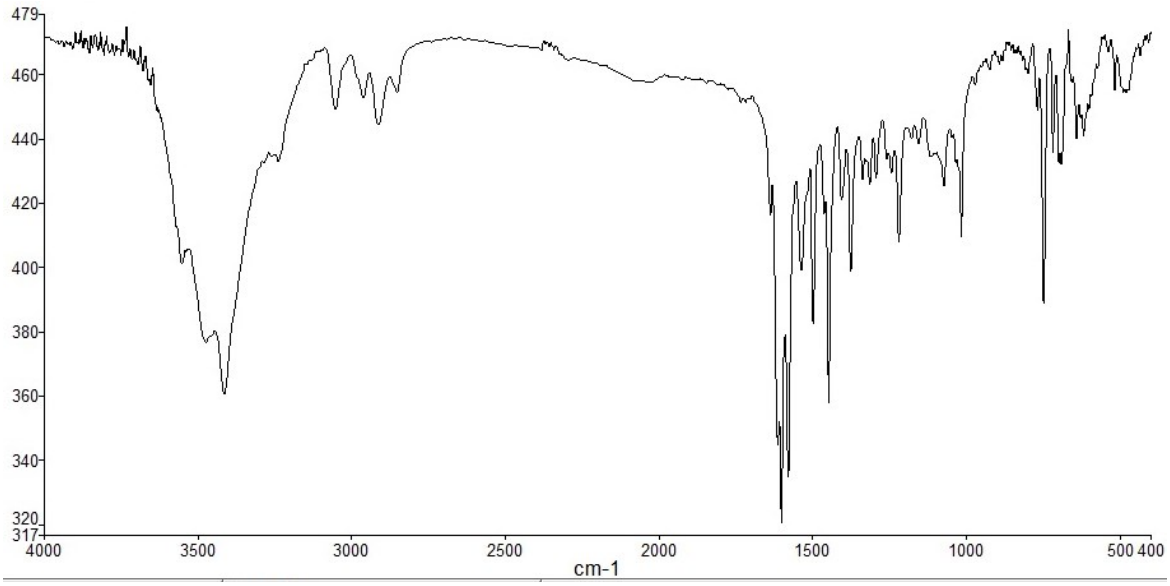


Figure S28. IR spectrum of **2**.

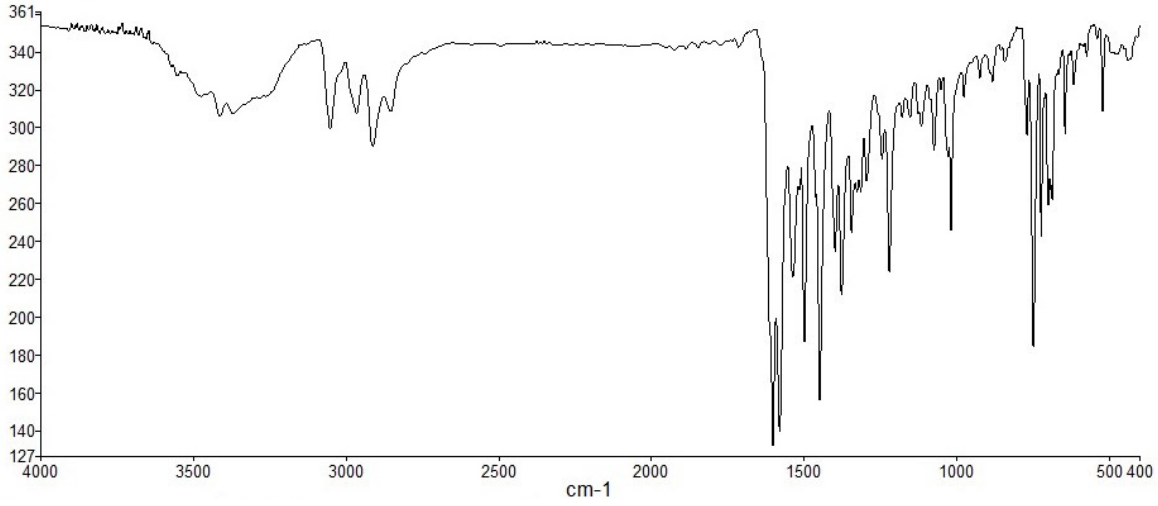


Figure S29. IR spectrum of **3**.

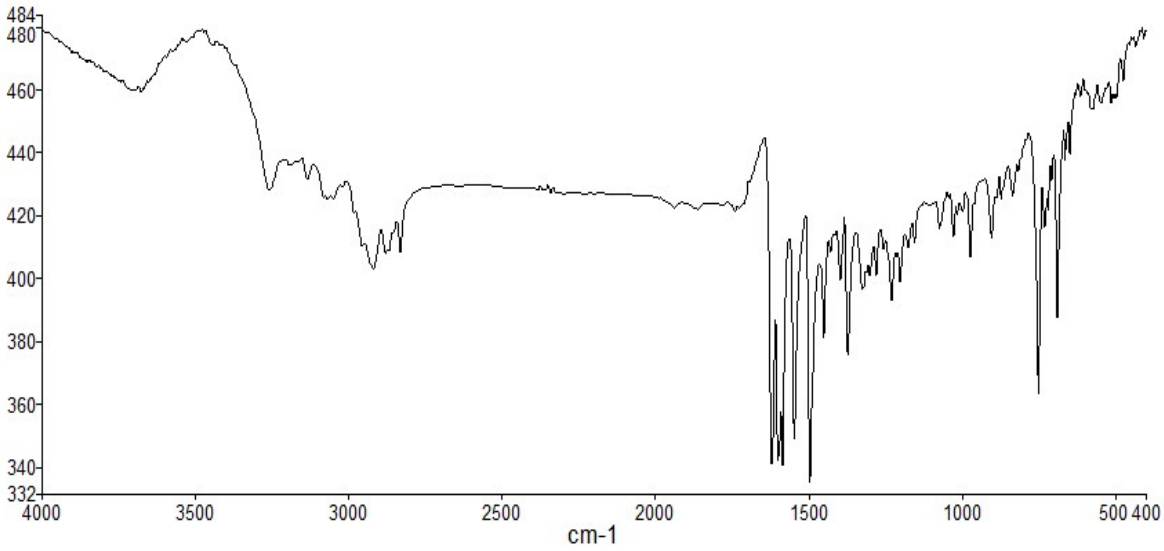


Figure S30. IR spectrum of **5**.

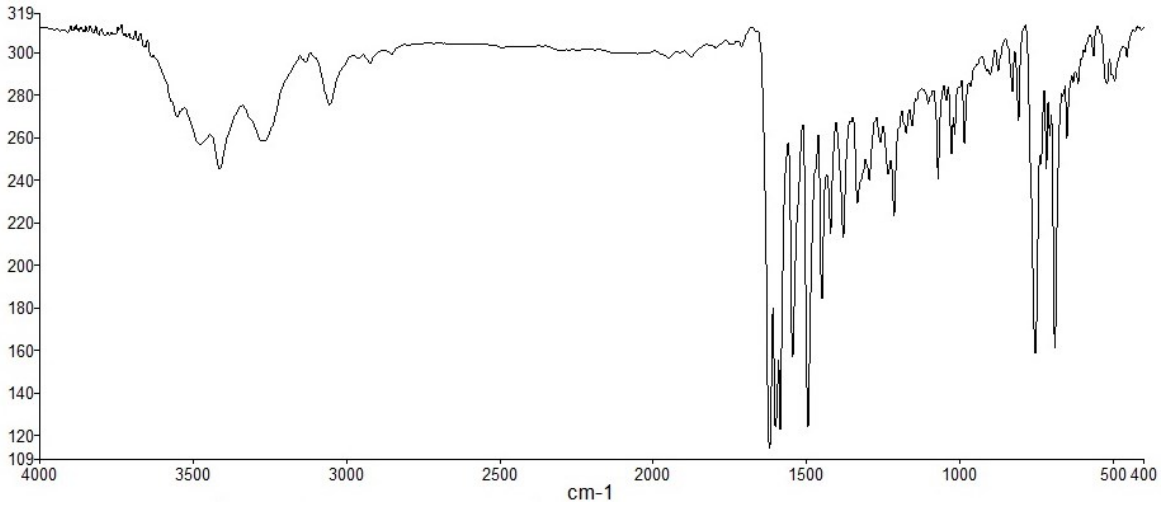


Figure S31. IR spectrum of **6**.

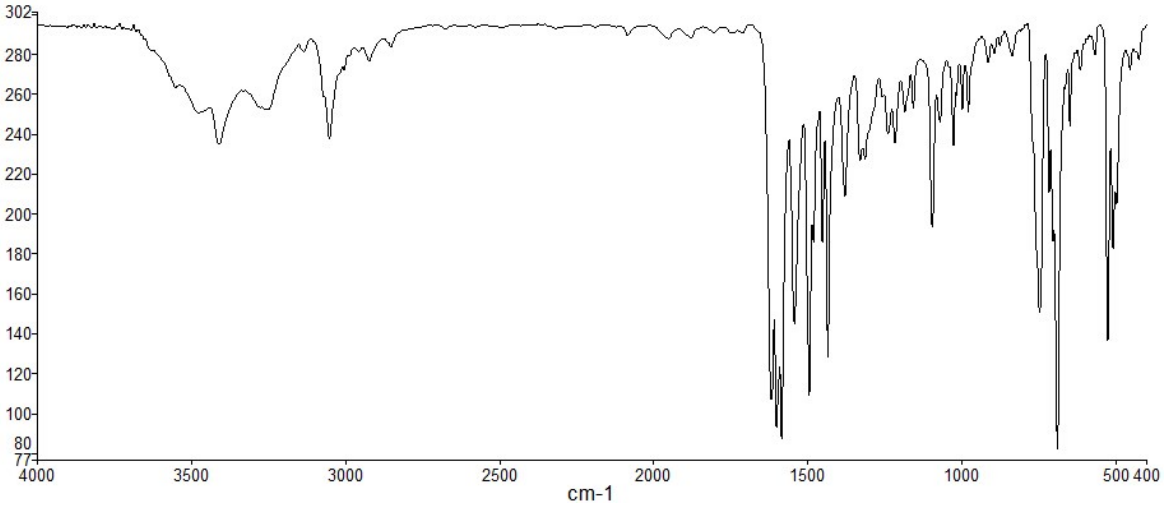


Figure S32. IR spectrum of **7**.

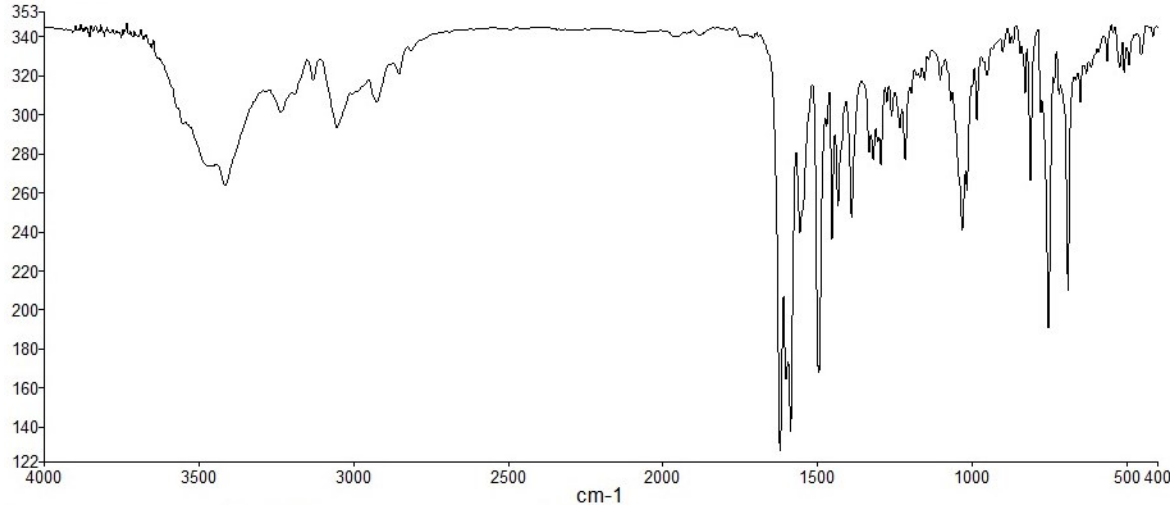


Figure S33. IR spectrum of **8**.

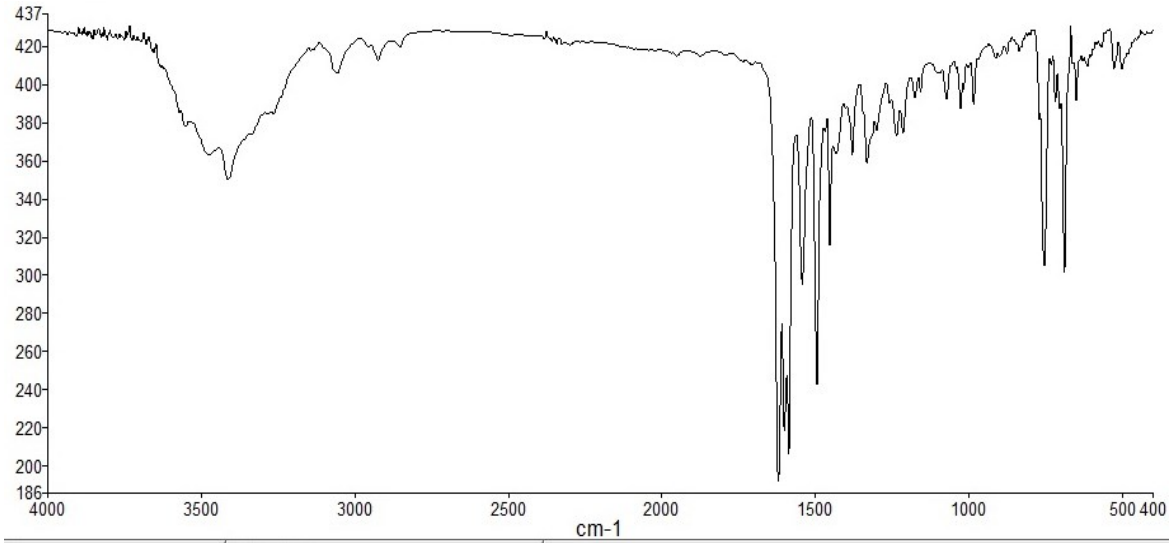


Figure S34. IR spectrum of **9**.

Table S1. Crystal data and structure refinement parameters for **1-4** and **6.**

	1	**3**	**4**	**2**	**6**
Empirical formula	$C_{30}H_{29}ClN_4Ru$	$C_{30}H_{30}ClN_4Ir$	$C_{30}H_{32}Cl_3N_4Ir$	$C_{91}H_{92}Cl_5N_{12}Rh_3$	$C_{25}H_{21}Br_2N_5Pd$
Formula weight	582.09	674.23	747.14	1839.74	657.69
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1	P-1
*a (*Å)	9.6026 (9)	13.700 (3)	9.9976 (9)	13.6235 (10)	9.6188 (11)
*b (*Å)	12.3020 (13)	15.904 (4)	11.8767 (12)	15.9331 (13)	11.9263 (14)
*c (*Å)	13.6024 (15)	21.409 (6)	13.6237 (14)	21.3560 (18)	12.2365 (13)
*α (*º)	100.477 (5)	69.083 (12)	98.645 (4)	69.077 (3)	77.662 (4)
*β (*º)	109.614 (4)	83.451 (12)	96.039 (5)	83.636 (4)	71.146 (5)
*γ (*º)	110.590 (5)	88.890 (13)	110.163 (4)	88.592 (3)	69.041 (4)
*V (*Å^3)	1332.5 (2)	4328 (2)	1479.6 (3)	4302.7 (6)	1232.9 (2)
Z	2	6	2	2	2
D_C (g cm^{-3})	1.451	1.552	1.677	1.420	1.772
μ (mm^{-1})	0.71	4.74	4.81	0.78	4.02
θ range (º)	2.9-28.3	2.9-26.6	2.9-26.4	2.9-26.5	3.3-28.4
Measured refls.	44857	94400	39096	62298	38069
Independent refls.	6549	16019	5978	15757	4647
R_{int}	0.079	0.100	0.084	0.100	0.053
S	1.11	1.13	1.19	1.12	1.23
R1/wR2	0.078/0.176	0.076/0.163	0.058/0.105	0.099/0.240	0.086/0.196
Δρmax/Δρmin (eÅ^{-3})	0.66/-0.71	1.77/-2.98	1.11/-0.87	0.94/-3.15	0.64/-0.82

Cartesian

Cat-PhBr-complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.810423	1.228815	-0.000002
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3	6	0	-2.927175	-0.000010	-0.000010
4	6	0	-2.221075	-1.219615	0.000002
5	6	0	-0.810410	-1.228809	0.000004
6	6	0	-0.130077	0.000017	-0.000008
7	1	0	-0.267772	2.168955	0.000006
8	1	0	-2.757888	2.164464	0.000011
9	1	0	-4.013695	-0.000037	-0.000003
10	1	0	-2.757867	-2.164473	0.000003
11	1	0	-0.267709	-2.168921	0.000013
12	35	0	1.851044	0.000001	0.000000

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.922625	2.348823	0.327553
2	7	0	2.298105	2.617362	0.569395
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4	7	0	1.892595	0.412604	0.428322
5	6	0	0.618040	0.993289	0.219690
6	7	0	4.186357	1.205825	0.948627
7	6	0	5.115875	0.464908	0.166929

8	6	0	6.378831	0.165965	0.729386
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10	6	0	7.045353	-0.959329	-1.337091
11	6	0	5.785145	-0.660877	-1.891981
12	6	0	4.823568	0.052531	-1.152912
13	6	0	0.040333	3.474243	0.256762
14	6	0	2.121253	-1.004301	0.571788
15	6	0	2.587221	-1.505882	1.802027
16	6	0	2.809312	-2.888168	1.947341
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21	6	0	-2.127470	4.451901	-0.269825
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25	46	0	-1.144126	0.011295	-0.000124
26	7	0	-2.622910	-0.683313	1.545639
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63	1	0	-1.308480	1.473705	-3.612486
64	35	0	-2.263084	-2.998500	-1.352195

İnt01

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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23	6	0	-0.738698	5.731805	0.110362

24	6	0	0.174204	4.672194	0.256627
25	46	0	-1.243677	-0.170373	-0.315862
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27	6	0	-1.012159	-0.387050	2.804623
28	6	0	-1.360992	-0.285392	4.160783
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40	1	0	2.772091	-4.766845	0.808842
41	1	0	1.801928	-3.938612	-1.341251
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43	1	0	-1.648646	2.189857	-1.251072
44	1	0	-3.260102	4.069555	-1.496702
45	1	0	-2.685725	6.344904	-0.627916
46	1	0	-0.476630	6.716654	0.487834
47	1	0	1.132306	4.829385	0.737427
48	1	0	-2.914348	0.338601	5.545742
49	1	0	-4.463933	1.070208	3.689956
50	1	0	-3.711691	0.812368	1.318345
51	1	0	-0.051040	-0.785736	2.501995
52	1	0	-0.659956	-0.613583	4.921039
53	6	0	-1.982881	-1.207694	-2.359825
54	6	0	-2.800140	-1.124867	-1.179378
55	6	0	-4.129335	-0.610903	-1.258956
56	6	0	-4.585505	-0.087813	-2.474947

57	6	0	-3.766499	-0.112978	-3.641370
58	6	0	-2.486277	-0.674989	-3.585495
59	1	0	-1.089267	-1.825807	-2.378791
60	1	0	-4.768014	-0.601587	-0.380533
61	1	0	-5.578693	0.354159	-2.524332
62	1	0	-4.151406	0.281562	-4.578396
63	1	0	-1.881245	-0.757263	-4.486355
64	35	0	-2.829247	-3.280977	0.028077

İnt02

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.568010	2.206211	-0.034096
2	7	0	1.918229	2.528555	0.255994
3	6	0	2.509696	1.342179	0.367791
4	7	0	1.574863	0.309777	0.147541
5	6	0	0.324586	0.864854	-0.116839
6	7	0	3.835504	1.176396	0.719280
7	6	0	4.804092	0.425893	-0.008418
8	6	0	6.050113	0.168892	0.607632
9	6	0	7.044722	-0.540275	-0.087384
10	6	0	6.805856	-1.013784	-1.394436
11	6	0	5.561026	-0.756879	-2.002335
12	6	0	4.563237	-0.034629	-1.322118
13	6	0	-0.363435	3.285615	-0.220779
14	6	0	1.817449	-1.111794	0.244111
15	6	0	2.436667	-1.638519	1.392181
16	6	0	2.659138	-3.025397	1.477461
17	6	0	2.255289	-3.875885	0.428376

18	6	0	1.625689	-3.334726	-0.710852
19	6	0	1.405774	-1.948769	-0.809330
20	6	0	-1.398227	3.156386	-1.168176
21	6	0	-2.302770	4.221695	-1.334392
22	6	0	-2.166176	5.405151	-0.580816
23	6	0	-1.112990	5.523499	0.349180
24	6	0	-0.206150	4.464106	0.533832
25	46	0	-1.485773	-0.198556	-0.510189
26	7	0	-1.816520	-0.507432	1.535509
27	6	0	-1.888791	-1.766784	2.050759
28	6	0	-2.096594	-2.000380	3.418345
29	6	0	-2.247624	-0.902864	4.286607
30	6	0	-2.179861	0.397243	3.750374
31	6	0	-1.959206	0.557479	2.374795
32	1	0	4.190797	1.848477	1.391343
33	1	0	6.234033	0.519866	1.620391
34	1	0	8.001133	-0.728167	0.394046
35	1	0	7.574371	-1.566528	-1.927568
36	1	0	5.366441	-1.107160	-3.012934
37	1	0	3.622025	0.180988	-1.819536
38	1	0	2.736171	-0.981870	2.203182
39	1	0	3.138199	-3.438187	2.361031
40	1	0	2.427258	-4.946605	0.498989
41	1	0	1.309864	-3.986520	-1.520919
42	1	0	0.920641	-1.518456	-1.680332
43	1	0	-1.476123	2.247474	-1.761780
44	1	0	-3.105015	4.130802	-2.062301
45	1	0	-2.865495	6.225345	-0.719785
46	1	0	-0.998669	6.434154	0.931085
47	1	0	0.606116	4.545226	1.248279
48	1	0	-2.414172	-1.055626	5.348533
49	1	0	-2.292485	1.274106	4.378814
50	1	0	-1.896793	1.541540	1.926312

51	1	0	-1.782081	-2.582695	1.347527
52	1	0	-2.141495	-3.020359	3.784758
53	6	0	-3.163827	-2.295860	-1.920247
54	6	0	-3.188564	-1.241525	-0.965924
55	6	0	-4.440896	-0.953738	-0.357674
56	6	0	-5.610234	-1.673151	-0.688775
57	6	0	-5.558302	-2.719530	-1.633573
58	6	0	-4.326844	-3.030228	-2.245411
59	1	0	-2.228967	-2.562147	-2.412288
60	1	0	-4.514212	-0.159133	0.383665
61	1	0	-6.554903	-1.420315	-0.209161
62	1	0	-6.456336	-3.279800	-1.885524
63	1	0	-4.270263	-3.838487	-2.973333
64	8	0	-1.168720	0.122386	-2.502588
65	1	0	-1.912339	-0.285601	-2.996477

İnt02-PhHOBOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.941876	-0.815860	1.993113
2	7	0	-2.193636	-1.425268	2.264392
3	6	0	-2.976066	-0.992385	1.279254
4	7	0	-2.247990	-0.150528	0.413943
5	6	0	-0.935160	-0.041562	0.867996
6	7	0	-4.322508	-1.286056	1.184695
7	6	0	-4.980048	-1.838768	0.047324
8	6	0	-6.393455	-1.863259	0.039884
9	6	0	-7.080872	-2.426876	-1.048725
10	6	0	-6.371870	-2.958074	-2.146373
11	6	0	-4.963354	-2.929376	-2.134045

12	6	0	-4.264052	-2.381860	-1.042715
13	6	0	0.147979	-1.073631	2.894652
14	6	0	-2.765515	0.571200	-0.726339
15	6	0	-3.906367	1.380884	-0.579533
16	6	0	-4.394765	2.087869	-1.693891
17	6	0	-3.740615	1.991747	-2.938891
18	6	0	-2.592680	1.183903	-3.068140
19	6	0	-2.101165	0.467217	-1.961979
20	6	0	1.459128	-1.183081	2.390283
21	6	0	2.514006	-1.418968	3.292066
22	6	0	2.262251	-1.567903	4.671089
23	6	0	0.940556	-1.479435	5.153437
24	6	0	-0.123272	-1.230649	4.267290
25	46	0	0.639526	1.078861	-0.046658
26	7	0	-0.042126	2.865100	0.809757
27	6	0	-0.399061	3.923666	0.029166
28	6	0	-0.873874	5.125150	0.575908
29	6	0	-0.974749	5.250135	1.974247
30	6	0	-0.597691	4.158002	2.778817
31	6	0	-0.141294	2.982945	2.164442
32	1	0	-4.810594	-1.355900	2.071530
33	1	0	-6.945234	-1.442965	0.877499
34	1	0	-8.167815	-2.444418	-1.041865
35	1	0	-6.905705	-3.387928	-2.989327
36	1	0	-4.403402	-3.343893	-2.968590
37	1	0	-3.178061	-2.397585	-1.037954
38	1	0	-4.400672	1.460929	0.383848
39	1	0	-5.276230	2.714163	-1.587334
40	1	0	-4.119845	2.540825	-3.796606
41	1	0	-2.084013	1.107790	-4.025322
42	1	0	-1.219145	-0.160064	-2.047991
43	1	0	1.633956	-1.087417	1.319864
44	1	0	3.530726	-1.495247	2.915169

45	1	0	3.082360	-1.755322	5.359055
46	1	0	0.737659	-1.597518	6.214466
47	1	0	-1.143037	-1.155410	4.629440
48	1	0	-1.334870	6.170532	2.423641
49	1	0	-0.655008	4.207217	3.860889
50	1	0	0.153878	2.121025	2.750303
51	1	0	-0.293754	3.792145	-1.040049
52	1	0	-1.151873	5.939017	-0.085152
53	6	0	2.377222	1.911419	-2.387389
54	6	0	2.152979	2.080324	-0.993369
55	6	0	3.027182	2.963135	-0.302862
56	6	0	4.076181	3.637828	-0.965382
57	6	0	4.274069	3.458900	-2.350714
58	6	0	3.415722	2.594182	-3.059949
59	1	0	1.732957	1.248974	-2.964246
60	1	0	2.894952	3.131945	0.765082
61	1	0	4.732362	4.301413	-0.403752
62	1	0	5.077534	3.982281	-2.864904
63	1	0	3.553976	2.448924	-4.130533
64	8	0	1.305693	-0.673980	-0.862522
65	1	0	2.124949	-0.499815	-1.374006
66	6	0	5.999455	-2.527361	0.030496
67	6	0	4.696130	-3.056958	0.093077
68	6	0	3.868624	-3.118604	-1.058800
69	6	0	4.403882	-2.634762	-2.281701
70	6	0	5.703542	-2.099825	-2.350875
71	6	0	6.505079	-2.044676	-1.192753
72	1	0	6.615886	-2.492490	0.925565
73	1	0	4.337213	-3.432127	1.050379
74	1	0	3.792710	-2.680383	-3.179462
75	1	0	6.091186	-1.731042	-3.297685
76	1	0	7.510962	-1.634307	-1.243202
77	5	0	2.424540	-3.710455	-1.012940

78	8	0	1.770845	-3.960175	-2.210388
79	1	0	0.862019	-4.313584	-2.162070
80	8	0	1.761183	-4.078400	0.151647
81	1	0	2.129863	-3.849330	1.023084

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.850413	-0.814728	2.087268
2	7	0	-2.129576	-1.379392	2.324883
3	6	0	-2.863083	-0.946371	1.303937
4	7	0	-2.079741	-0.147872	0.446535
5	6	0	-0.778736	-0.069881	0.943600
6	7	0	-4.213512	-1.201676	1.168801
7	6	0	-4.851260	-1.752064	0.019030
8	6	0	-6.263721	-1.732137	-0.033709
9	6	0	-6.933862	-2.291860	-1.134991
10	6	0	-6.207613	-2.863330	-2.200640
11	6	0	-4.800043	-2.879150	-2.143049
12	6	0	-4.118626	-2.335825	-1.038364
13	6	0	0.187410	-1.082714	3.047093
14	6	0	-2.546576	0.578489	-0.712810
15	6	0	-3.659574	1.430852	-0.595050
16	6	0	-4.101097	2.145576	-1.723656
17	6	0	-3.428189	2.015495	-2.955396
18	6	0	-2.309752	1.163832	-3.056816
19	6	0	-1.866947	0.438734	-1.935807

20	6	0	1.528983	-1.172563	2.626172
21	6	0	2.525227	-1.430480	3.586615
22	6	0	2.189286	-1.614130	4.943037
23	6	0	0.839345	-1.538164	5.342235
24	6	0	-0.167694	-1.272440	4.396926
25	46	0	0.829610	1.043131	0.069231
26	7	0	-0.047465	2.844944	0.671254
27	6	0	-0.445400	3.766583	-0.249860
28	6	0	-1.028434	4.986378	0.123580
29	6	0	-1.200852	5.274239	1.490603
30	6	0	-0.784750	4.321454	2.439901
31	6	0	-0.216876	3.118586	1.995637
32	1	0	-4.732276	-1.241864	2.039947
33	1	0	-6.828189	-1.280642	0.778795
34	1	0	-8.020468	-2.275121	-1.163004
35	1	0	-6.727814	-3.290047	-3.053635
36	1	0	-4.227470	-3.325368	-2.952297
37	1	0	-3.034455	-2.386684	-0.997629
38	1	0	-4.169103	1.537838	0.357723
39	1	0	-4.960583	2.804749	-1.638126
40	1	0	-3.770563	2.571096	-3.824259
41	1	0	-1.786995	1.059316	-4.003577
42	1	0	-1.011527	-0.224677	-2.005944
43	1	0	1.778452	-1.041652	1.573717
44	1	0	3.563116	-1.498739	3.270225
45	1	0	2.964939	-1.818126	5.676353
46	1	0	0.569663	-1.681354	6.385225
47	1	0	-1.208046	-1.210730	4.696606
48	1	0	-1.645265	6.212946	1.806985
49	1	0	-0.895658	4.498663	3.504264
50	1	0	0.111380	2.359339	2.694916
51	1	0	-0.286124	3.510061	-1.289378
52	1	0	-1.334048	5.689081	-0.644143

53	6	0	2.688112	1.875926	-2.176665
54	6	0	2.359105	2.081370	-0.809272
55	6	0	3.139539	3.026424	-0.090755
56	6	0	4.202688	3.726447	-0.702499
57	6	0	4.507432	3.510060	-2.062811
58	6	0	3.741484	2.583409	-2.798942
59	1	0	2.116273	1.165845	-2.772666
60	1	0	2.922459	3.225081	0.958108
61	1	0	4.786413	4.438931	-0.121279
62	1	0	5.322148	4.052601	-2.537847
63	1	0	3.962859	2.408915	-3.850947
64	8	0	1.751502	-0.700629	-0.516410
65	1	0	2.579174	-0.460301	-0.984344
66	6	0	5.510181	-3.467160	-0.305558
67	6	0	4.106705	-3.458686	-0.182104
68	6	0	3.270828	-3.058126	-1.256621
69	6	0	3.902559	-2.679905	-2.470509
70	6	0	5.304400	-2.683648	-2.602452
71	6	0	6.113732	-3.076646	-1.517393
72	1	0	6.127787	-3.778268	0.534009
73	1	0	3.669246	-3.772485	0.764874
74	1	0	3.285863	-2.383376	-3.315602
75	1	0	5.763676	-2.385770	-3.542540
76	1	0	7.196986	-3.081778	-1.615438
77	5	0	1.704377	-3.063991	-1.140981
78	8	0	0.965538	-3.009547	-2.326035
79	1	0	-0.005021	-3.052791	-2.229527
80	8	0	1.007044	-3.484580	-0.002174
81	1	0	1.427909	-3.391109	0.870645

İnt03

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.637823	-0.032132	2.243009
2	7	0	1.982079	0.131072	2.660364
3	6	0	2.688818	-0.236402	1.596531
4	7	0	1.831773	-0.618753	0.548110
5	6	0	0.514508	-0.442323	0.945264
6	7	0	4.069684	-0.257333	1.543535
7	6	0	4.843104	0.476257	0.596490
8	6	0	6.228189	0.210233	0.505811
9	6	0	7.024095	0.936866	-0.397048
10	6	0	6.448685	1.921905	-1.226590
11	6	0	5.066108	2.178959	-1.132166
12	6	0	4.259369	1.470587	-0.222224
13	6	0	-0.400030	0.247988	3.195884
14	6	0	2.233158	-1.202615	-0.712191
15	6	0	3.096382	-2.315140	-0.703934
16	6	0	3.469807	-2.906508	-1.924279
17	6	0	2.971559	-2.396089	-3.140599
18	6	0	2.102370	-1.286986	-3.129707
19	6	0	1.730607	-0.677953	-1.915798
20	6	0	-1.626179	0.794955	2.770831
21	6	0	-2.631929	1.042395	3.723071
22	6	0	-2.412085	0.768887	5.087654
23	6	0	-1.171118	0.242271	5.500871
24	6	0	-0.161321	-0.020930	4.558343
25	46	0	-1.234424	-0.771016	-0.220902
26	7	0	-1.132136	-2.809125	0.096834
27	6	0	-0.782588	-3.648117	-0.917692
28	6	0	-0.698579	-5.035314	-0.731570
29	6	0	-0.989659	-5.577076	0.534651
30	6	0	-1.353150	-4.704348	1.577727

31	6	0	-1.412708	-3.326500	1.325622
32	1	0	4.543362	-0.578334	2.380932
33	1	0	6.673917	-0.557887	1.133650
34	1	0	8.089618	0.728787	-0.456135
35	1	0	7.065181	2.478275	-1.927303
36	1	0	4.612025	2.942249	-1.759606
37	1	0	3.199896	1.704286	-0.141809
38	1	0	3.465519	-2.714145	0.236035
39	1	0	4.135755	-3.765256	-1.923231
40	1	0	3.256695	-2.857665	-4.082413
41	1	0	1.717604	-0.888904	-4.065322
42	1	0	1.078975	0.193224	-1.909774
43	1	0	-1.780824	1.031914	1.723454
44	1	0	-3.580733	1.461766	3.398454
45	1	0	-3.191687	0.967824	5.818019
46	1	0	-0.990340	0.032030	6.551638
47	1	0	0.793807	-0.430931	4.867945
48	1	0	-0.935801	-6.648091	0.703422
49	1	0	-1.586400	-5.075421	2.569778
50	1	0	-1.685617	-2.620861	2.100662
51	1	0	-0.575400	-3.191101	-1.876798
52	1	0	-0.414970	-5.668465	-1.565204
53	6	0	-3.023330	-0.659549	-2.676356
54	6	0	-2.941444	-1.064320	-1.318280
55	6	0	-4.096866	-1.649789	-0.737862
56	6	0	-5.287798	-1.816607	-1.477870
57	6	0	-5.348715	-1.410090	-2.827352
58	6	0	-4.209890	-0.833627	-3.424836
59	1	0	-2.161484	-0.211180	-3.167457
60	1	0	-4.077381	-1.981967	0.299435
61	1	0	-6.160699	-2.263282	-1.004436
62	1	0	-6.263964	-1.541287	-3.400568
63	1	0	-4.242530	-0.518171	-4.466501

64	8	0	-1.480367	1.291164	-0.568156
65	1	0	-2.332509	1.428561	-1.024825
66	6	0	-2.675096	5.438014	0.429276
67	6	0	-2.001643	4.203027	0.336596
68	6	0	-1.269354	3.828343	-0.823736
69	6	0	-1.258585	4.757520	-1.895433
70	6	0	-1.926865	5.997758	-1.816887
71	6	0	-2.638963	6.344156	-0.650806
72	1	0	-3.225238	5.691334	1.333737
73	1	0	-2.050864	3.518204	1.182937
74	1	0	-0.721923	4.502629	-2.807745
75	1	0	-1.895289	6.687075	-2.658890
76	1	0	-3.157555	7.298475	-0.585510
77	5	0	-0.450629	2.421452	-0.905666
78	8	0	0.072912	2.103036	-2.255365
79	1	0	0.894410	2.582240	-2.474647
80	8	0	0.674494	2.354267	0.056807
81	1	0	0.527005	2.840704	0.890183

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.925681	1.899398	-0.978625
2	7	0	2.240884	2.374252	-0.771506
3	6	0	2.850771	1.372124	-0.147291
4	7	0	1.961136	0.291977	0.021536
5	6	0	0.710366	0.625766	-0.512412
6	7	0	4.143947	1.440335	0.330853
7	6	0	5.195747	0.522124	0.039294
8	6	0	6.375573	0.589781	0.814384

9	6	0	7.450705	-0.270711	0.533256
10	6	0	7.357793	-1.215476	-0.510148
11	6	0	6.178231	-1.279361	-1.277803
12	6	0	5.101666	-0.412208	-1.015373
13	6	0	-0.010896	2.800824	-1.597588
14	6	0	2.271544	-0.927304	0.740041
15	6	0	2.640454	-0.840855	2.095712
16	6	0	2.968387	-2.014667	2.796857
17	6	0	2.924100	-3.264424	2.146144
18	6	0	2.555027	-3.335496	0.788448
19	6	0	2.230801	-2.165380	0.076445
20	6	0	-1.094189	2.303277	-2.345456
21	6	0	-1.998829	3.215842	-2.920447
22	6	0	-1.821364	4.604956	-2.765819
23	6	0	-0.719730	5.085987	-2.029356
24	6	0	0.189385	4.187884	-1.443624
25	46	0	-1.303330	-0.108929	0.094915
26	7	0	-1.074104	1.405404	1.616065
27	6	0	-0.430293	1.094638	2.774232
28	6	0	-0.304365	2.015607	3.824831
29	6	0	-0.862043	3.300137	3.678303
30	6	0	-1.531739	3.614975	2.481059
31	6	0	-1.621103	2.642721	1.472988
32	1	0	4.420360	2.346547	0.694773
33	1	0	6.446320	1.307380	1.628272
34	1	0	8.355580	-0.207524	1.132386
35	1	0	8.188225	-1.883161	-0.722046
36	1	0	6.096597	-1.995320	-2.091753
37	1	0	4.214605	-0.451368	-1.641069
38	1	0	2.678418	0.124557	2.591248
39	1	0	3.253964	-1.952929	3.843234
40	1	0	3.177629	-4.170377	2.689958
41	1	0	2.523417	-4.296266	0.281828

42	1	0	1.956144	-2.212760	-0.972970
43	1	0	-1.231790	1.239851	-2.518134
44	1	0	-2.835454	2.835712	-3.501010
45	1	0	-2.523729	5.300715	-3.217002
46	1	0	-0.568342	6.155179	-1.907523
47	1	0	1.036818	4.551043	-0.873536
48	1	0	-0.780301	4.032725	4.475467
49	1	0	-1.980472	4.590014	2.324640
50	1	0	-2.136651	2.841798	0.542114
51	1	0	-0.024620	0.093431	2.852025
52	1	0	0.216260	1.725714	4.731221
53	6	0	-3.275042	-1.239061	2.086537
54	6	0	-3.122770	-0.378249	0.974386
55	6	0	-4.230997	0.407408	0.577256
56	6	0	-5.461958	0.328667	1.264865
57	6	0	-5.605067	-0.538226	2.368433
58	6	0	-4.504628	-1.320126	2.777091
59	1	0	-2.442994	-1.856532	2.419371
60	1	0	-4.148689	1.078998	-0.276290
61	1	0	-6.302403	0.939351	0.938502
62	1	0	-6.552537	-0.601442	2.899311
63	1	0	-4.600397	-1.990373	3.630098
64	6	0	-1.837635	-1.912814	-1.138748
65	6	0	-3.241191	-2.044446	-1.402572
66	1	0	-3.750616	-1.232527	-1.917625
67	5	0	-1.009680	-1.647379	-2.895642
68	8	0	0.389232	-1.382349	-2.654068
69	1	0	0.516209	-0.689672	-1.971508
70	8	0	-1.225023	-2.907786	-3.587641
71	1	0	-0.690247	-3.651903	-3.252412
72	6	0	-1.244176	-3.013464	-0.435255
73	6	0	-3.975219	-3.194448	-1.072578
74	6	0	-3.336782	-4.261167	-0.404209

75	1	0	-3.898379	-5.156483	-0.144101
76	6	0	-1.968328	-4.164231	-0.073024
77	1	0	-1.475885	-4.981803	0.449830
78	1	0	-5.032137	-3.263864	-1.322018
79	1	0	-0.182520	-2.981055	-0.207759
80	8	0	-1.734430	-0.571383	-3.548463
81	1	0	-2.555085	-0.851040	-3.995446

İnt04

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.631686	2.196200	-0.530125
2	7	0	-2.001836	2.489520	-0.758280
3	6	0	-2.595799	1.303982	-0.712479
4	7	0	-1.651802	0.295260	-0.439272
5	6	0	-0.385266	0.865833	-0.299153
6	7	0	-3.935439	1.109310	-0.980198
7	6	0	-4.859765	0.391763	-0.165413
8	6	0	-6.117535	0.057559	-0.716893
9	6	0	-7.069928	-0.618447	0.064967
10	6	0	-6.775916	-0.982132	1.395814
11	6	0	-5.519646	-0.648440	1.939184
12	6	0	-4.564311	0.042207	1.170939
13	6	0	0.289516	3.302116	-0.587633
14	6	0	-1.910452	-1.128775	-0.460125
15	6	0	-2.451715	-1.706529	-1.623435
16	6	0	-2.703970	-3.090452	-1.652160
17	6	0	-2.407960	-3.888931	-0.528804
18	6	0	-1.860677	-3.297370	0.627542
19	6	0	-1.612834	-1.912865	0.667444

20	6	0	1.680711	3.093109	-0.498259
21	6	0	2.554019	4.190610	-0.576041
22	6	0	2.053630	5.496772	-0.744791
23	6	0	0.661701	5.695158	-0.832657
24	6	0	-0.223413	4.604881	-0.756822
25	46	0	1.399600	-0.201440	0.137596
26	7	0	1.629984	-0.718371	-1.988427
27	6	0	1.631361	-2.032577	-2.342697
28	6	0	1.747539	-2.449593	-3.677939
29	6	0	1.880744	-1.477726	-4.687834
30	6	0	1.886353	-0.118487	-4.320959
31	6	0	1.754151	0.221501	-2.965219
32	1	0	-4.330278	1.736974	-1.672873
33	1	0	-6.343485	0.323558	-1.746809
34	1	0	-8.036048	-0.866720	-0.367132
35	1	0	-7.511734	-1.509863	1.996186
36	1	0	-5.283344	-0.913895	2.966565
37	1	0	-3.613523	0.319933	1.616552
38	1	0	-2.669760	-1.089174	-2.489962
39	1	0	-3.122685	-3.541414	-2.547712
40	1	0	-2.602089	-4.957896	-0.554541
41	1	0	-1.631548	-3.908114	1.496663
42	1	0	-1.196565	-1.449180	1.554902
43	1	0	2.070960	2.088106	-0.350980
44	1	0	3.625291	4.021472	-0.504985
45	1	0	2.733933	6.341719	-0.805912
46	1	0	0.260643	6.697145	-0.960445
47	1	0	-1.293209	4.755997	-0.825958
48	1	0	1.977636	-1.770400	-5.729050
49	1	0	1.987194	0.666225	-5.063258
50	1	0	1.745086	1.258342	-2.650811
51	1	0	1.547827	-2.749062	-1.534820
52	1	0	1.739058	-3.508903	-3.912007

53	6	0	3.080909	-2.646665	0.845510
54	6	0	3.114294	-1.249588	0.582224
55	6	0	4.399396	-0.640130	0.558669
56	6	0	5.582645	-1.379846	0.783168
57	6	0	5.518419	-2.765735	1.038256
58	6	0	4.257199	-3.396627	1.067023
59	1	0	2.124407	-3.168773	0.885583
60	1	0	4.488210	0.429202	0.366352
61	1	0	6.548162	-0.875675	0.759178
62	1	0	6.427241	-3.338618	1.211605
63	1	0	4.188979	-4.466063	1.263665
64	6	0	1.213865	0.177154	2.147597
65	6	0	1.198477	1.496974	2.675303
66	6	0	1.038350	-0.880489	3.082558
67	6	0	1.018559	1.748616	4.054391
68	1	0	1.327892	2.350015	2.013174
69	6	0	0.845695	-0.637496	4.459960
70	1	0	1.063952	-1.912848	2.739469
71	6	0	0.836812	0.682107	4.957782
72	1	0	1.017357	2.775678	4.417693
73	1	0	0.709844	-1.476890	5.140946
74	1	0	0.693494	0.873315	6.019284

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.759546	1.981008	-1.058414
2	7	0	-2.135922	2.243634	-1.294625
3	6	0	-2.735355	1.104231	-0.973025
4	7	0	-1.789557	0.161793	-0.525775

5	6	0	-0.503288	0.725289	-0.550723
6	7	0	-4.088837	0.879671	-1.141318
7	6	0	-4.988106	0.387956	-0.152387
8	6	0	-6.280390	-0.011607	-0.564216
9	6	0	-7.210388	-0.469993	0.384561
10	6	0	-6.861441	-0.550283	1.749015
11	6	0	-5.571735	-0.152597	2.153439
12	6	0	-4.637470	0.322641	1.214679
13	6	0	0.173706	3.029761	-1.361261
14	6	0	-2.056806	-1.224490	-0.219265
15	6	0	-2.675072	-2.036730	-1.188063
16	6	0	-2.927451	-3.389868	-0.895185
17	6	0	-2.552547	-3.927974	0.352421
18	6	0	-1.926190	-3.105633	1.310786
19	6	0	-1.679715	-1.749564	1.029054
20	6	0	1.543596	2.742624	-1.526565
21	6	0	2.438574	3.783081	-1.829867
22	6	0	1.976767	5.105939	-1.980111
23	6	0	0.603455	5.380832	-1.822170
24	6	0	-0.301454	4.348934	-1.514715
25	46	0	1.313049	-0.170599	0.130370
26	7	0	1.694599	-1.422636	-1.807250
27	6	0	2.619542	-2.422234	-1.796650
28	6	0	2.921387	-3.185245	-2.937745
29	6	0	2.249219	-2.905991	-4.143254
30	6	0	1.294025	-1.871196	-4.159296
31	6	0	1.045005	-1.158533	-2.974378
32	1	0	-4.503676	1.338939	-1.945299
33	1	0	-6.549628	0.035155	-1.616876
34	1	0	-8.202735	-0.770123	0.057317
35	1	0	-7.580381	-0.910319	2.479702
36	1	0	-5.292056	-0.199393	3.202971
37	1	0	-3.659735	0.656046	1.550094

38	1	0	-2.951558	-1.621158	-2.152571
39	1	0	-3.406353	-4.019714	-1.639963
40	1	0	-2.745603	-4.974129	0.574498
41	1	0	-1.635957	-3.514970	2.274693
42	1	0	-1.206757	-1.106200	1.762906
43	1	0	1.898367	1.722468	-1.408687
44	1	0	3.494323	3.556853	-1.955487
45	1	0	2.672531	5.906135	-2.217593
46	1	0	0.234289	6.396788	-1.935836
47	1	0	-1.357871	4.556434	-1.394063
48	1	0	2.462832	-3.476838	-5.042247
49	1	0	0.750760	-1.618717	-5.064236
50	1	0	0.314054	-0.358123	-2.947900
51	1	0	3.117045	-2.605698	-0.850373
52	1	0	3.664230	-3.974134	-2.876908
53	6	0	2.975262	-2.052914	1.803094
54	6	0	2.984702	-0.730610	1.263621
55	6	0	4.249082	-0.220853	0.837676
56	6	0	5.422405	-0.991980	0.921043
57	6	0	5.385274	-2.301733	1.449510
58	6	0	4.149524	-2.823895	1.890127
59	1	0	2.042116	-2.482121	2.162735
60	1	0	4.315264	0.790727	0.441888
61	1	0	6.365819	-0.572783	0.575229
62	1	0	6.293421	-2.895720	1.519813
63	1	0	4.100410	-3.831592	2.299289
64	6	0	1.792909	0.531721	2.062400
65	6	0	2.273091	1.874784	2.165546
66	6	0	1.044123	0.039011	3.175743
67	6	0	1.994891	2.676667	3.286818
68	1	0	2.866721	2.297135	1.357718
69	6	0	0.767063	0.840907	4.297406
70	1	0	0.687477	-0.988953	3.172031

71	6	0	1.235577	2.171242	4.365387
72	1	0	2.368640	3.699034	3.318415
73	1	0	0.185147	0.426926	5.119488
74	1	0	1.022842	2.791113	5.233196

Ph-Ph_lin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.210930	1.491197
2	6	0	0.000000	0.000000	0.750279
3	6	0	0.000000	-1.210930	1.491197
4	6	0	0.000000	-1.213033	2.897154
5	6	0	0.000000	0.000000	3.613275
6	6	0	0.000000	1.213033	2.897154
7	1	0	0.000000	2.169215	0.982474
8	1	0	0.000000	-2.169215	0.982474
9	1	0	0.000000	-2.160548	3.430642
10	1	0	0.000000	0.000000	4.700317
11	1	0	0.000000	2.160548	3.430642
12	6	0	0.000000	0.000000	-0.750279
13	6	0	0.000000	1.210930	-1.491197
14	6	0	0.000000	-1.210930	-1.491197
15	6	0	0.000000	1.213033	-2.897154
16	1	0	0.000000	2.169215	-0.982474
17	6	0	0.000000	-1.213033	-2.897154
18	1	0	0.000000	-2.169215	-0.982474
19	6	0	0.000000	0.000000	-3.613275
20	1	0	0.000000	2.160548	-3.430642
21	1	0	0.000000	-2.160548	-3.430642
22	1	0	0.000000	0.000000	-4.700317

Cat-Pd0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.060561	2.109584	-0.168455
2	7	0	-1.417790	2.495711	-0.313860
3	6	0	-2.071090	1.346710	-0.424834
4	7	0	-1.181164	0.262921	-0.337560
5	6	0	0.136383	0.737731	-0.165554
6	7	0	-3.430498	1.265310	-0.669272
7	6	0	-4.376550	0.518582	0.087980
8	6	0	-5.682386	0.370021	-0.434118
9	6	0	-6.656369	-0.332425	0.295830
10	6	0	-6.340105	-0.906658	1.544936
11	6	0	-5.037099	-0.757055	2.059698
12	6	0	-4.057667	-0.043256	1.344616
13	6	0	0.910745	3.161759	-0.065562
14	6	0	-1.521116	-1.127163	-0.528474
15	6	0	-2.173259	-1.522563	-1.710908
16	6	0	-2.495602	-2.879462	-1.902572
17	6	0	-2.158731	-3.834290	-0.922377
18	6	0	-1.499835	-3.426969	0.255839
19	6	0	-1.181179	-2.071679	0.457629
20	6	0	2.199374	2.909654	0.448696
21	6	0	3.132197	3.958655	0.530354
22	6	0	2.788337	5.260693	0.115070

23	6	0	1.493759	5.505407	-0.385617
24	6	0	0.553070	4.463957	-0.476939
25	46	0	1.781778	-0.370749	-0.005980
26	7	0	3.511246	-1.592498	0.122660
27	6	0	3.416158	-2.949791	-0.010680
28	6	0	4.530960	-3.796598	0.085527
29	6	0	5.799332	-3.235308	0.328659
30	6	0	5.903064	-1.837794	0.466474
31	6	0	4.744932	-1.052716	0.357805
32	1	0	-3.802046	1.991494	-1.272540
33	1	0	-5.928095	0.799247	-1.402680
34	1	0	-7.658013	-0.436366	-0.113871
35	1	0	-7.093370	-1.453942	2.104820
36	1	0	-4.781297	-1.185658	3.025537
37	1	0	-3.067974	0.088341	1.772061
38	1	0	-2.420376	-0.785771	-2.469344
39	1	0	-2.999087	-3.187705	-2.814859
40	1	0	-2.405884	-4.881663	-1.074249
41	1	0	-1.238391	-4.158645	1.015547
42	1	0	-0.679038	-1.747669	1.363473
43	1	0	2.459051	1.901509	0.764929
44	1	0	4.124667	3.757444	0.925831
45	1	0	3.512292	6.068269	0.183373
46	1	0	1.213952	6.505112	-0.707921
47	1	0	-0.442218	4.650853	-0.861704
48	1	0	6.679087	-3.866866	0.407849
49	1	0	6.858536	-1.359193	0.654130
50	1	0	4.787765	0.025376	0.456979
51	1	0	2.425023	-3.345811	-0.197754
52	1	0	4.401091	-4.867746	-0.028000

Cat-Pd0_PhBr_cmplx

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.661478	2.320430	-0.965623
2	7	0	2.021140	2.439381	-1.353268
3	6	0	2.672496	1.674490	-0.487153
4	7	0	1.775278	1.070576	0.409536
5	6	0	0.457246	1.476285	0.113804
6	7	0	4.051553	1.570913	-0.450502
7	6	0	4.804768	0.362918	-0.472892
8	6	0	6.189443	0.434309	-0.194601
9	6	0	6.977271	-0.728562	-0.239869
10	6	0	6.395554	-1.976422	-0.547220
11	6	0	5.015104	-2.042243	-0.821227
12	6	0	4.219211	-0.882096	-0.794265
13	6	0	-0.300228	3.082001	-1.711832
14	6	0	2.136373	0.267200	1.553930
15	6	0	3.003964	0.800628	2.524634
16	6	0	3.346635	0.023580	3.647368
17	6	0	2.817604	-1.273674	3.800550
18	6	0	1.945250	-1.795272	2.823302
19	6	0	1.603075	-1.027033	1.695592
20	6	0	-1.673693	2.767415	-1.655875
21	6	0	-2.592857	3.534214	-2.393469
22	6	0	-2.154371	4.605754	-3.196856
23	6	0	-0.778468	4.905464	-3.255069
24	6	0	0.150676	4.149283	-2.518354
25	46	0	-1.188414	0.962419	1.113675
26	7	0	-2.890721	0.467983	2.281403
27	6	0	-2.879312	-0.622852	3.105061
28	6	0	-3.981843	-0.981229	3.895632
29	6	0	-5.146908	-0.191918	3.845767

30	6	0	-5.163468	0.933298	2.999348
31	6	0	-4.024259	1.230367	2.235560
32	1	0	4.551595	2.422151	-0.684536
33	1	0	6.640357	1.391630	0.056454
34	1	0	8.041551	-0.660489	-0.028720
35	1	0	7.005588	-2.874987	-0.576438
36	1	0	4.554977	-2.995507	-1.069304
37	1	0	3.163492	-0.947930	-1.040520
38	1	0	3.399147	1.805518	2.408875
39	1	0	4.015571	0.432841	4.399588
40	1	0	3.081205	-1.870330	4.669859
41	1	0	1.535979	-2.795683	2.935530
42	1	0	0.939438	-1.423295	0.933923
43	1	0	-2.007347	1.942200	-1.030665
44	1	0	-3.650509	3.287492	-2.344407
45	1	0	-2.868894	5.192827	-3.767584
46	1	0	-0.425555	5.728357	-3.871378
47	1	0	1.208291	4.379254	-2.562363
48	1	0	-6.014195	-0.445401	4.447984
49	1	0	-6.037745	1.571755	2.927309
50	1	0	-4.000362	2.088335	1.574062
51	1	0	-1.965553	-1.205238	3.119585
52	1	0	-3.921662	-1.857437	4.532679
53	6	0	-2.563526	-1.835693	-1.340437
54	6	0	-1.972104	-2.933401	-1.984842
55	6	0	-2.700010	-3.788863	-2.828218
56	6	0	-4.072132	-3.529867	-3.029193
57	6	0	-4.691399	-2.434668	-2.393887
58	6	0	-3.936770	-1.592475	-1.553080
59	1	0	-1.987978	-1.178936	-0.689891
60	1	0	-2.223120	-4.632431	-3.317416
61	1	0	-4.646555	-4.184200	-3.679370
62	1	0	-5.748570	-2.240294	-2.552618

63	1	0	-4.407029	-0.745701	-1.059838
64	35	0	-0.043317	-3.291610	-1.695541

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.452103	2.174304	-0.310800
2	7	0	1.769614	2.602407	-0.013794
3	6	0	2.438030	1.466444	0.181369
4	7	0	1.581055	0.363065	-0.000950
5	6	0	0.306064	0.817852	-0.323189
6	7	0	3.756643	1.416360	0.577120
7	6	0	4.787314	0.624711	-0.012421
8	6	0	5.999539	0.474329	0.697811
9	6	0	7.053303	-0.268291	0.137830
10	6	0	6.905928	-0.880172	-1.124501
11	6	0	5.694239	-0.727499	-1.826805
12	6	0	4.638603	0.027713	-1.283518
13	6	0	-0.551935	3.176551	-0.539546
14	6	0	1.887544	-1.031434	0.225092
15	6	0	2.443286	-1.430799	1.454200
16	6	0	2.708718	-2.794355	1.675571
17	6	0	2.408473	-3.748469	0.682051
18	6	0	1.844439	-3.334924	-0.541376
19	6	0	1.586640	-1.972004	-0.776626
20	6	0	-1.641670	2.908929	-1.390741
21	6	0	-2.623006	3.896924	-1.586852
22	6	0	-2.509349	5.150999	-0.954689
23	6	0	-1.403111	5.413307	-0.121345
24	6	0	-0.420812	4.429702	0.090180

25	46	0	-1.434099	-0.423802	-0.561491
26	7	0	-2.077880	-0.257652	1.394767
27	6	0	-1.693315	-1.187162	2.313887
28	6	0	-2.079561	-1.087878	3.657674
29	6	0	-2.884538	-0.006658	4.063511
30	6	0	-3.277642	0.945584	3.104574
31	6	0	-2.858640	0.791626	1.775600
32	1	0	4.055507	2.185707	1.167733
33	1	0	6.111613	0.932150	1.677798
34	1	0	7.983676	-0.374424	0.689877
35	1	0	7.719722	-1.458918	-1.552359
36	1	0	5.571124	-1.184538	-2.805397
37	1	0	3.724949	0.163198	-1.855053
38	1	0	2.658244	-0.695393	2.223416
39	1	0	3.138466	-3.109534	2.622275
40	1	0	2.611561	-4.800959	0.859608
41	1	0	1.613156	-4.065407	-1.311430
42	1	0	1.174558	-1.642886	-1.726806
43	1	0	-1.715171	1.957844	-1.908211
44	1	0	-3.464091	3.690307	-2.242830
45	1	0	-3.266341	5.913679	-1.114584
46	1	0	-1.305215	6.379248	0.366376
47	1	0	0.429963	4.623039	0.733673
48	1	0	-3.197518	0.090541	5.098295
49	1	0	-3.897333	1.794487	3.371277
50	1	0	-3.135711	1.502180	1.007124
51	1	0	-1.077808	-2.003381	1.958458
52	1	0	-1.754020	-1.845831	4.361444
53	6	0	-4.301398	-1.079545	-1.171539
54	6	0	-3.022952	-1.614908	-0.899261
55	6	0	-2.806395	-3.006594	-1.020239
56	6	0	-3.851411	-3.850631	-1.457351
57	6	0	-5.120452	-3.311311	-1.753424

58	6	0	-5.344055	-1.926173	-1.609428
59	1	0	-4.493575	-0.014044	-1.056356
60	1	0	-1.834152	-3.438245	-0.785917
61	1	0	-3.675601	-4.919604	-1.558774
62	1	0	-5.926223	-3.962574	-2.084032
63	1	0	-6.323248	-1.506342	-1.830414
