Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Cooperative Ruthenium Complex Catalyzed Multicomponent Synthesis of Pyrimidines

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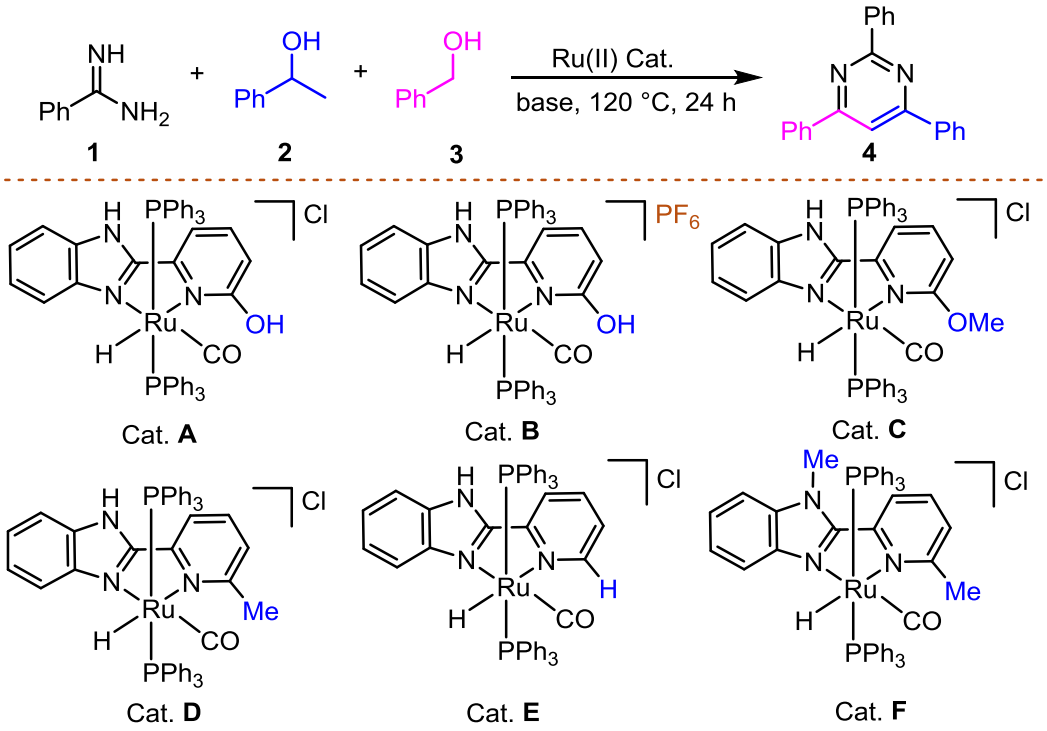
1. Optimization Details

Table S1. Optimization of Reaction Conditions[a]



Entry	Amidine: 1° Alc: 2° Alc	Base (equiv.)	Ru(II) cat	Solvent	Yield (%)[a]
1	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **A**	toluene	61
2	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **A**	*tert*-amyl alcohol	42
3	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **A**	diglyme	21
4	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **A**	dioxane	79
5	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **B**	dioxane	31
6	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **C**	dioxane	43
7	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **D**	dioxane	51
8	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **E**	dioxane	28
9	1:1.3:1.3	KO^{t}Bu (0.5)	Cat. **F**	dioxane	37
10	1:1.3:1.3	KO^{t}Bu (0.5)	$RuHClCO(PPh_3)_3$	dioxane	39
11	1:1.3:1.3	KO^{t}Bu (0.5)	-	dioxane	<10
12	1:1.3:1.3	KOH (0.5)	Cat. **A**	dioxane	41
13	1:1.3:1.3	NaOH (0.5)	Cat. **A**	dioxane	28
14	1:1.3:1.3	Cs_2CO_3 (0.5)	Cat. **A**	dioxane	<10
15	1:1.3:1.3	K_2CO_3 (0.5)	Cat. **A**	dioxane	<10
16	**1:1.3:1.3**	**KO^{t}Bu (1.0)**	**Cat. A**	**dioxane**	**95**
17	1:1.3:1.3	KO^{t}Bu (1.0)	Cat. **A**	dioxane	61[b]
18	1:1.3:1.3	KO^{t}Bu (1.0)	Cat. **A**	dioxane	41[c]
19	1:1:1	KO^{t}Bu (1.0)	Cat. **A**	dioxane	71

[a]Reaction Conditions: benzamidine (0.25 mmol), 1-phenylethanol (0.325 mmol), benzyl alcohol (0.325 mmol), cat **A** (1.0 mol%). The amount (equiv.) of KO^{t}Bu were given with respect to the benzamidine substrate. Yields were determined by ^{1}H-NMR spectroscopy using 1,3,5-trimethoxy benzene as internal standard. [b]Heated for 12 h. [c]Using 0.5 mol% cat. **A**.

2. General Procedure for Synthesis of pyrimidines and Determination of Yield

In a Schlenk tube amidine (0.5 mmol), primary alcohol (0.65 mmol), secondary alcohol (0.65 mmol), cat. A (1.0 mol%), KO^{t}Bu (0.5 mmol) and dioxane (3.0 mL) were taken. The tube was sealed and reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Yield was determined by the analysis of the ^{1}H-NMR spectra of the crude reaction mixture using $CDCl_3$ as NMR solvent. Final products were purified by silica-gel column chromatography using hexane/ethyl acetate as eluent. (**Caution**: *All the catalytic reactions were carried out inside the fume hood and after the reactions Schlenk tubes were carefully opened under proper ventilation to release the hydrogen gas produced in the reactions.*)

After the reaction, it was cooled to room temperature and then 1,3,5-trimethoxy benzene (0.5 equiv. with respect to banzamidine) was added as internal standard. Then the reaction mixture was filtered through a small plug of neutral alumina and small portion was taken for determination of yield. In a typical example, as in Table S1, entry 16, the ^{1}H-NMR spectra of the crude reaction mixture is shown below.

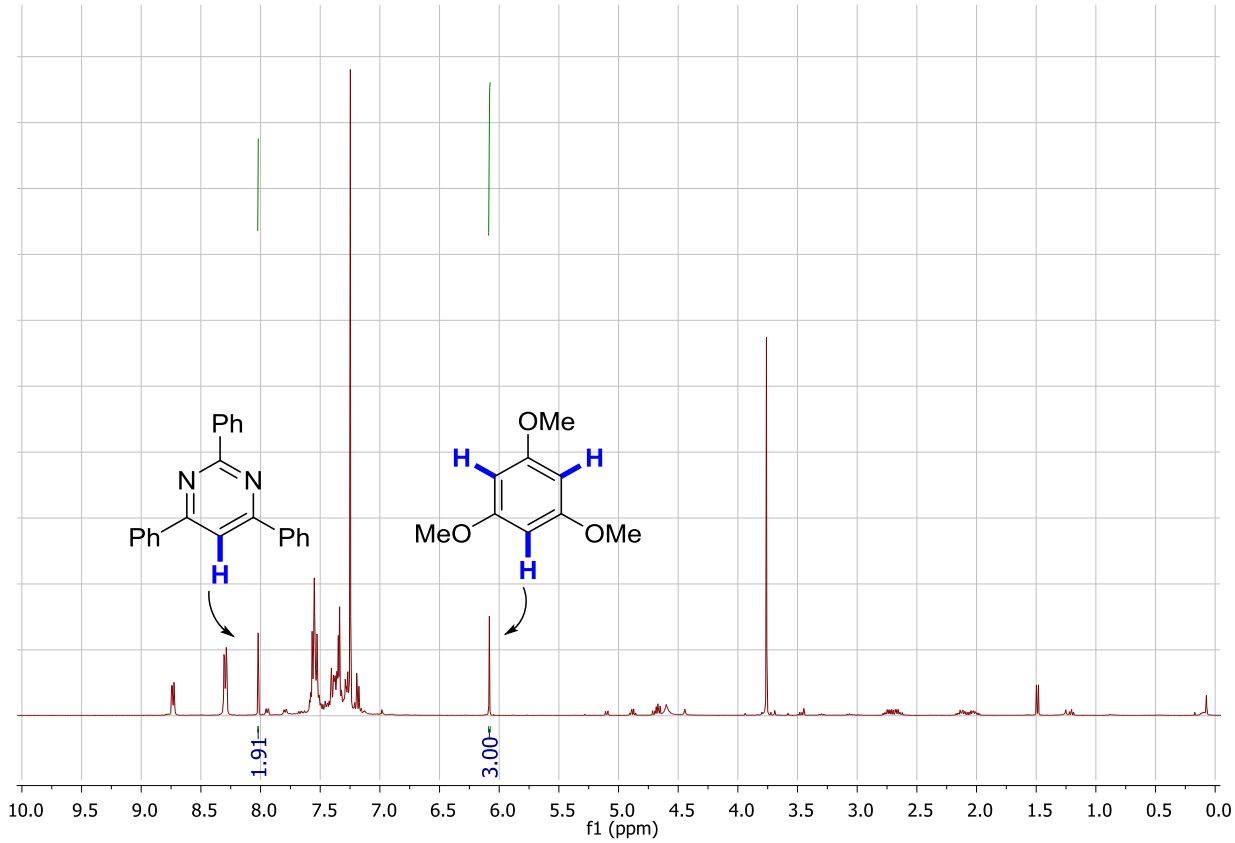
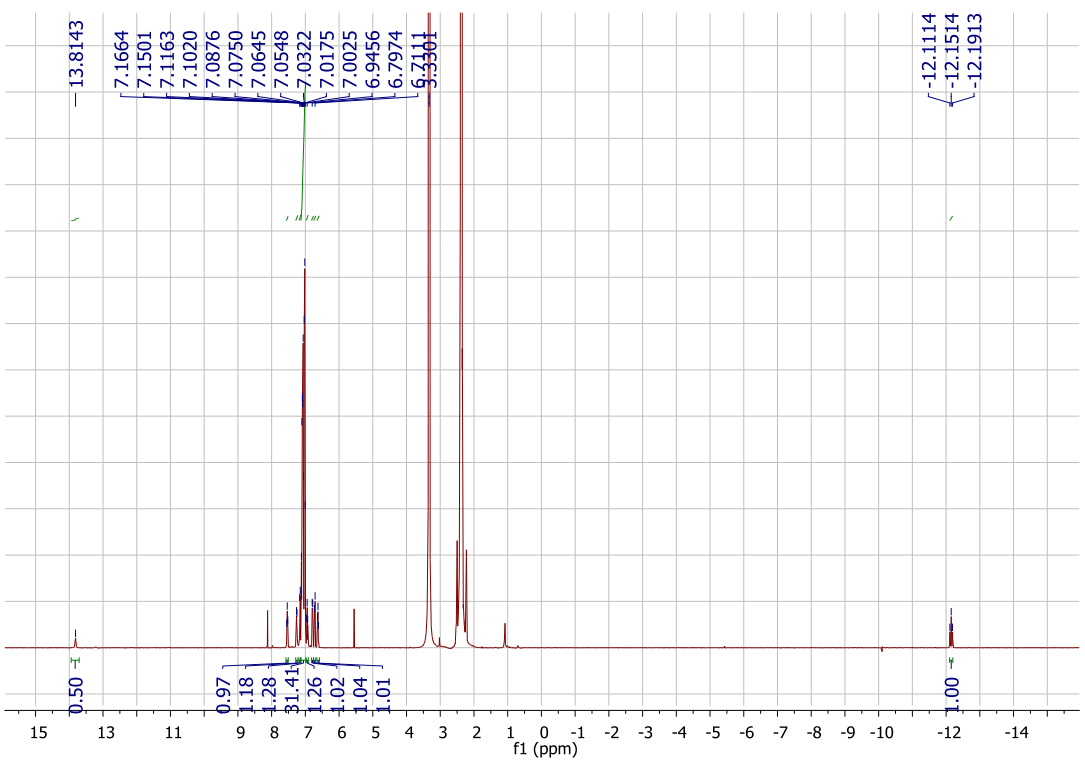


Figure S1. ^{1}H-NMR spectra of the crude reaction mixture as in Table S1, entry 16

3. ^{1}H-NMR and ^{31}P-NMR Spectra of Metal Complexes

(A)



(B)

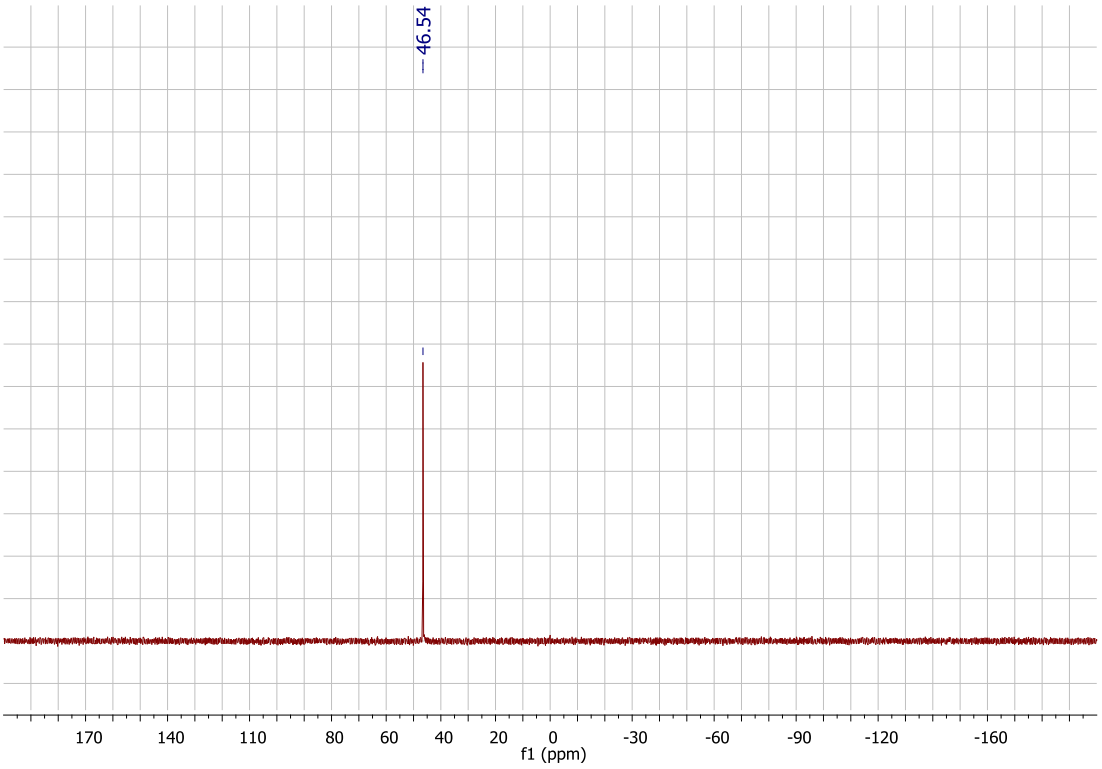


Figure S2. A) ^{1}H-NMR Spectra of complex **A**. B) ^{31}P-NMR Spectra of complex **A.**

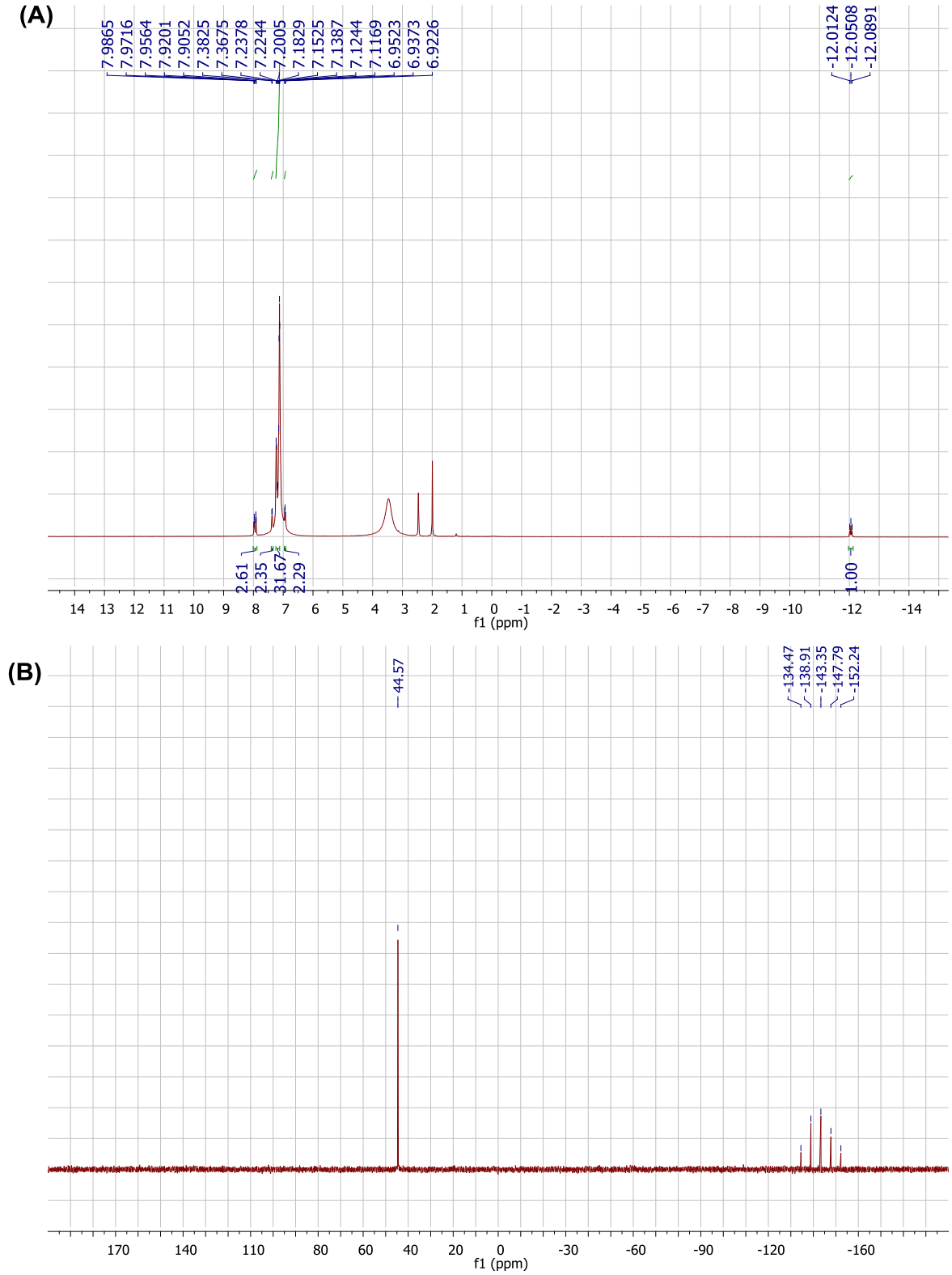


Figure S3. A) ^{1}H-NMR Spectra of complex **B**. B) ^{31}P-NMR Spectra of complex **B.**

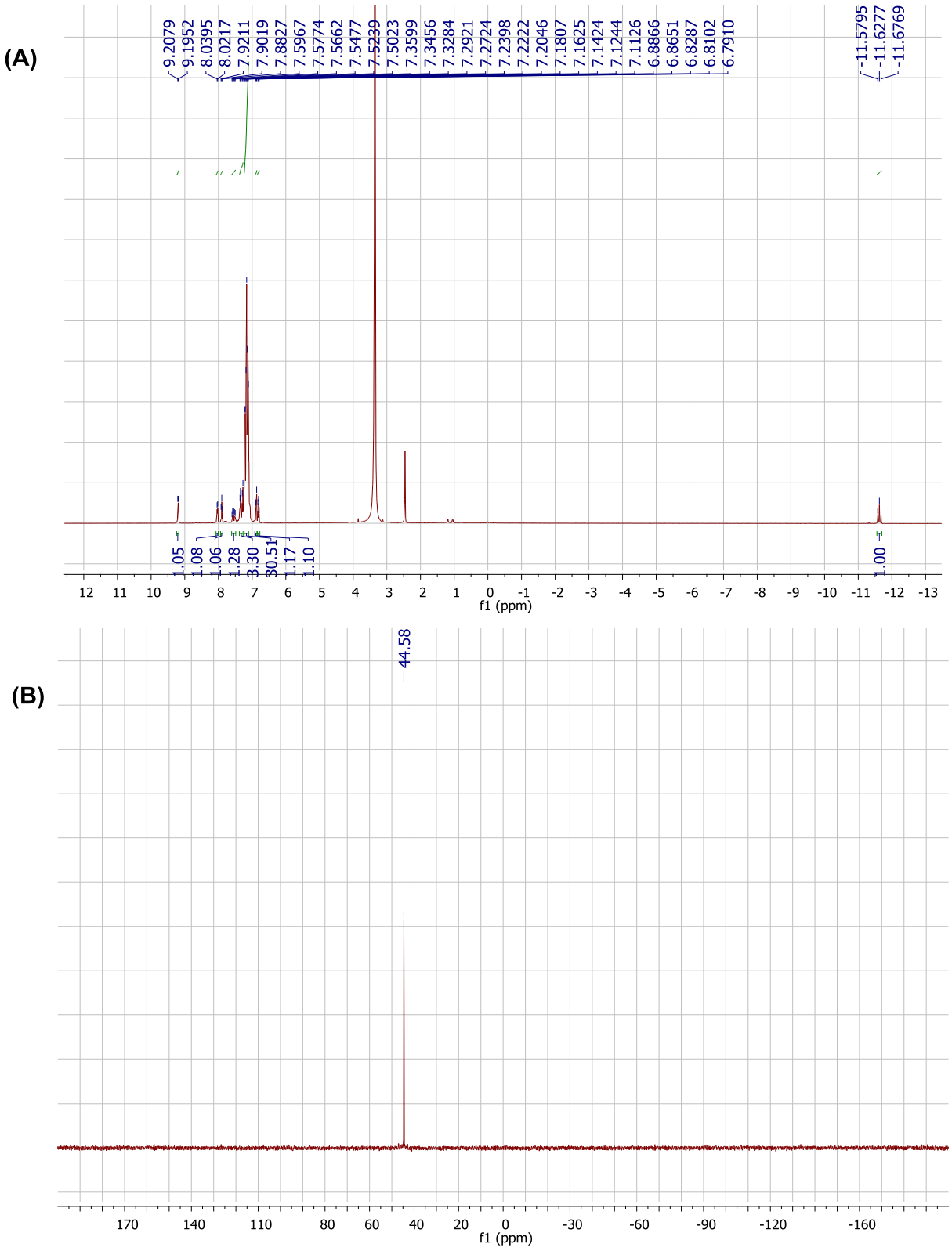


Figure S4. A) ^{1}H-NMR Spectra of complex **E**. B) ^{31}P-NMR Spectra of complex **E.**

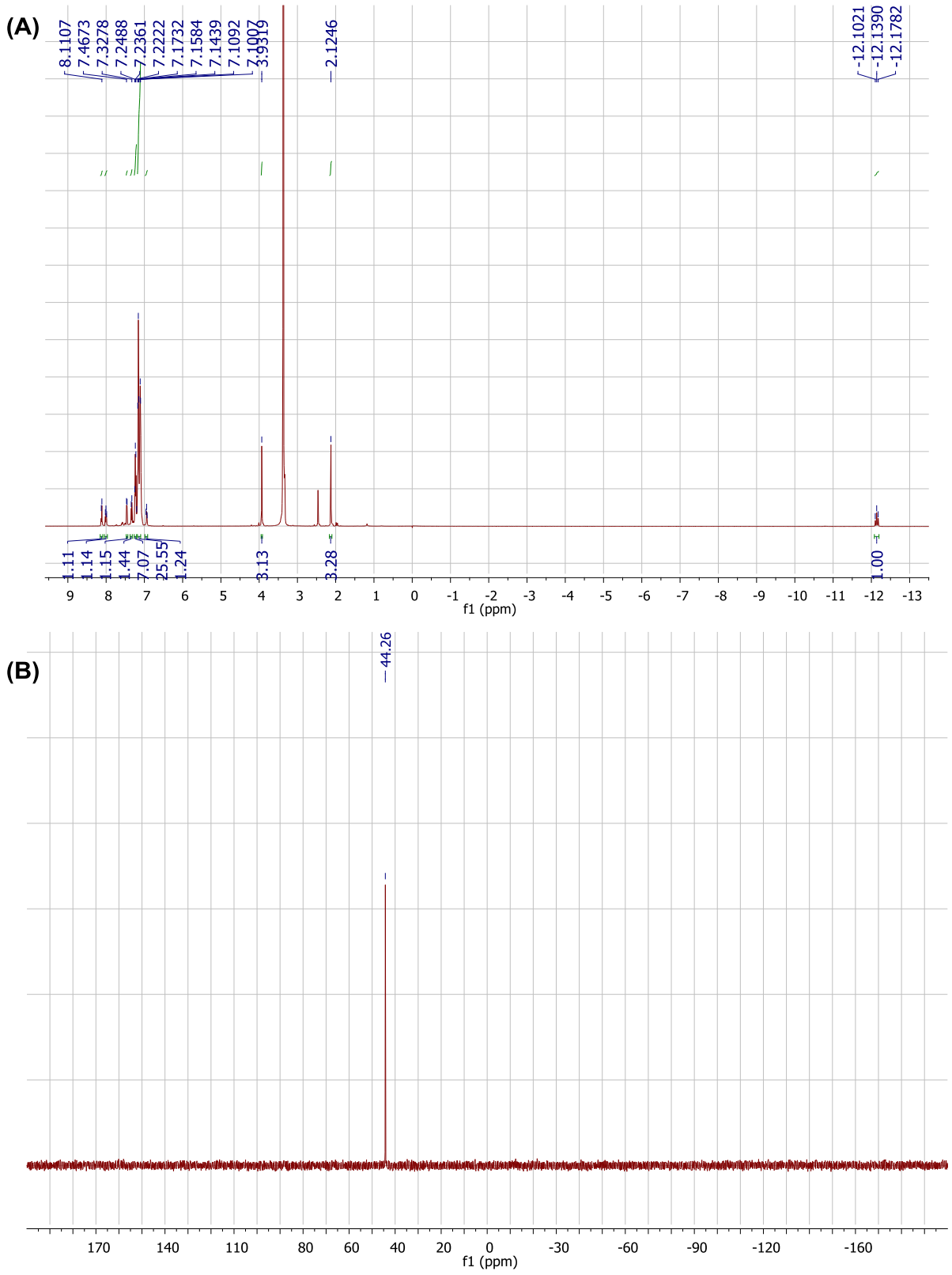


Figure S5. A) ^{1}H-NMR Spectra of complex **F**. B) ^{31}P-NMR Spectra of complex **F**.

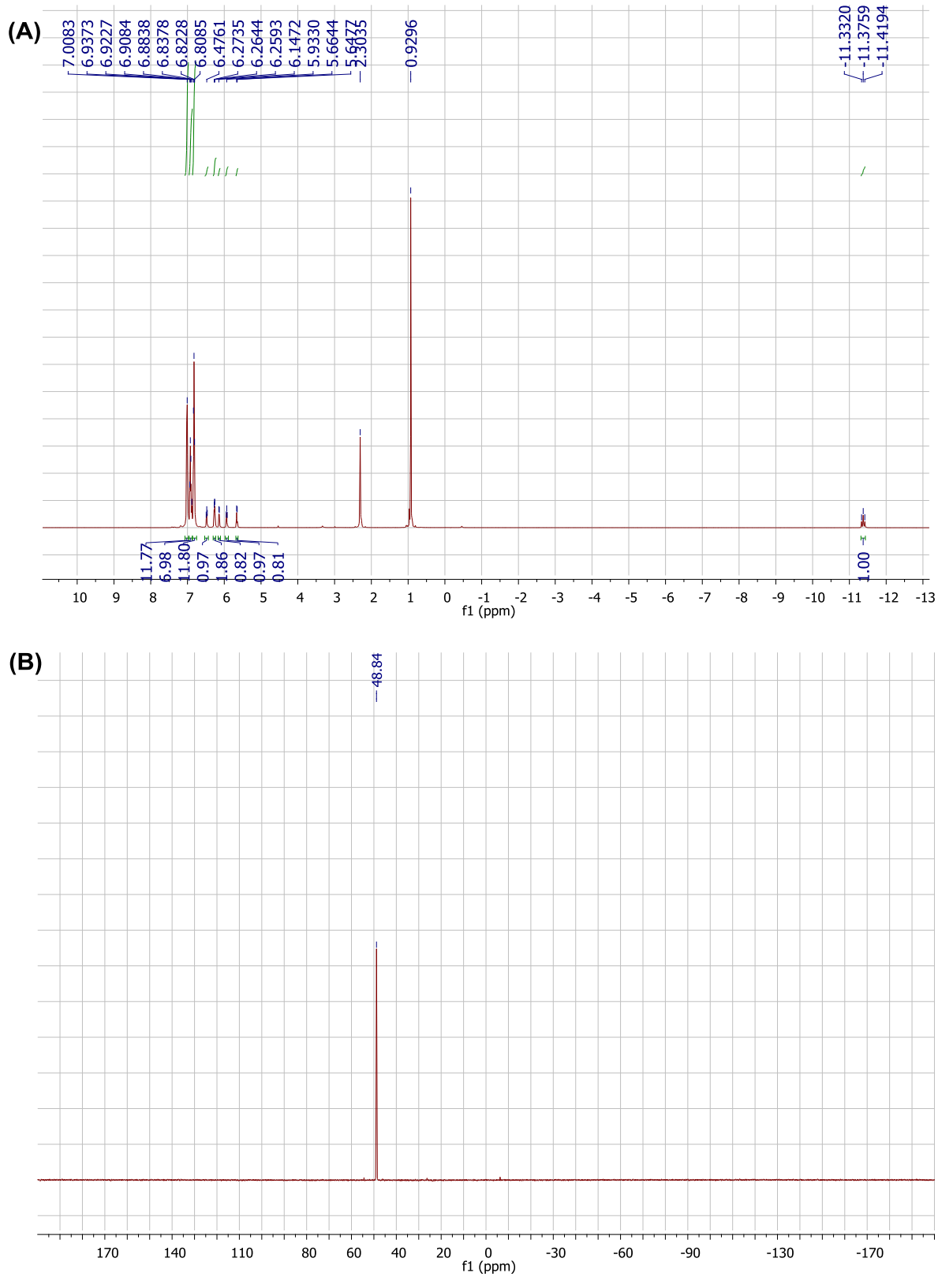


Figure S6. A) ^{1}H-NMR Spectra of complex **A'**. B) ^{31}P-NMR Spectra of complex **A'**.

4. ESI-MS Spectra of Complex A and B

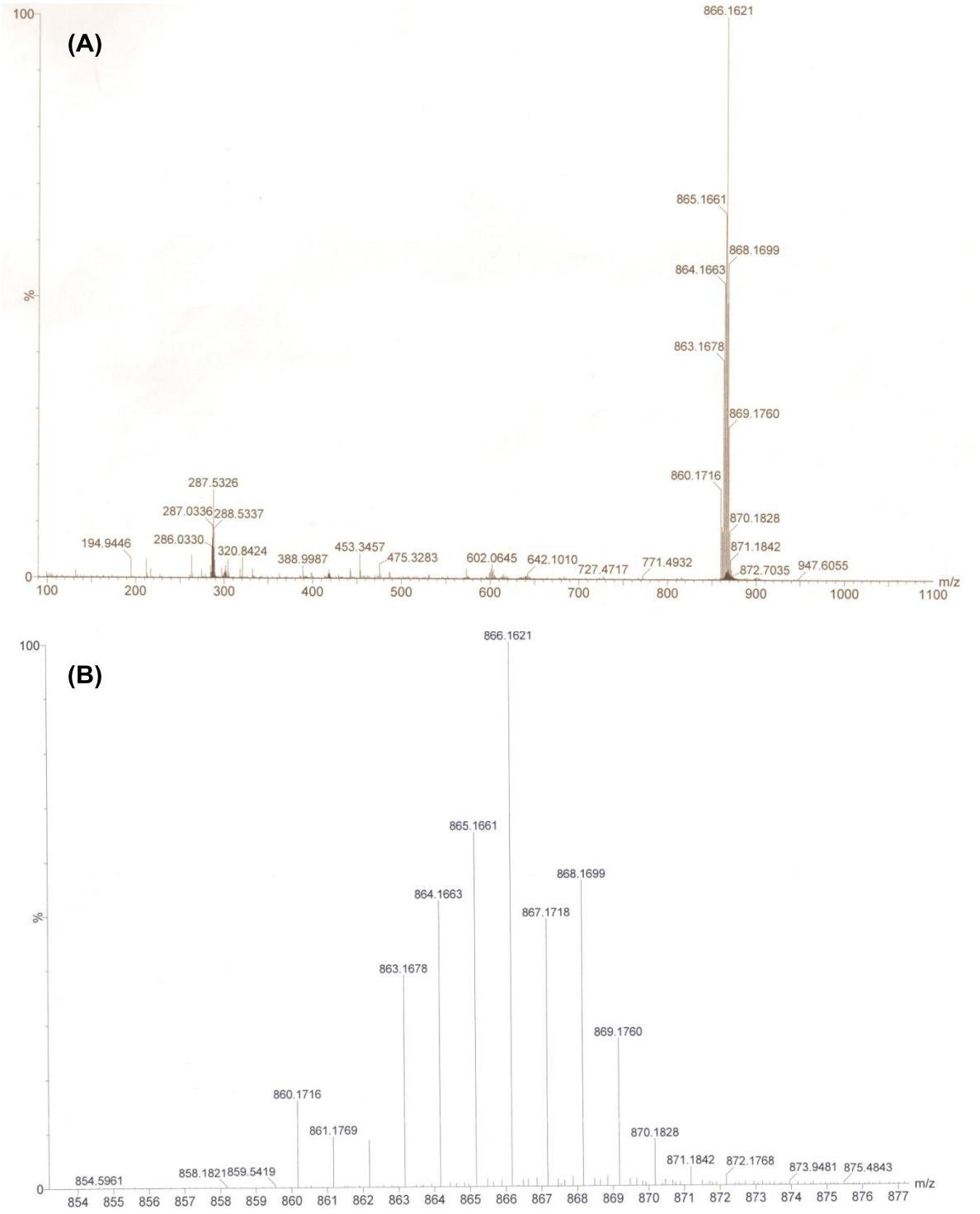


Figure S7. A) ESI-MS spectra of complex **A**. B) Expansion of the Spectra of complex **A**

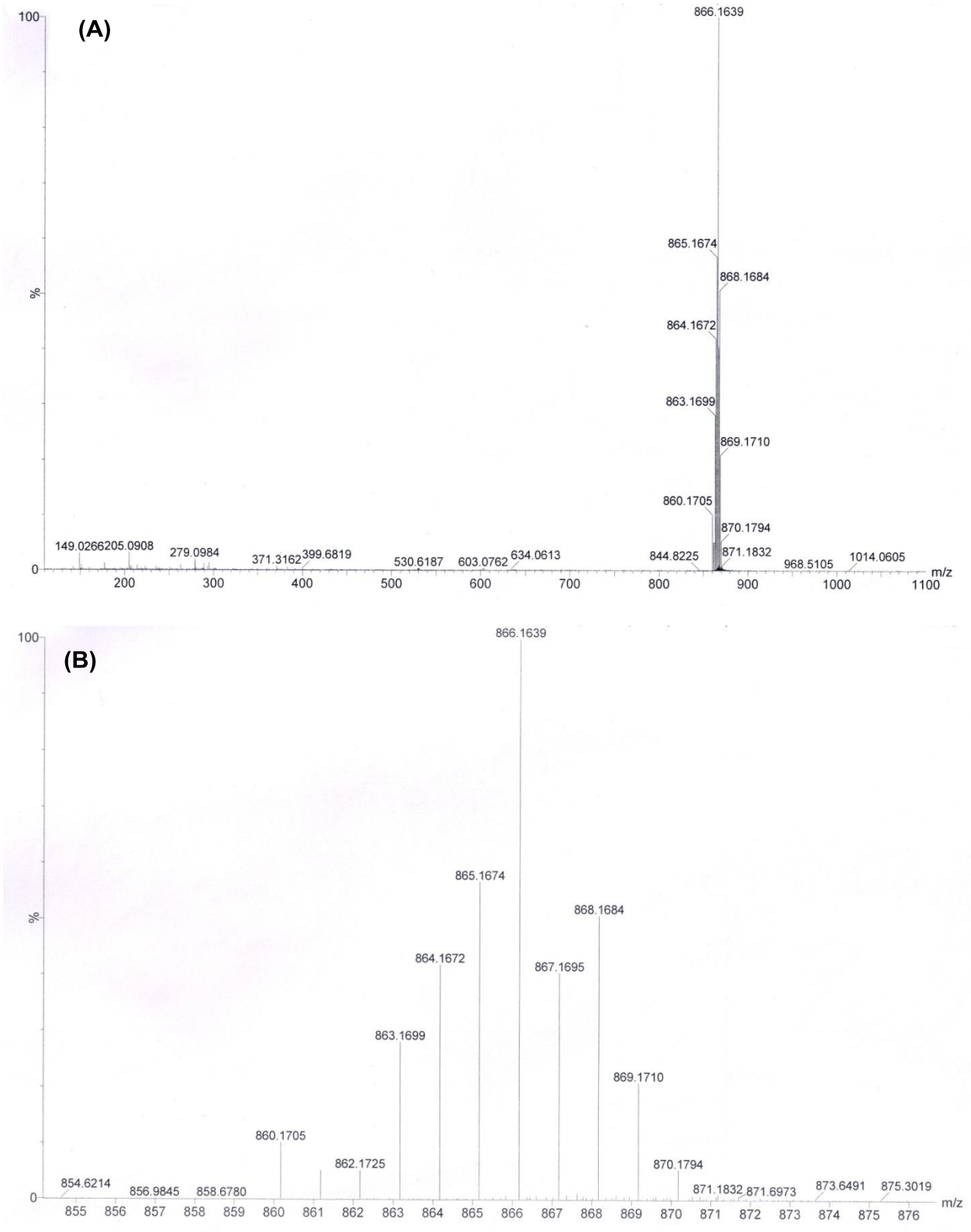


Figure S8. A) ESI-MS spectra of complex **B**. B) Expansion of the Spectra of complex **B**

5. X-Ray Structure Determination Data

Single-crystal X-ray data of all the complexes were collected at 100 K by using a Bruker SMART APEX II CCD diffractometer. MoKα radiation (λ =0.71073 Å). The program SMART was used for collecting frames of data, indexing reflections, and determining lattice parameters, SAINT for integration of the intensity of reflections and scaling, SADABS for absorption correction, and SHELXTL for space group and structure determination and least-squares refinements on F^2. [1, 2] The crystal structure were solved and refined by full-matrix least-squares methods against F^2 by using the program SHELXL-2014[3] using Olex-2 software.[4] All the non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen positions were fixed at calculated positions and refined isotropically. The few lattice solvent molecules of all crystals could not be modelled satisfactorily due to the presence of severe disorder. Therefore, PLATON/SQUEEZE program has been performed to discard those disordered solvents molecules.[5] For all other solvent molecules that are located successfully are modelled as described above. The figures have been generated using Mercury 3.7 software (30% probability thermal ellipsoids).[6] The crystallographic information file were deposited in Cambridge Structural Database (CCDC) and the CCDC number of complex **A**, **C**, **D** and **E** are CCDC 1937945, CCDC 1954543, CCDC 1953620 and CCDC 1953618 respectively.

In a Schlenk tube amidine (0.5 mmol), primary alcohol (0.65 mmol), secondary alcohol (0.65 mmol), cat. A (1.0 mol%), KO^{t}Bu (0.5 mmol) and dioxane (3.0 mL) were taken. The tube was sealed and reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. After the reaction, it was cooled to room temperature and then 1,3,5-trimethoxy benzene was added as internal standard. Then the reaction mixture was filtered through a small plug of neutral alumina and small portion was taken for determination of yield. yield was determined by the analysis of the ^{1}H-NMR spectra of the crude reaction mixture using $CDCl_3$ as NMR solvent. Final products were purified by silica-gel column chromatography using hexane/ethyl acetate as eluent.

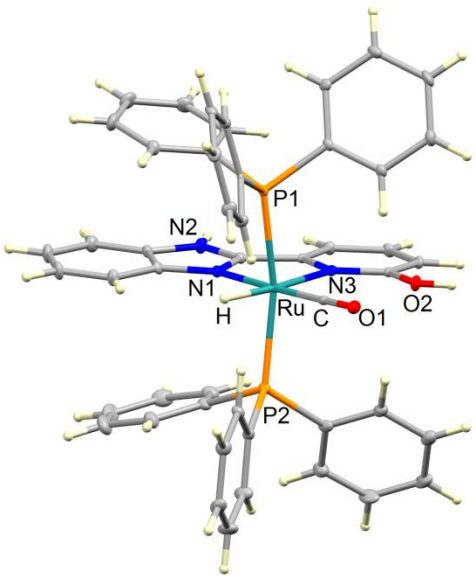


Figure S9. Solid state structure of complex **A** (30% thermal ellipsoids, Cl counter anion and solvent molecules were omitted for clarity).

Single crystals suitable for X-ray diffraction were grown in CH_2Cl_2/diethyl ether by slow evaporation process at ambient temperature. One water molecule was co-crystallized during the crystallization process as solvent impurity.

Table S2. Crystallographic Data and Refinement Parameters for complex A.

Identification code	Complex A
Empirical formula	$C_{49}H_{42}ClN_3O_3P_2Ru$
Formula weight	919.31
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	12.1744(3)
b/Å	12.4671(3)
c/Å	16.7201(4)
α/°	70.5040(10)
β/°	73.1360(10)
γ/°	73.7020(10)
Volume/Å^3	2241.36(10)
Z	2
ρ_{calc}g/cm^3	1.362
μ/mm^{-1}	0.525
F(000)	944.0
Crystal size/mm^3	0.24 × 0.21 × 0.19
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.206 to 49.996
Index ranges	$-14 \leq h \leq 14$, $-14 \leq k \leq 14$, $-19 \leq l \leq 19$
Reflections collected	27029
Independent reflections	7848 [R_{int} = 0.0497, R_{sigma} = 0.0551]
Data/restraints/parameters	7848/166/528
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.0847
Final R indexes [all data]	R_1 = 0.0509, wR_2 = 0.0903
Largest diff. peak/hole / e Å^{-3}	1.02/-0.85

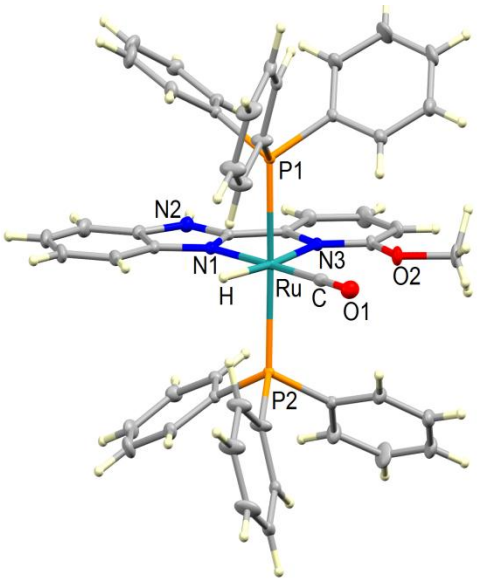


Figure S10. Solid state structure of complex **C** (30% thermal ellipsoids, Cl counter anion and solvent molecules were omitted for clarity).

Single crystals suitable for X-ray diffraction were grown in CH_2Cl_2/n-hexane by slow evaporation process at ambient temperature. One dichloromethane molecule was co-crystallized during the crystallization process as solvent impurity.

Table S3. **Crystallographic Data and Refinement Parameters for complex C**

Identification code	16sepa_a
Empirical formula	$C_{51}H_{44}Cl_3N_3O_2P_2Ru$
Formula weight	1000.25
Temperature/K	273.15
Crystal system	orthorhombic
Space group	Pnma
a/Å	19.4234(8)
b/Å	14.5749(7)
c/Å	16.5414(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4682.8(4)
Z	4
ρ_{calc}g/cm^3	1.419
μ/mm^{-1}	0.618
F(000)	2048.0
Crystal size/mm^3	0.2 ×0.2 × 0.2

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.354 to 56.608
Index ranges	$-25 \leq h \leq 25$, $-19 \leq k \leq 19$, $-22 \leq l \leq 22$
Reflections collected	68913
Independent reflections	6035 [R_{int} = 0.0789, R_{sigma} = 0.0360]
Data/restraints/parameters	6035/12/326
Goodness-of-fit on F^2	1.078
Final R indexes [I>=2σ (I)]	R_1 = 0.0494, wR_2 = 0.0891
Final R indexes [all data]	R_1 = 0.0679, wR_2 = 0.0985
Largest diff. peak/hole / e $Å^{-3}$	1.04/-1.24

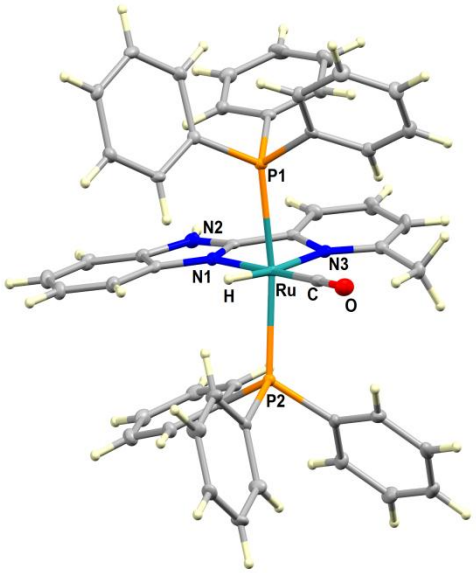


Figure S11. Solid state structure of complex **D** (30% thermal ellipsoids, Cl counter anion and solvent molecules were omitted for clarity).

Single crystals suitable for X-ray diffraction were grown in CH_2Cl_2/benzene by slow evaporation process at ambient temperature. One half of benzene molecule was co-crystallized during the crystallization process as solvent impurity. Half of benzene molecule was present because of mirror symmetry.

Table S4. **Crystallographic Data and Refinement Parameters for complex D**

Identification code	Complex_**D**
Empirical formula	$C_{53}H_{45}ClN_3OP_2Ru$
Formula weight	937.37
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$

a/Å	9.806(5)
b/Å	22.261(5)
c/Å	19.795(5)
α/°	90.000(5)
β/°	95.099(5)
γ/°	90.000(5)
Volume/Å^3	4304(3)
Z	4
ρ_{calc}g/cm^3	1.447
μ/mm^{-1}	0.545
F(000)	1928.0
Crystal size/mm^3	0.01 × 0.01 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.132 to 56.744
Index ranges	-13 ≤ h ≤ 10, -29 ≤ k ≤ 29, -26 ≤ l ≤ 26
Reflections collected	43395
Independent reflections	10744 [R_{int} = 0.1038, R_{sigma} = 0.1174]
Data/restraints/parameters	10744/0/555
Goodness-of-fit on F^2	1.007
Final R indexes [I>=2σ (I)]	R_1 = 0.0566, wR_2 = 0.1133
Final R indexes [all data]	R_1 = 0.1194, wR_2 = 0.1334
Largest diff. peak/hole / e Å^{-3}	1.11/-0.73

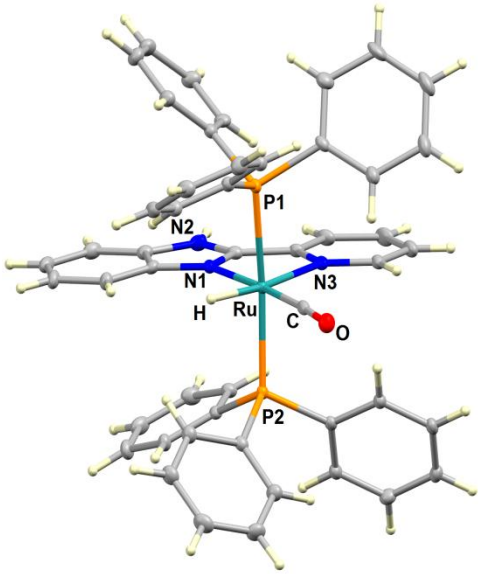


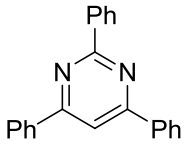
Figure S12. Solid state structure of complex **E** (30% thermal ellipsoids, Cl counter anion and solvent molecules were omitted for clarity).

Single crystals suitable for X-ray diffraction were grown in CH_2Cl_2/benzene by slow evaporation process at ambient temperature. In asymmetric unit of the crystal, two half of benzene molecules were co-crystallized during the crystallization process as solvent impurity.

Table S5. **Crystallographic Data and Refinement Parameters for complex E**

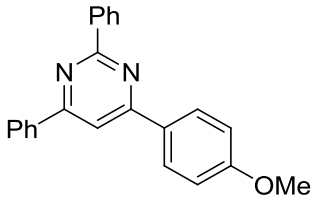
Identification code	Complex_**E**
Empirical formula	$C_{55}H_{46}ClN_3OP_2Ru$
Formula weight	963.41
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.693(5)
b/Å	24.331(5)
c/Å	19.244(5)
α/°	90.000(5)
β/°	91.923(5)
γ/°	90.000(5)
Volume/Å^3	4536(3)
Z	4
ρ_{calc}g/cm^3	1.411
μ/mm^{-1}	0.519
F(000)	1984.0
Crystal size/mm^3	0.01 × 0.01 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.526 to 56.6
Index ranges	$-12 \leq h \leq 12$, $-32 \leq k \leq 32$, $-25 \leq l \leq 25$
Reflections collected	71173
Independent reflections	11255 [R_{int} = 0.1061, R_{sigma} = 0.0735]
Data/restraints/parameters	11255/0/572
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0502, wR_2 = 0.1122
Final R indexes [all data]	R_1 = 0.0977, wR_2 = 0.1406
Largest diff. peak/hole / e Å^{-3}	2.41/-1.24

6. Characterization Data of Products



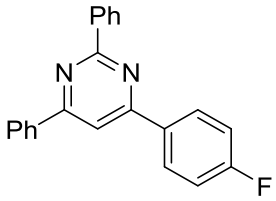
2,4,6-Triphenylpyrimidine (4)[7]

140 mg; 91% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.75-8.73 (m, 2H), 8.31-8.28 (m, 4H), 8.01 (s, 1H), 7.58-7.52 (m, 9H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 164.87, 164.64, 138.30, 137.68, 130.85, 130.72, 129.10, 128.59, 127.39, 110.38. **GC-MS** (M^+) = 308.1.



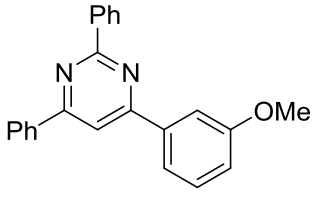
4-(4-Methoxyphenyl)-2,6-diphenylpyrimidine (5)[7]

150 mg; 89% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.73-8.70 (m, 2H), 8.29-8.26 (m, 4H), 7.94 (s, 1H), 7.56-7.52 (m, 6H), 7.08-7.04 (m, 2H), 3.89 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.57, 164.44, 164.30, 162.01, 138.39, 137.80, 130.78, 130.70, 130.05, 128.97, 128.79, 128.60, 128.45, 127.43, 127.25, 114.46, 114.21, 109.54, 55.64. **GC-MS** (M^+) = 338.1.



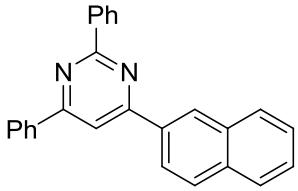
4-(4-Fluorophenyl)-2,6-diphenylpyrimidine (6)[7]

112 mg; 69% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.72-8.69 (m, 2H), 8.30-8.26 (m, 4H), 7.95 (s, 1H), 7.56-7.52 (m, 6H), 7.22 (d, $J_{H,H}$ = 8.7 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 165.93, 164.94, 164.60, 163.71, 163.44, 138.11, 137.52, 130.72,130.93, 130.80, 129.43, 129.34, 129.01,128.54, 127.36, 116.13,115.91, 109.96. **GC-MS** (M^+) = 326.1.



4-(3-Methoxyphenyl)-2,6-diphenylpyrimidine (7)

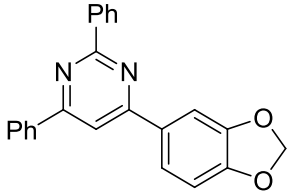
157 mg; 93% yield; white solid; **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.73-8.71 (m, 2H), 8.29-8.27 (m, 2H), 7.99 (s, 1H), 7.89 (t, $J_{H,H}$ = 8.7 Hz, 1H), 7.82 (dd, $J_{H,H}$ = 7.7 Hz, 0.9 Hz, 1H), 7.56-7.51 (m, 6H), 7.47 (t, $J_{H,H}$ = 7.9 Hz, 1H), 7.09-7.07 (m, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 164.90, 164.67, 164.59, 160.29, 139.16, 138.23, 137.64, 129.02, 128.58, 128.54, 127.39, 119.74, 116.46, 112.93, 110.57, 55.58. **HRMS** (ESI): Calcd. for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1497; found: 339.1499.



4-(Naphthalen-2-yl)-2,6-diphenylpyrimidine (8)[8]

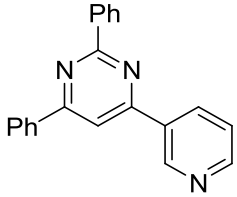
170 mg; 95% yield; white solid; **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.79-8.77 (m, 3H), 8.39 (dd, $J_{H,H}$ = 8.5 Hz, 1.6 Hz, 1H), 8.33 (dd, $J_{H,H}$ = 7.8 Hz, 1.7 Hz, 2H), 8.13 (s, 1H), 8.04-8.0 (m, 2H), 7.92-7.90 (m, 1H), 7.60-7.54 (m, 8H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 164.84, 164.70, 164.64, 138.29, 137.65, 134.91, 134.70, 133.39, 130.87, 130.74, 129.11, 129.0, 128.74, 128.61, 128.55, 127.87, 127.47, 127.40, 126.65, 124.32, 110.56.

GC-MS (M^+) = 358.1.



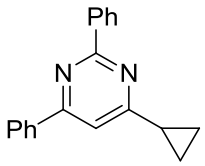
4-(Benzo[d][1,3]dioxol-5-yl)-2,6-diphenylpyrimidine (9)[8]

155 mg; 88% yield; light yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.72-8.69 (m, 2H), 8.27-8.25 (m, 2H), 7.87 (s, 1H), 7.83-7.79 (m, 2H), 7.56-7.52 (m, 6H), 6.94 (d, $J_{H,H}$ = 8.1 Hz, 1H), 6.04 (s, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 164.63, 164.39, 164.04, 150.07, 148.55, 130.65, 128.94, 128.54, 128.48, 127.33, 121.90, 109.59, 108.59, 107.57, 101.68. **GC-MS** (M^+) = 352.1.



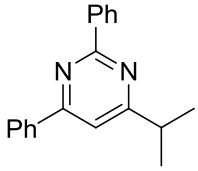
2,4-Diphenyl-6-(pyridin-3-yl)pyrimidine (10)[7]

121 mg; 78% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 9.45 (d, $J_{H,H}$ = 1.7 Hz, 1H), 8.77 (dd, $J_{H,H}$ = 4.8 Hz, 1.6 Hz, 1H), 8.72-8.69 (m, 2H), 8.59 (dt, $J_{H,H}$ = 8.0 Hz, 2.0 Hz, 1H), 8.30-8.27 (m, 2H), 8.01 (s, 1H), 7.58-7.51 (m, 6H), 7.49 (qd, $J_{H,H}$ = 4.7 Hz, 0.5 Hz, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 165.21, 164.84, 162.49, 151.60, 148.70, 137.81, 137.18, 134.84, 133.26, 131.16, 131.0, 129.11, 129.08, 128.61, 128.55, 127.39, 123.82, 110.32. **GC-MS** (M^+) = 309.1.



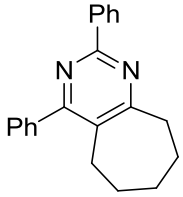
4-Cyclopropyl-2,6-diphenylpyrimidine (11)[9]

96 mg; 71% yield; light yellow gel; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.60-8.58 (m, 2H), 8.23-8.21 (m, 2H), 7.55-7.48 (m, 6H), 7.47 (s, 1H), 2.15-2.09 (m, 1H), 1.39-1.35 (m, 2H), 1.17-1.12 (m, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 172.22, 163.94, 162.87, 138.24, 137.49, 130.43, 130.32, 128.77, 128.28, 128.24, 127.15, 112.42, 17.30, 10.90. **GC-MS** (M^+) = 272.1.



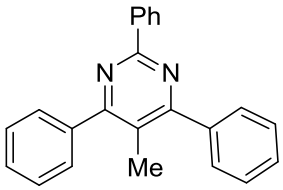
4-Isopropyl-2,6-diphenylpyrimidine (12)[10]

79 mg; 58% yield; yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.64-8.61 (m, 2H), 8.22-8.20 (m, 2H), 7.55-7.47 (m, 6H), 7.47 (s, 1H), 3.13 (sept, $J_{H,H}$ = 6.9 Hz, 1H), 1.41 (d, $J_{H,H}$ = 6.9 Hz, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 176.40, 164.13, 164.04, 138.42, 137.72, 130.62, 130.47, 128.92, 128.47, 127.30, 111.64, 36.44, 22.03. **GC-MS** (M^+) = 274.1.



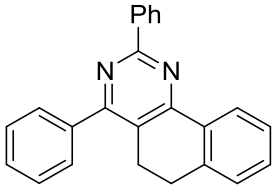
2,4-Diphenyl-6,7,8,9-tetrahydro-5H-cyclohepta[d]pyrimidine (13)

122 mg; 81% yield; colourless gel; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.48 (dd, $J_{H,H}$ = 7.9 Hz, 2.2 Hz, 2H), 7.60-7.58 (m, 2H), 7.49-7.44 (m, 6H), 3.17-3.15 (m, 2H), 2.89-2.86 (m, 2H), 1.93 (quint, $J_{H,H}$ = 5.6 Hz, 2H), 1.82 (quint, $J_{H,H}$ = 5.0 Hz, 2H), 1.71 (quint, $J_{H,H}$ = 5.5 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ = 172.81, 164.43, 161.17, 139.37, 138.25, 130.48, 130.06, 129.34, 128.77, 128.42, 128.29, 128.18, 39.44, 32.34, 29.23, 27.85, 26.22. **HRMS** (ESI): Calcd. for $C_{21}H_{21}N_2$ $[M+H]^+$: 301.1705; found: 301.1709.



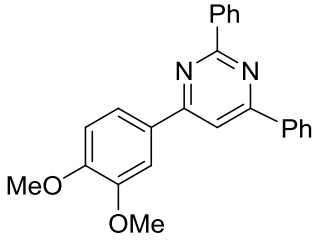
5-Methyl-2,4,6-triphenylpyrimidine (14)[11]

135 mg; 57% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.56 (d, $J_{H,H}$ = 5.2 Hz, 2H), 7.74 (d, $J_{H,H}$ = 7.6 Hz, 4H), 7.50-7.45 (m, 9H), 2.39 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ = 167.02, 161.57, 139.32, 138.0, 129.45, 129.19, 128.44, 128.37, 123.25, 17.82. **GC-MS** (M^+) = 322.1.



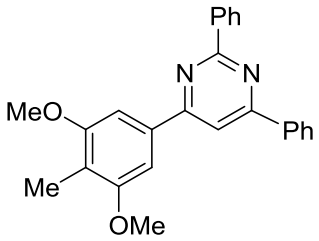
2,4-Diphenyl-5,6-dihydrobenzo[h]quinazoline (15)[12]

44 mg; 92% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.67 (d, $J_{H,H}$ = 7.2 Hz, 2H), 8.63-8.61 (m, 1H), 7.75 (dd, $J_{H,H}$ = 8.1 Hz, 1.8 Hz, 2H), 7.54-7.44 (m, 8H), 7.28-7.27 (m, 1H), 3.12-3.08 (m, 2H), 2.91 (t, $J_{H,H}$ = 7.8 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.35, 162.21, 160.19, 139.18, 138.41, 138.29, 133.45, 130.89, 130.30, 129.31, 128.46, 128.37, 128.24, 127.81, 127.35, 126.12, 123.54, 27.90, 24.86. **GC-MS** (M^+) = 334.1.



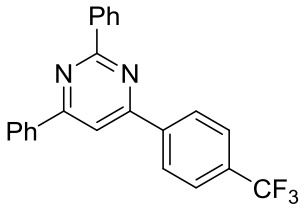
4-(3,4-Dimethoxyphenyl)-2,6-diphenylpyrimidine (18)

145 mg; 79% yield; yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.70 (d, $J_{H,H}$ = 6.4 Hz, 2H), 8.28 (d, $J_{H,H}$ = 6.2 Hz, 2H), 7.94 (s, 2H), 7.83 (d, $J_{H,H}$ = 8.4 Hz, 1H), 7.56-7.51 (m, 6H), 7.01 (d, $J_{H,H}$ = 8.5 Hz, 1H), 4.06 (s, 3H), 3.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.61, 164.43, 164.35, 151.61, 149.46, 137.75, 130.67, 128.97, 128.52, 127.36, 120.44, 111.14, 110.22, 109.73, 56.19. **HRMS** (ESI): Calcd. for $C_{24}H_{21}N_2O_2$ $[M+H]^+$: 369.1603; found: 369.1609.



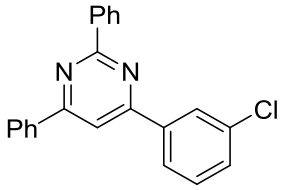
4-(3,5-Dimethoxy-4-methylphenyl)-2,6-diphenylpyrimidine (19)

136 mg; 71% yield; yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.71-8.68 (m, 2H), 8.29-8.27 (m, 2H), 7.92 (s, 1H), 7.57-7.52 (m, 8H), 4.02 (s, 6H), 3.94 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.87, 164.54, 164.49, 153.73, 140.72, 138.14, 137.61, 133.15, 130.91, 130.79, 129.02, 128.56, 128.52, 127.39, 110.24, 61.12, 56.50. **HRMS** (ESI): Calcd. for $C_{25}H_{23}N_2O_2$ $[M+H]^+$: 383.1760; found: 383.1765.



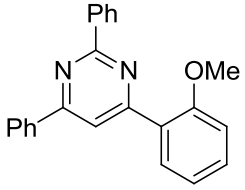
2,4-Diphenyl-6-(4-(trifluoromethyl)phenyl)pyrimidine (21)[13]

120 mg; 64% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.72-8.69 (m, 2H), 8.36 (d, $J_{H,H}$ = 8.2 Hz, 2H), 8.29-8.27 (m, 2H), 7.99 (s, 1H), 7.80 (d, $J_{H,H}$ = 8.3 Hz, 2H), 7.57-7.53 (m, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 165.26, 164.79, 163.33, 140.98, 137.88, 137.25, 131.13, 130.97, 129.06, 128.60, 128.57, 127.70, 127.39, 125.93, 125.90, 110.60. **GC-MS** (M^+) = 376.1.



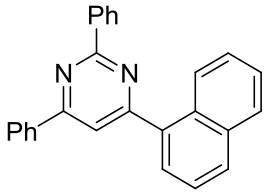
4-(3-Chlorophenyl)-2,6-diphenylpyrimidine (22)[14]

89 mg; 52% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.72-8.69 (m, 2H), 8.29-8.26 (m, 3H), 8.15-8.12 (dt, $J_{H,H}$ = 6.8 Hz, 1.5 Hz, 1H), 7.95 (s, 1H), 7.56-7.48 (m, 8H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 165.13, 164.70, 163.39, 139.45, 137.96, 137.34, 135.18, 131.04, 130.89, 130.78, 129.03, 128.58, 127.50, 127.38, 125.42, 110.33. **GC-MS** (M^+) = 342.1.



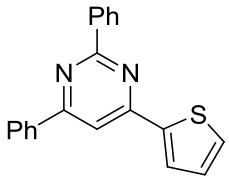
4-(2-Methoxyphenyl)-2,6-diphenylpyrimidine (23)[15]

103 mg; 61% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.72-8.70 (m, 2H), 8.30 (s, 1H), 8.29-8.24 (m, 3H), 7.57-7.46 (m, 7H), 7.17 (t, $J_{H,H}$ = 7.9 Hz, 1H), 7.06 (d, $J_{H,H}$ = 7.9 Hz, 1H), 3.95 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.29, 163.70, 163.50, 158.16, 138.49, 138.0, 131.60, 131.43, 130.57, 130.47, 128.92, 128.47, 128.43, 127.48, 127.07, 121.27, 115.50, 111.69, 55.85. **GC-MS** (M^+) = 338.1



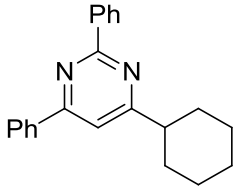
4-(Naphthalen-1-yl)-2,6-diphenylpyrimidine (24)[13]

163 mg; 91% yield; yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.74-8.72 (m, 2H), 8.39-8.37 (m, 1H), 8.33-8.31 (m, 2H), 8.0 (d, $J_{H,H}$ = 8.4 Hz, 1H), 7.98-7.96 (m, 1H), 7.91 (s, 1H), 7.81 (d, $J_{H,H}$ = 7.1 Hz, 1H), 7.64-7.53 (m, 9H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 167.53, 164.47, 164.38, 138.12, 137.34, 136.92, 134.09, 130.98, 130.79, 130.22, 129.03, 128.63, 127.94, 127.39, 126.99, 126.27, 125.52, 125.38, 115.42**. GC-MS** (M^+) = 358.1.



2,4-Diphenyl-6-(thiophen-2-yl)pyrimidine (25)[8]

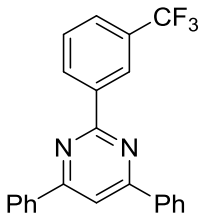
93 mg; 59% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.69-8.66 (m, 2H), 8.27-8.25 (m, 2H), 7.91 (dd, $J_{H,H}$ = 3.8 Hz, 1.0 Hz, 1H), 7.85 (s, 1H), 7.56-7.51 (m, 7H), 7.20 (dd, $J_{H,H}$ = 4.9 Hz, 3.8 Hz, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 164.65, 164.52, 159.77, 143.45, 137.81, 137.42, 130.92, 130.82, 129.89, 128.99, 128.52, 128.39, 127.32, 127.14, 108.51. **GC-MS** (M^+) = 314.1.



4-Cyclohexyl-2,6-diphenylpyrimidine (27)[16]

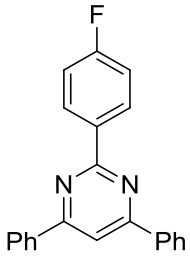
132 mg; 84% yield; yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.62-8.60 (m, 2H), 8.22-8.20 (m, 2H), 7.52-7.48 (m, 6H), 7.45 (s, 1H), 2.79 (tt, $J_{H,H}$ = 11.8 Hz, 3.4 Hz, 1H), 2.06 (dd, $J_{H,H}$ = 13.4 Hz, 1.6 Hz, 2H), 1.91 (dt, $J_{H,H}$ = 13.0 Hz, 3.3 Hz, 2H), 1.82-1.77 (m, 1H), 1.72-1.62 (m, 2H), 1.52-1.31 (m, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 175.48, 164.13, 163.94, 138.50,

137.77, 130.58, 130.41, 128.90, 128.46, 127.28, 46.43, 32.29, 26.44, 26.13. **GC-MS** (M^+) = 314.1.



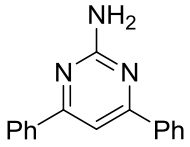
4,6-Diphenyl-2-(3-(trifluoromethyl)phenyl)pyrimidine (28)

105 mg; 56% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.98 (s, 1H), 8.91 (d, $J_{H,H}$ = 7.8 Hz, 1H), 8.29-8.27 (m, 4H), 8.05 (s, 1H), 7.76 (d, $J_{H,H}$ = 7.6 Hz, 1H), 7.65 (t, $J_{H,H}$ = 7.7 Hz, 1H), 7.60-7.55 (m, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 165.11, 163.25, 139.06, 137.28, 131.76, 131.11, 129.11, 129.01, 127.40, 127.18, 125.38, 110.99. **HRMS** (ESI): Calcd. for $C_{23}H_{16}F_3N_2$ $[M+H]_+$: 377.1266; found: 377.1271.



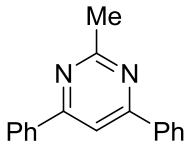
2-(4-Fluorophenyl)-4,6-diphenylpyrimidine (29)

104 mg; 64% yield; white solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.74-8.71 (m, 2H), 8.28-8.26 (m, 4H), 8.0 (s, 1H), 7.58-7.54 (m, 6H), 7.20 (t, $J_{H,H}$ = 8.6 Hz, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 166.07, 164.91, 163.72, 163.58, 137.54, 134.42, 130.92, 130.71, 130.62, 129.03, 127.36, 115.55, 115.33, 110.28. **HRMS** (ESI): Calcd. for $C_{22}H_{16}FN_2$ $[M+H]^+$: 327.1298; found: 327.1306.



4,6-Diphenylpyrimidin-2-amine (30)[17]

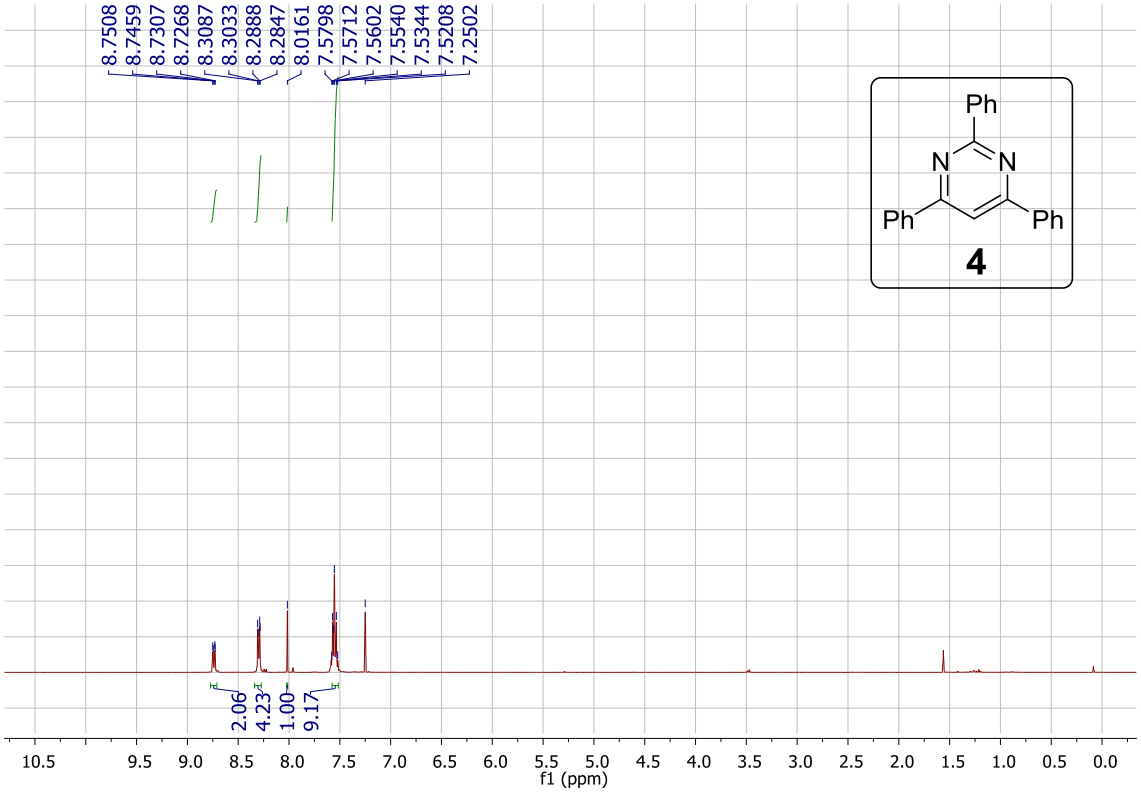
77 mg; 62% yield; brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.06-8.03 (m, 4H), 7.50-7.48 (m, 6H), 7.46 (s, 1H), 5.23 (brs, 2H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 166.34, 163.68, 137.83, 130.56, 128.87, 127.20, 104.45. **GC-MS** (M^+) = 247.1.

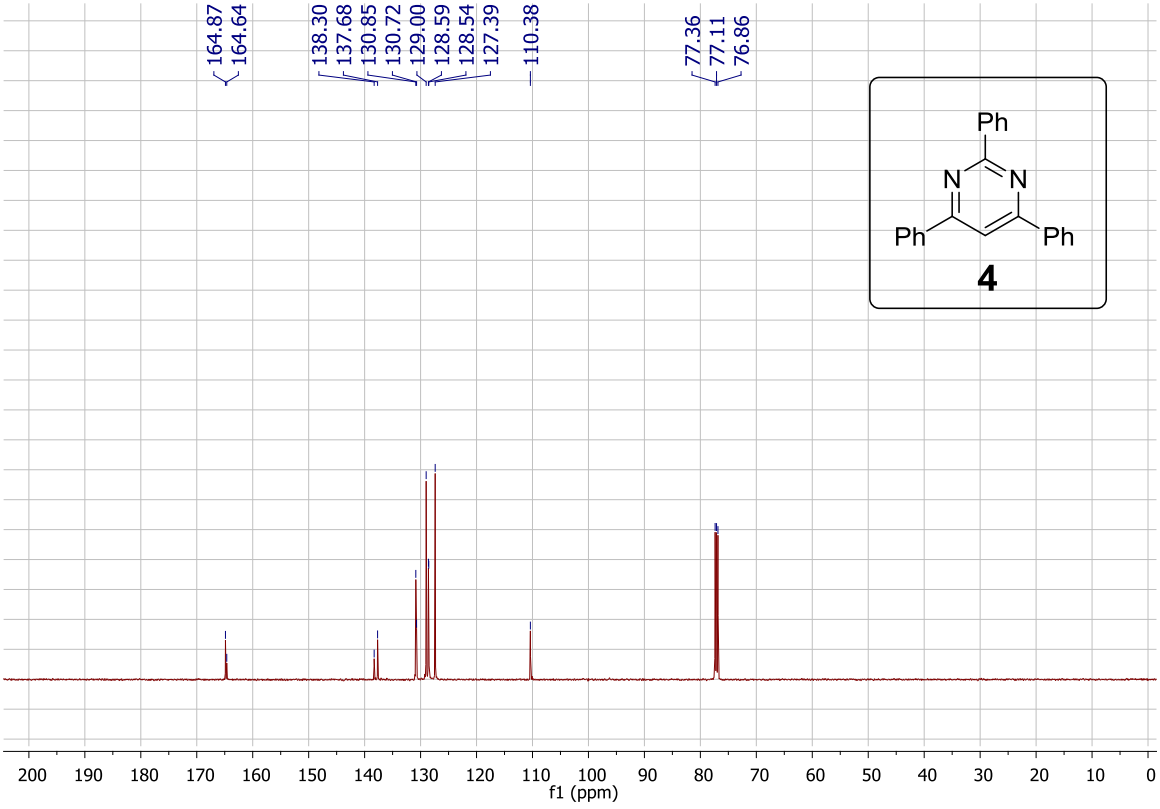


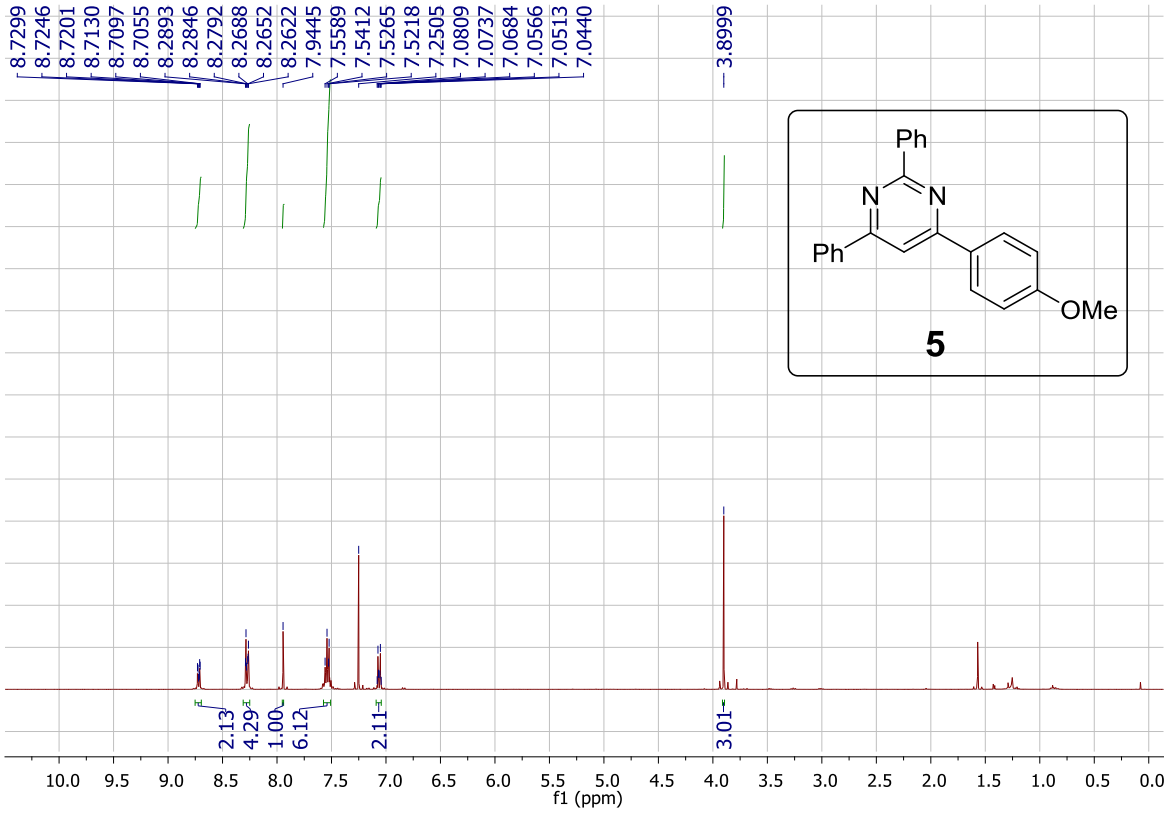
2-Methyl-4,6-diphenylpyrimidine (31)[13]

82 mg; 67% yield; brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.13-8.11 (m, 4H), 7.88 (s, 1H), 7.52-7.51 (m, 6H), 2.86 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 168.66, 164.98, 137.60, 130.72, 129.03, 127.35, 110.21, 26.60. **GC-MS** (M^+) = 246.1.

7. Copies of ^{1}H and ^{13}C NMR Spectra of the Products



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8.7097
8.7055
8.2893
8.2846
8.2792
8.2688
8.2652
8.2622
7.9445
7.5589
7.5412
7.5265
7.5218
7.2505
7.0809
7.0737
7.0684
7.0566
7.0513
7.0440
3.8999
Ph
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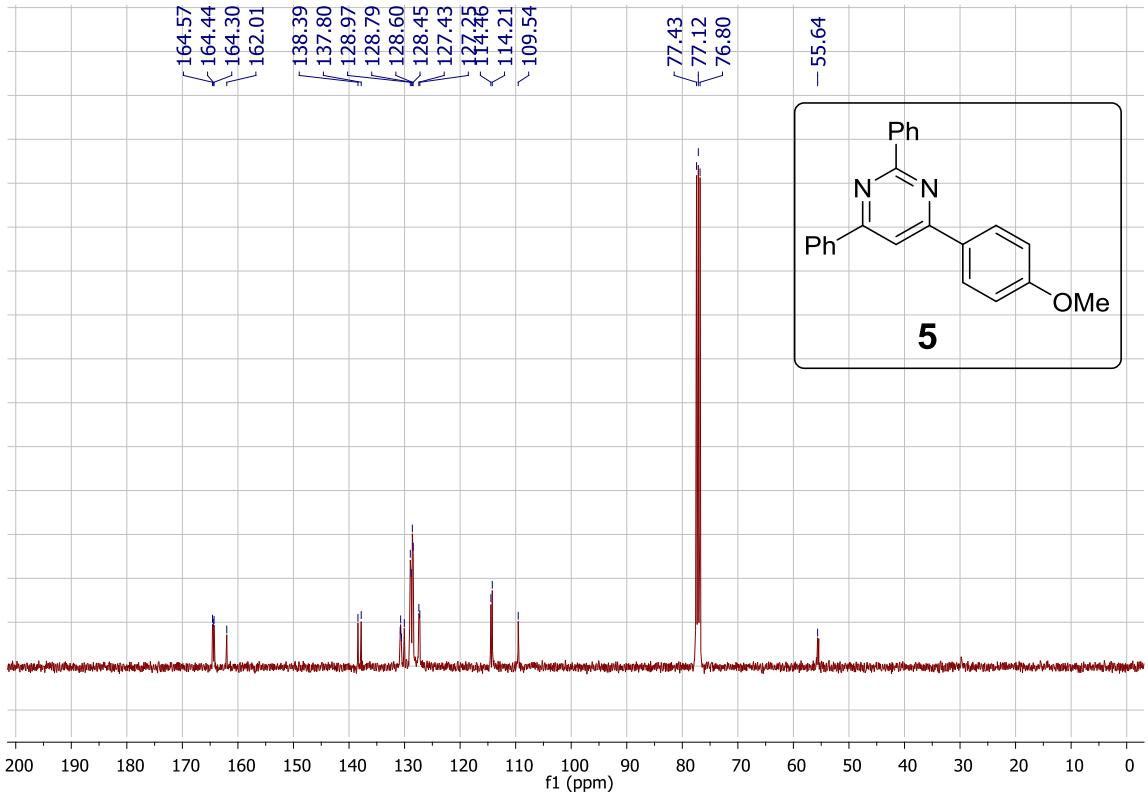
N
Ph
OMe
5
2.13
4.29
1.00
6.12
2.11
3.01
f1 (ppm)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164.44
164.30
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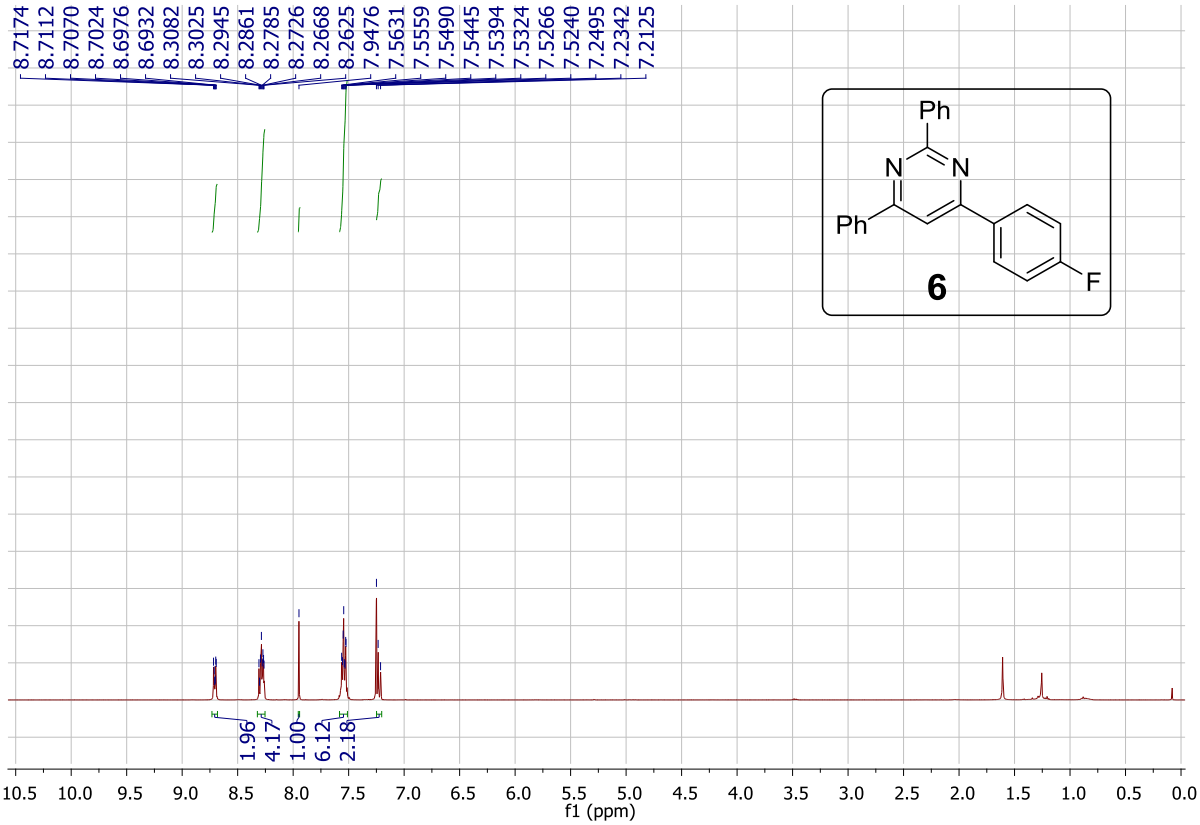
138.39
137.80
128.97
128.79
128.60
128.45
127.43
114.21
109.54
77.43
77.12
76.80
55.64
Ph
N
N
Ph
OMe
5
f1 (ppm)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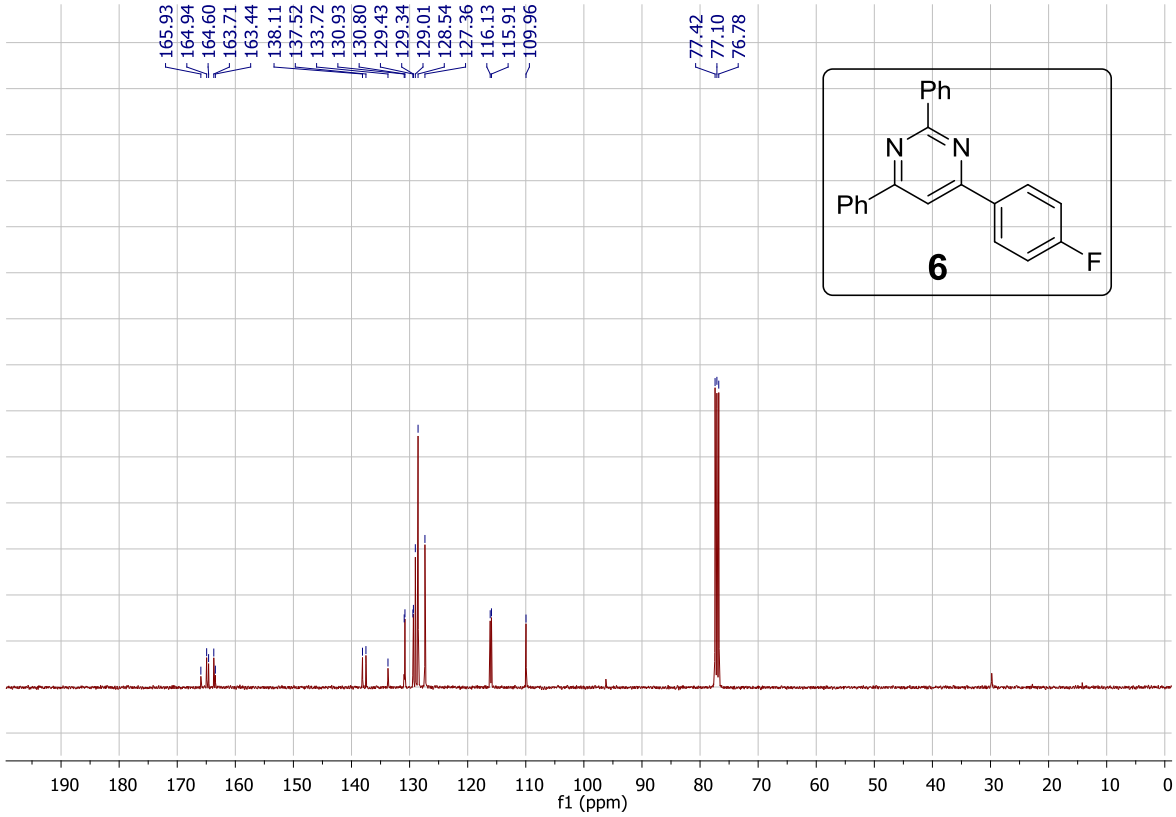
8.6976
8.6932
8.3082
8.3025
8.2945
8.2861
8.2785
8.2726
8.2668
8.2625
7.9476
7.5631
7.5559
7.5490
7.5445
7.5394
7.5324
7.5266
7.5240
7.2495
7.2342
7.2125
1.96
4.17
1.00
6.12
2.18
Ph
N
N
Ph
F
6
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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164.94
164.60
163.71
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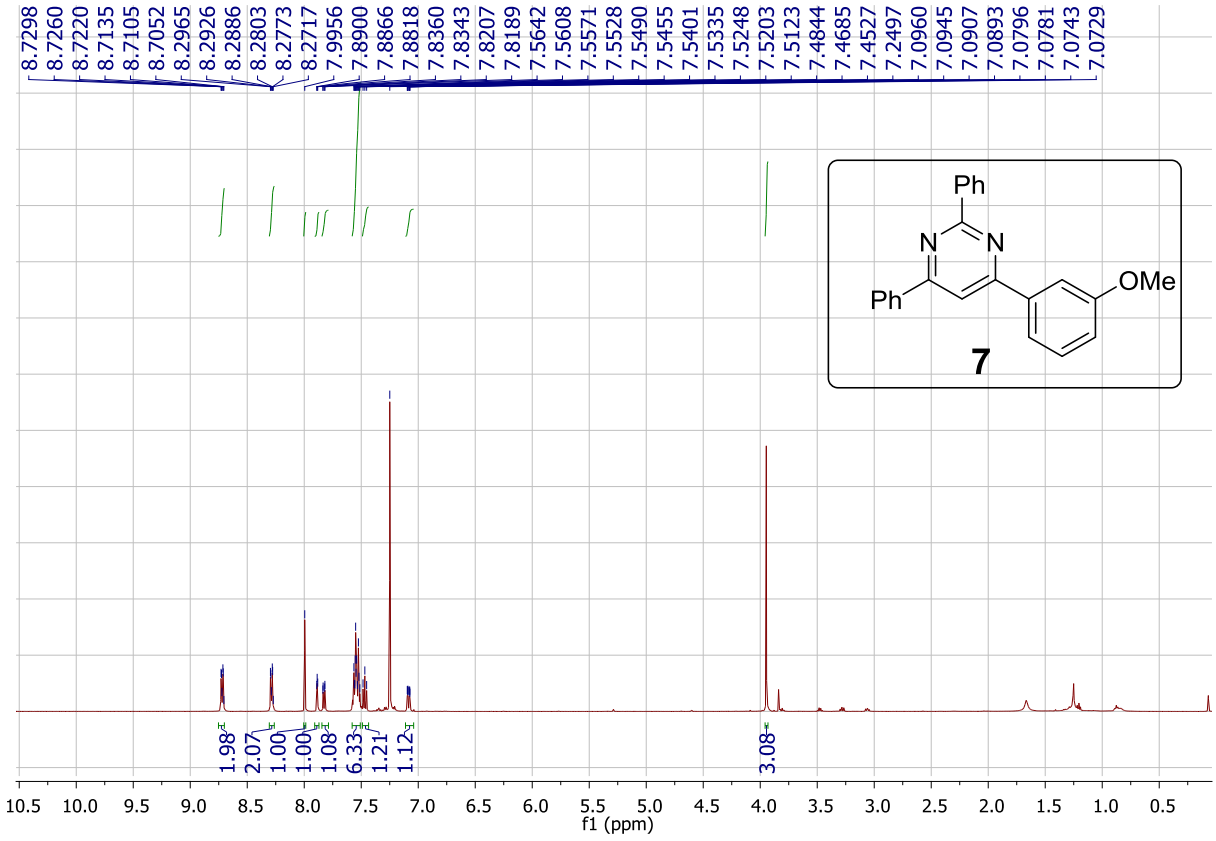
138.11
137.52
133.72
130.93
130.80
129.43
129.34
129.01
128.54
127.36
116.13
115.91
109.96
77.42
77.10
76.78
Ph
N
N
Ph
F
6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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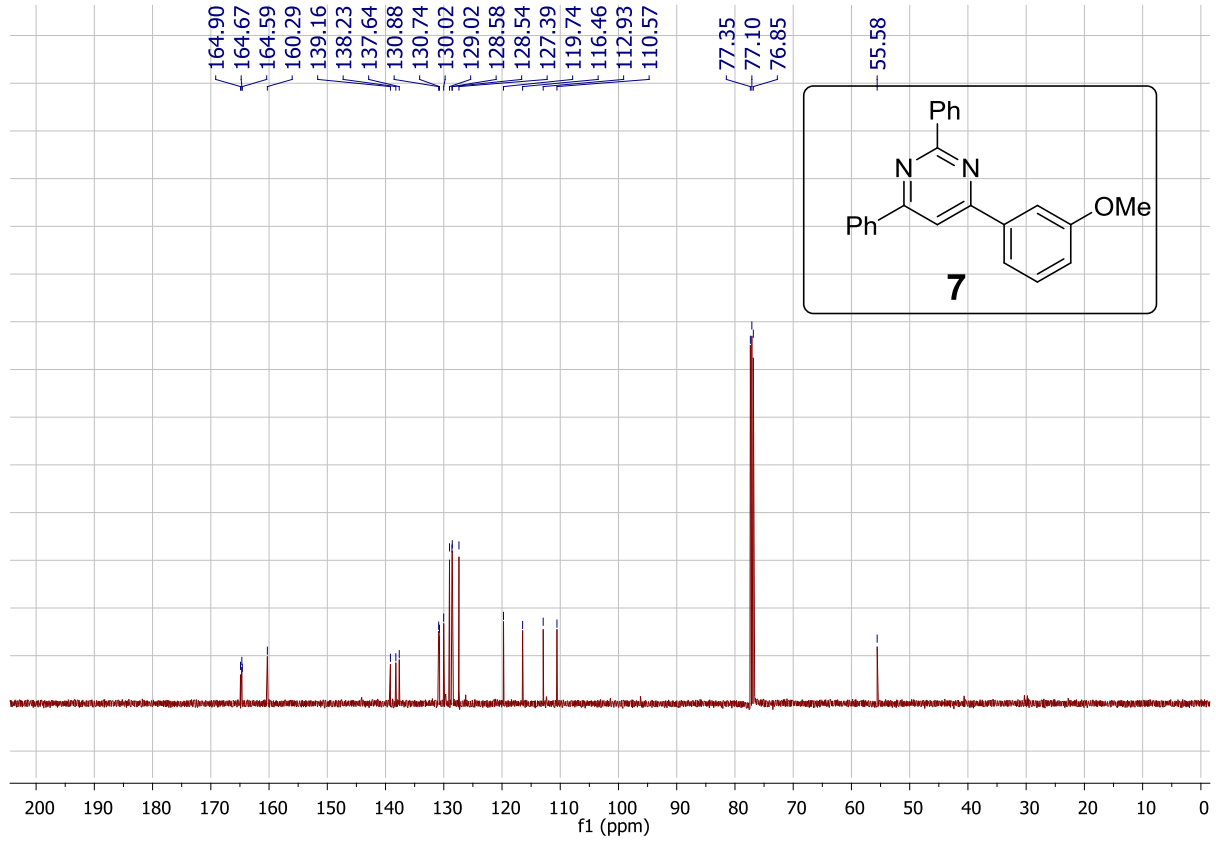
8.2717
7.9956
7.8900
7.8866
7.8818
7.8360
7.8343
7.8207
7.8189
7.5642
7.5608
7.5571
7.5528
7.5490
7.5455
7.5401
7.5335
7.5248
7.5203
7.5123
7.4844
7.4685
7.4527
7.2497
7.0960
7.0945
7.0907
7.0893
7.0796
7.0781
7.0743
7.0729
Ph
N
N
Ph
OMe
7
1.98
2.07
1.00
1.00
1.08
6.33
1.21
1.12
3.08
10.5 10.0 9.5 9.0 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
f1 (ppm)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139.16
138.23
137.64
130.88
130.74
130.02
129.02
128.58
128.54
127.39
119.74
116.46
112.93
110.57
77.35
77.10
76.85
55.58
Ph
N
N
Ph
OMe
7
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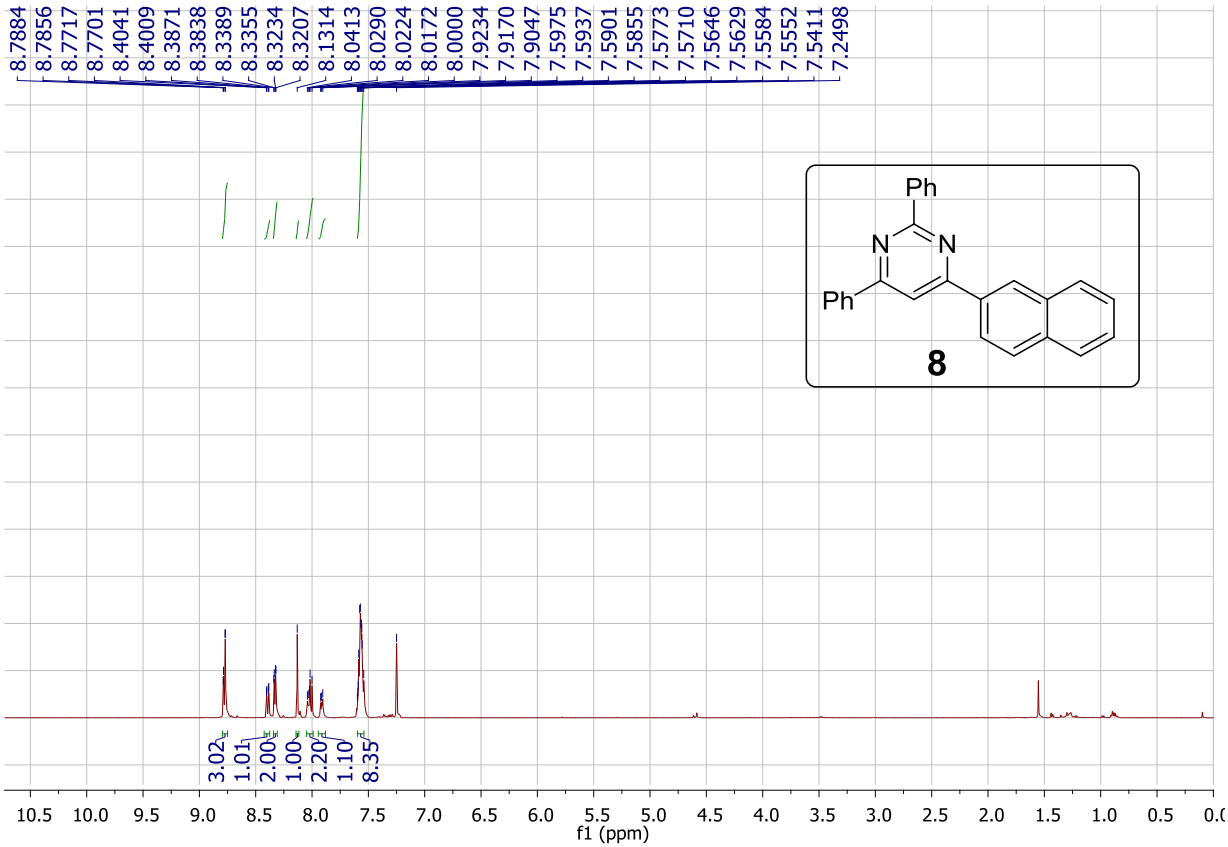
f1 (ppm)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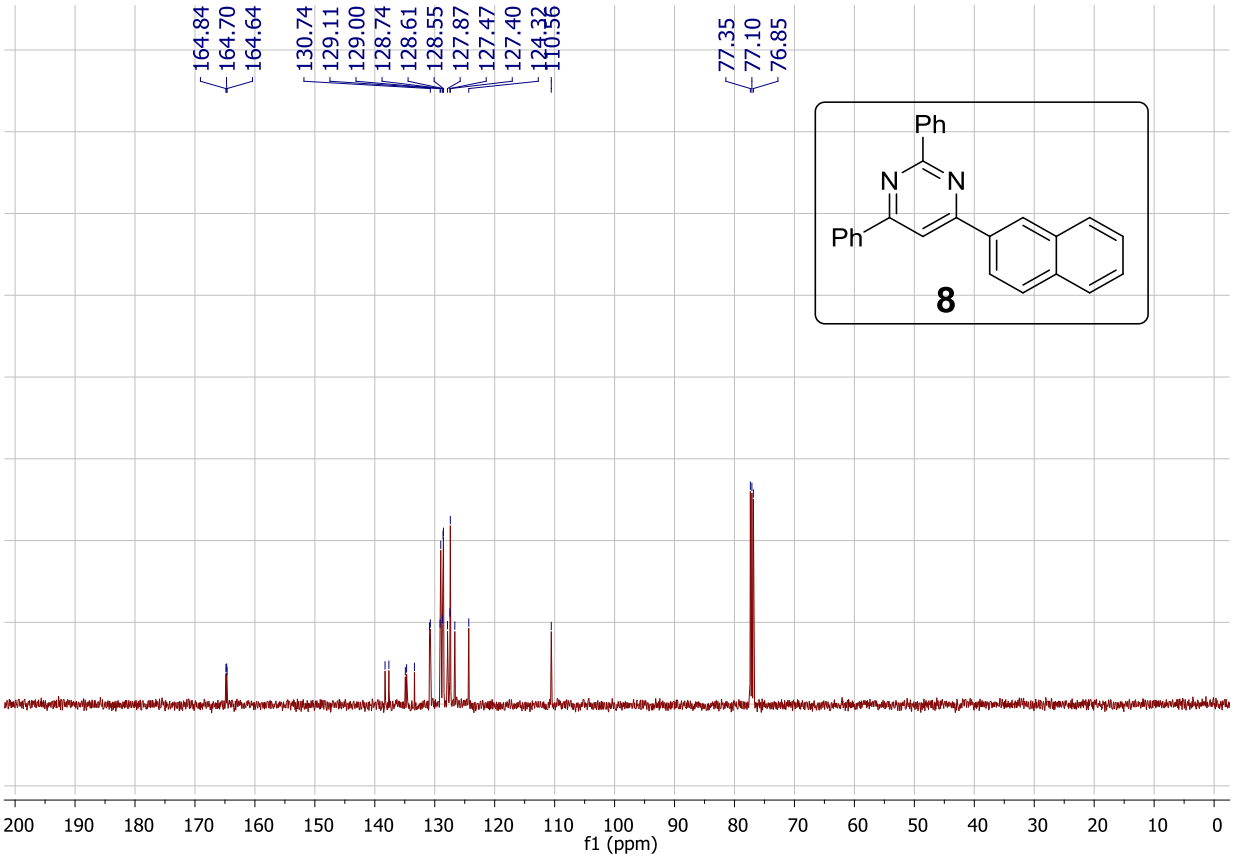
8.4009
8.3871
8.3838
8.3389
8.3355
8.3234
8.3207
8.1314
8.0413
8.0290
8.0224
8.0172
8.0000
7.9234
7.9170
7.9047
7.5975
7.5937
7.5901
7.5855
7.5773
7.5710
7.5646
7.5629
7.5584
7.5552
7.5411
7.2498
Ph
N
N
Ph
8
3.02
1.01
2.00
1.00
2.20
1.10
8.35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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164.64
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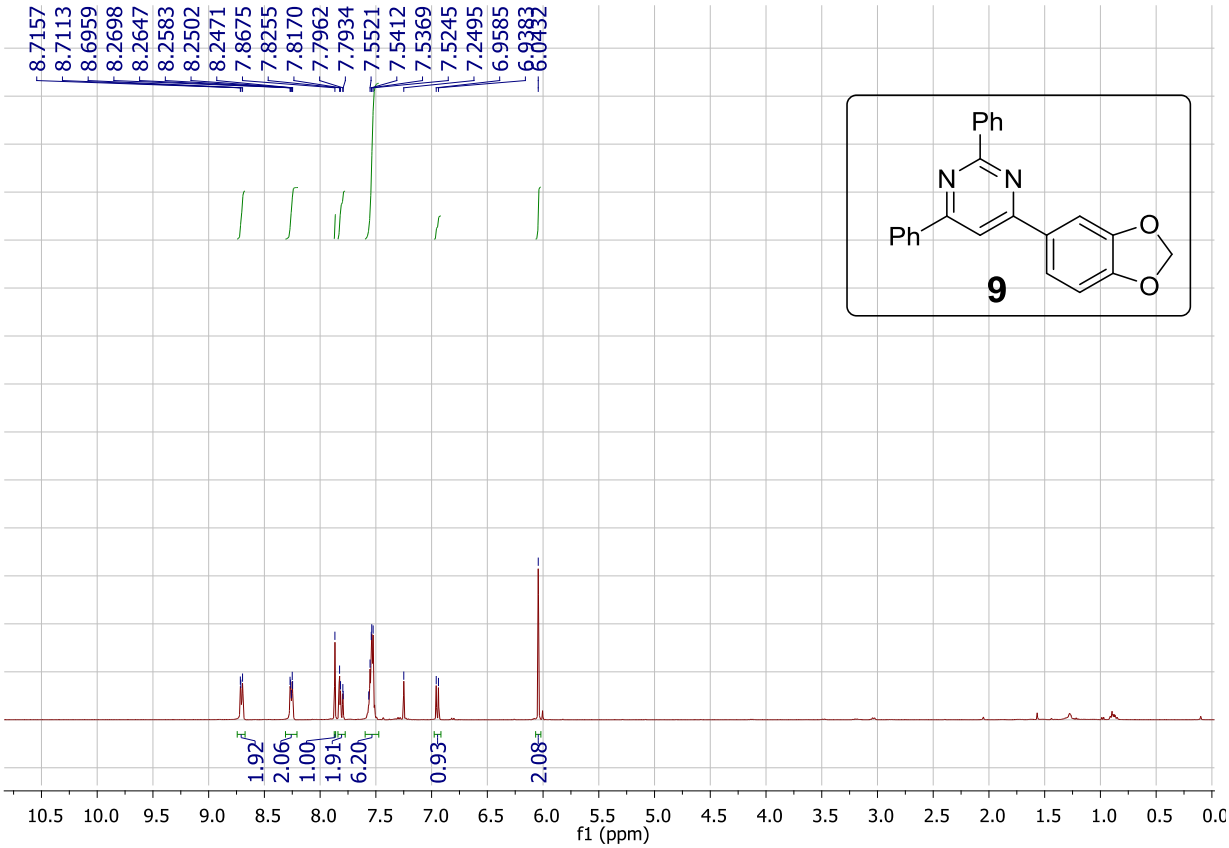
129.11
129.00
128.74
128.61
128.55
127.87
127.47
127.40
124.32
110.56
77.35
77.10
76.85
Ph
N
N
Ph
8
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.6959
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8.2647
8.2583
8.2502
8.2471
7.8675
7.8255
7.8170
7.7962
7.7934
7.5521
7.5412
7.5369
7.5245
7.2495
6.9585
6.9383
6.0432
1.92
2.06
1.00
1.91
6.20
0.93
2.08
f1 (ppm)
Ph
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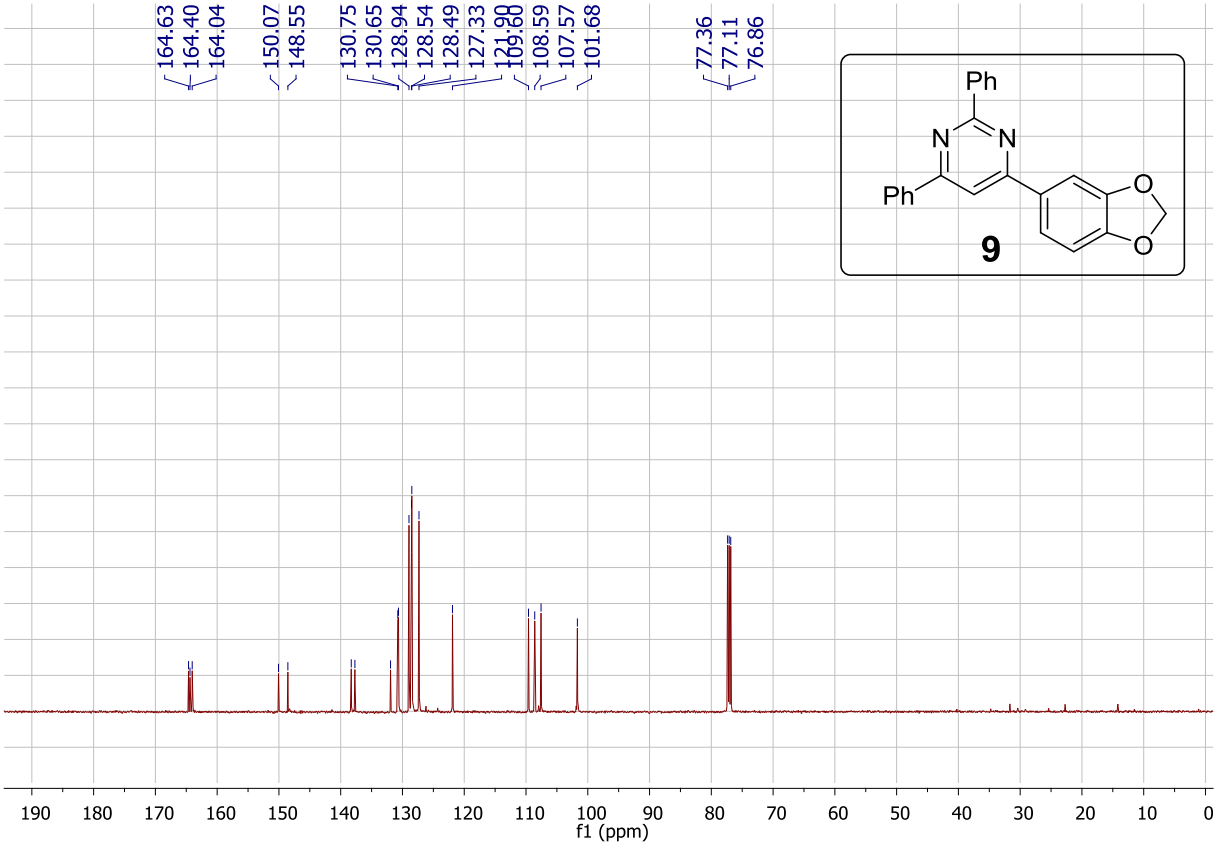
N
Ph
O
O
9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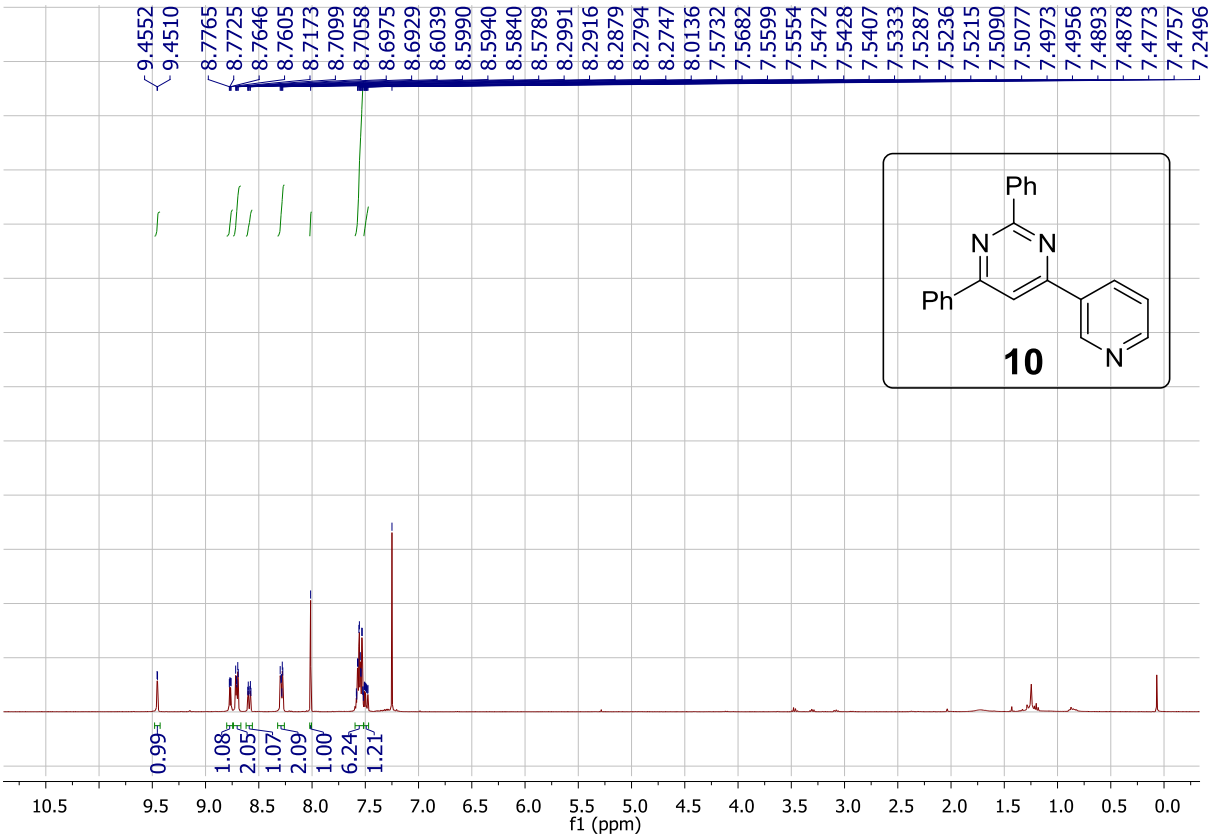
164.04
150.07
148.55
130.75
130.65
128.94
128.54
128.49
127.33
121.90
109.60
108.59
107.57
101.68
77.36
77.11
76.86
f1 (ppm)
Ph
N
N
Ph
O
O
9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9.4510
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8.7725
8.7646
8.7605
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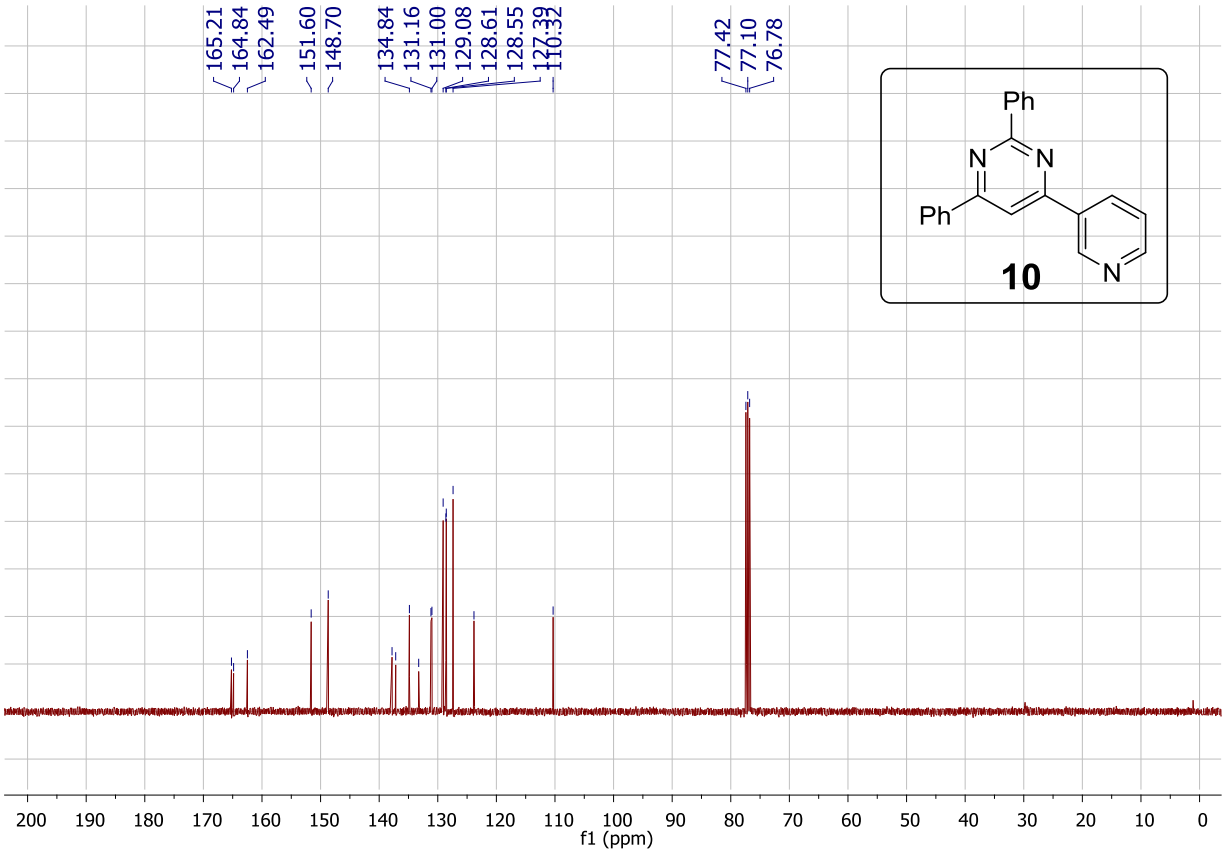
8.6929
8.6039
8.5990
8.5940
8.5840
8.5789
8.2991
8.2916
8.2879
8.2794
8.2747
8.0136
7.5732
7.5682
7.5599
7.5554
7.5472
7.5428
7.5407
7.5333
7.5287
7.5236
7.5215
7.5090
7.5077
7.4973
7.4956
7.4893
7.4878
7.4773
7.4757
7.2496
Ph
N
N
Ph
N
10
0.99
1.08
2.05
1.07
2.09
1.00
6.24
1.21
10.5
9.5
9.0
8.5
8.0
7.5
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)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151.60
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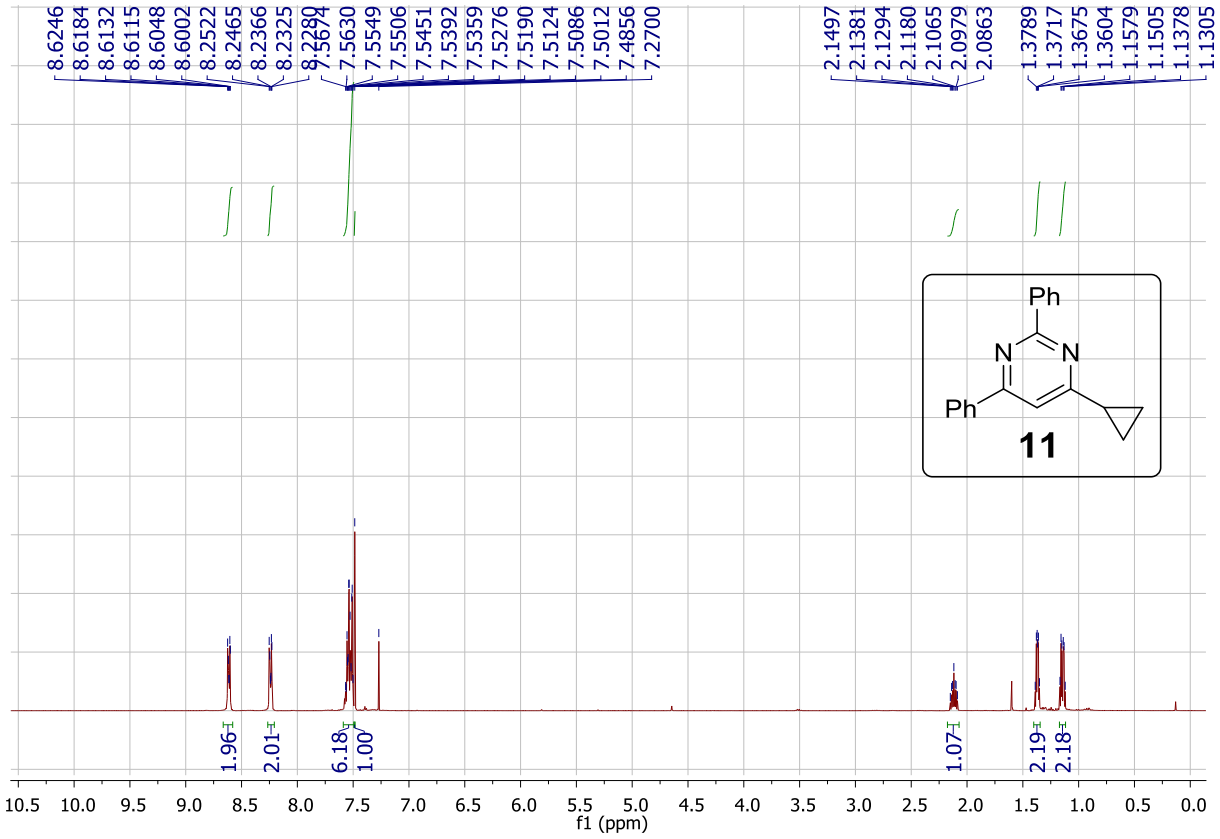
134.84
131.16
131.00
129.08
128.61
128.55
127.39
110.32
77.42
77.10
76.78
Ph
N
N
Ph
N
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.2465
8.2366
8.2325
7.5630
7.5549
7.5506
7.5451
7.5392
7.5359
7.5276
7.5190
7.5124
7.5086
7.5012
7.4856
7.2700
2.1497
2.1381
2.1294
2.1180
2.1065
2.0979
2.0863
1.3789
1.3717
1.3675
1.3604
1.1579
1.1505
1.1378
1.1305
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Ph
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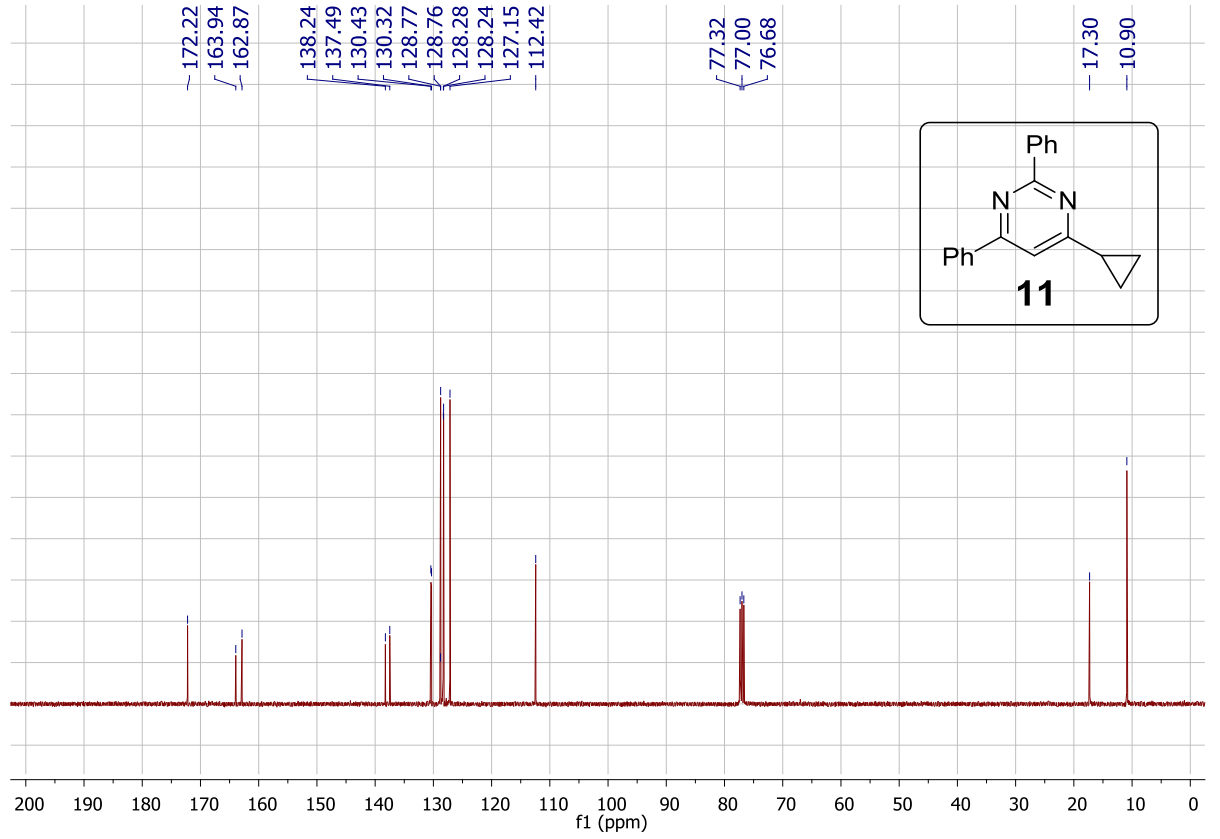
6.18
1.00
1.07
2.19
2.18
f1 (ppm)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130.43
130.32
128.77
128.76
128.28
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77.32
77.00
76.68
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10.90
Ph
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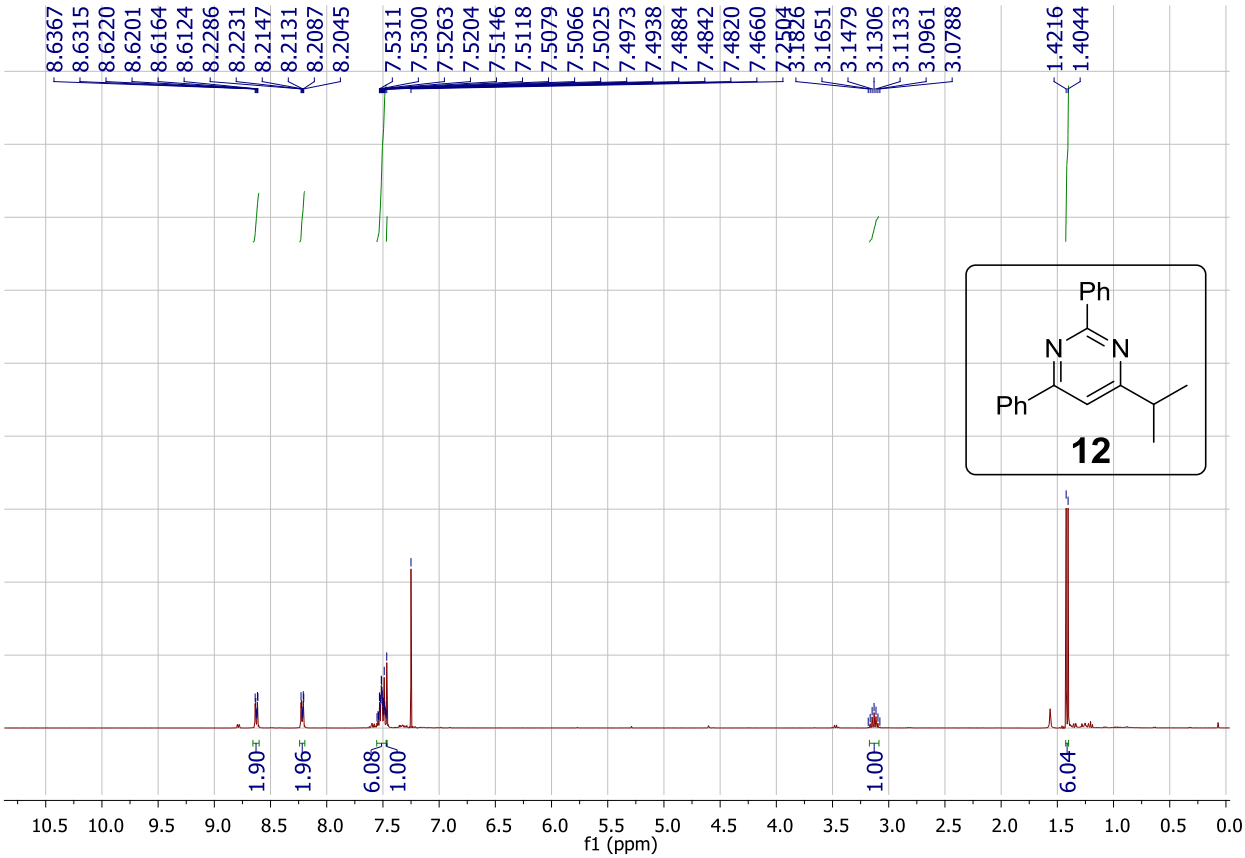
N
Ph
11
f1 (ppm)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8.6124
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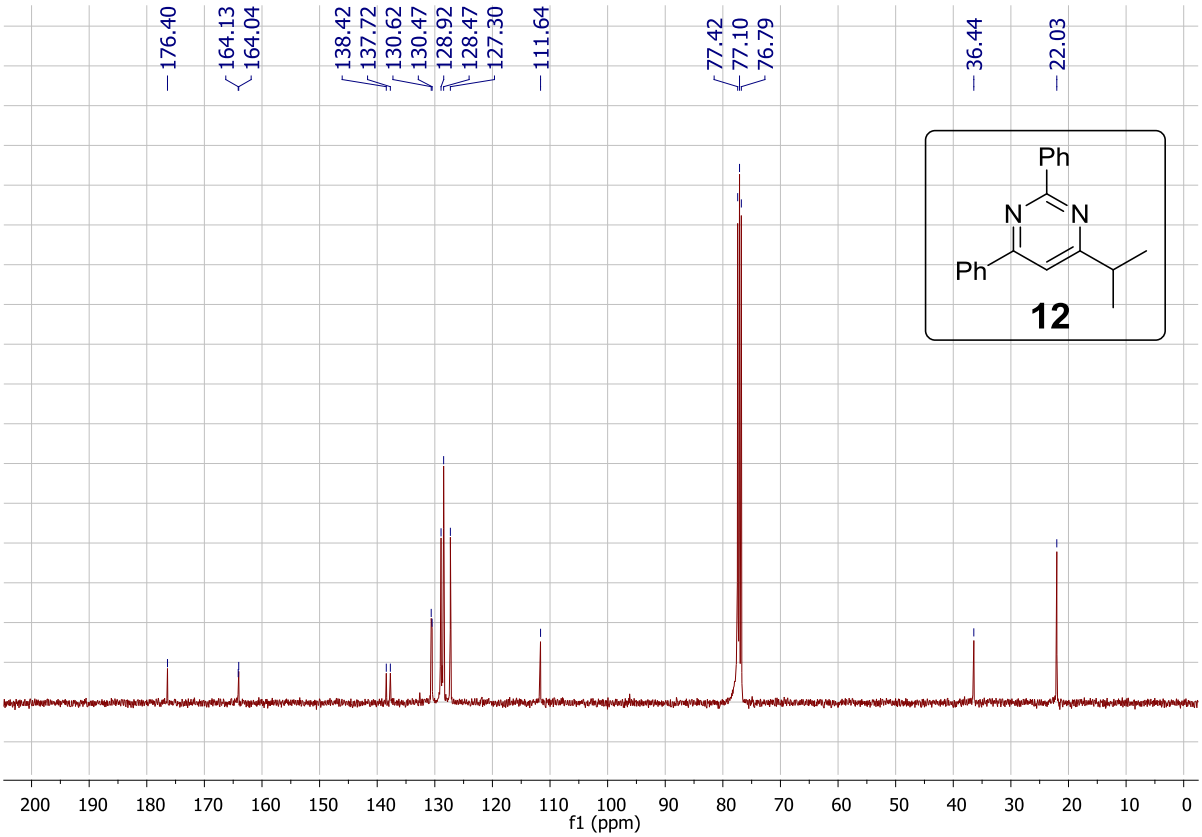
8.2231
8.2147
8.2131
8.2087
8.2045
7.5311
7.5300
7.5263
7.5204
7.5146
7.5118
7.5079
7.5066
7.5025
7.4973
7.4938
7.4884
7.4842
7.4820
7.4660
3.1651
3.1479
3.1306
3.1133
3.0961
3.0788
1.4216
1.4044
Ph
N
N
Ph
12
1.90
1.96
6.08
1.00
1.00
6.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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164.04
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137.72
130.62
130.47
128.92
128.47
127.30
111.64
77.42
77.10
76.79
36.44
22.03
Ph
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N
Ph
12
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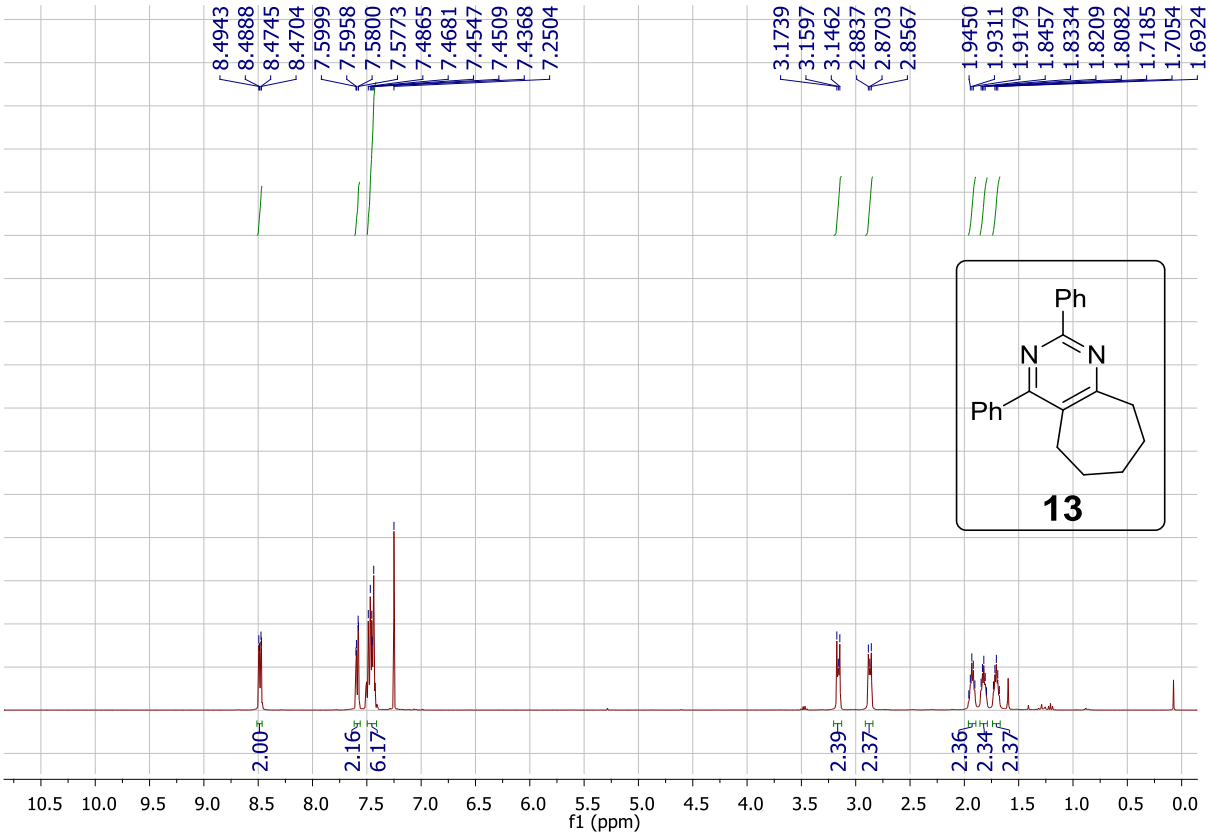
f1 (ppm)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7.4547
7.4509
7.4368
7.2504
3.1739
3.1597
3.1462
2.8837
2.8703
2.8567
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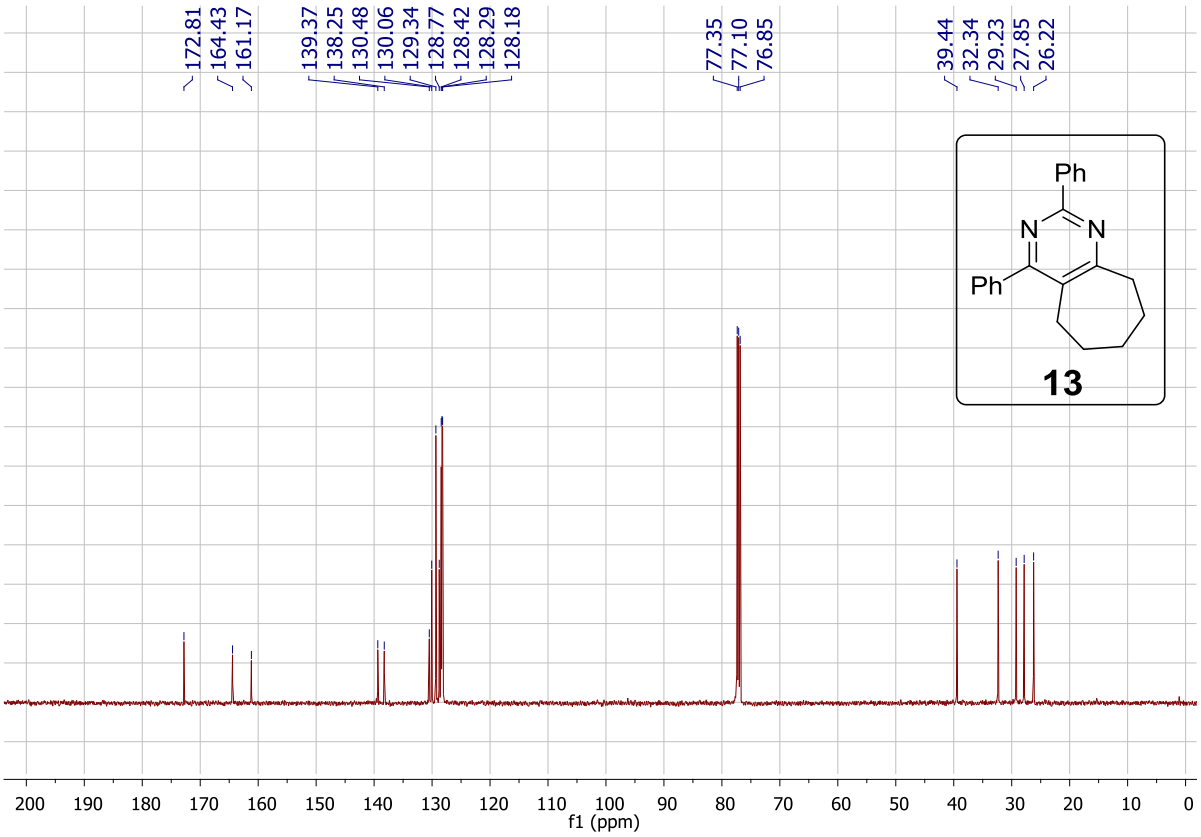
1.9311
1.9179
1.8457
1.8334
1.8209
1.8082
1.7185
1.7054
1.6924
Ph
N
N
Ph
13
2.00
2.16
6.17
2.39
2.37
2.36
2.34
2.37
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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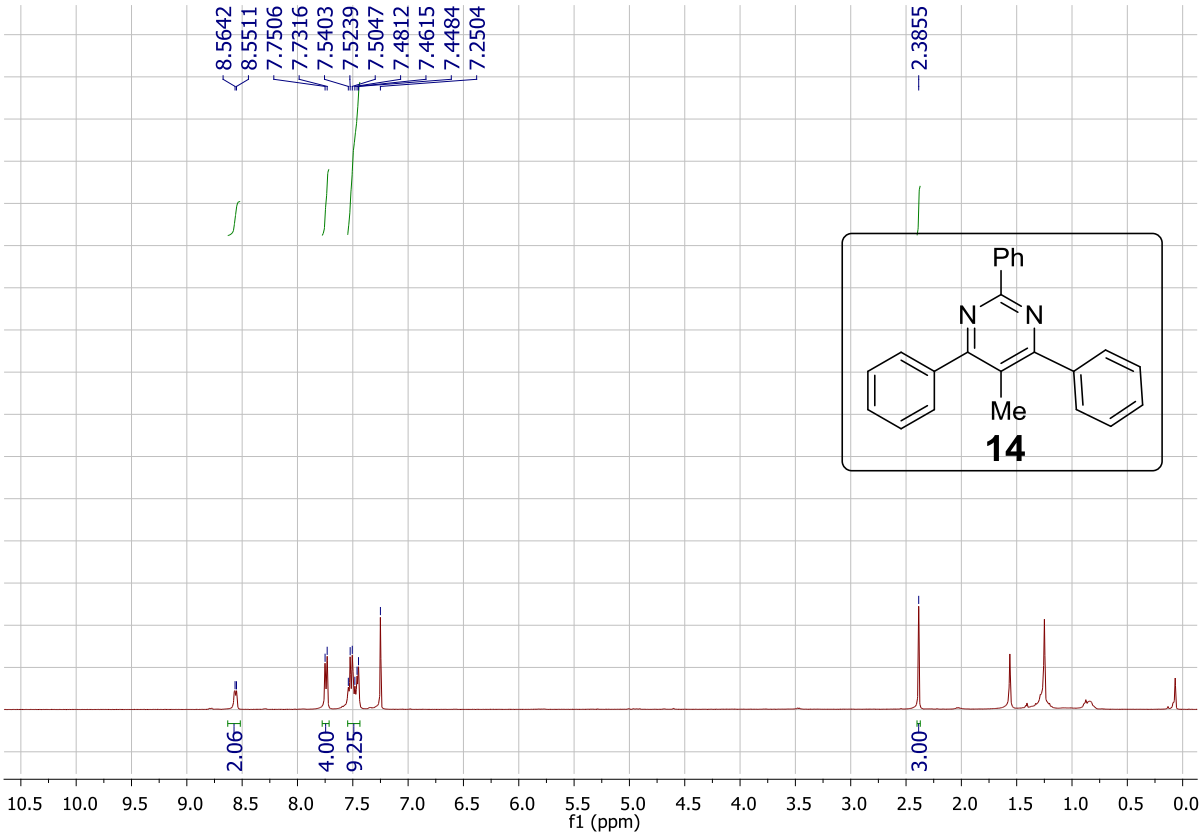
139.37
138.25
130.48
130.06
129.34
128.77
128.42
128.29
128.18
77.35
77.10
76.85
39.44
32.34
29.23
27.85
26.22
Ph
N
N
Ph
13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5047
7.4812
7.4615
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2.3855
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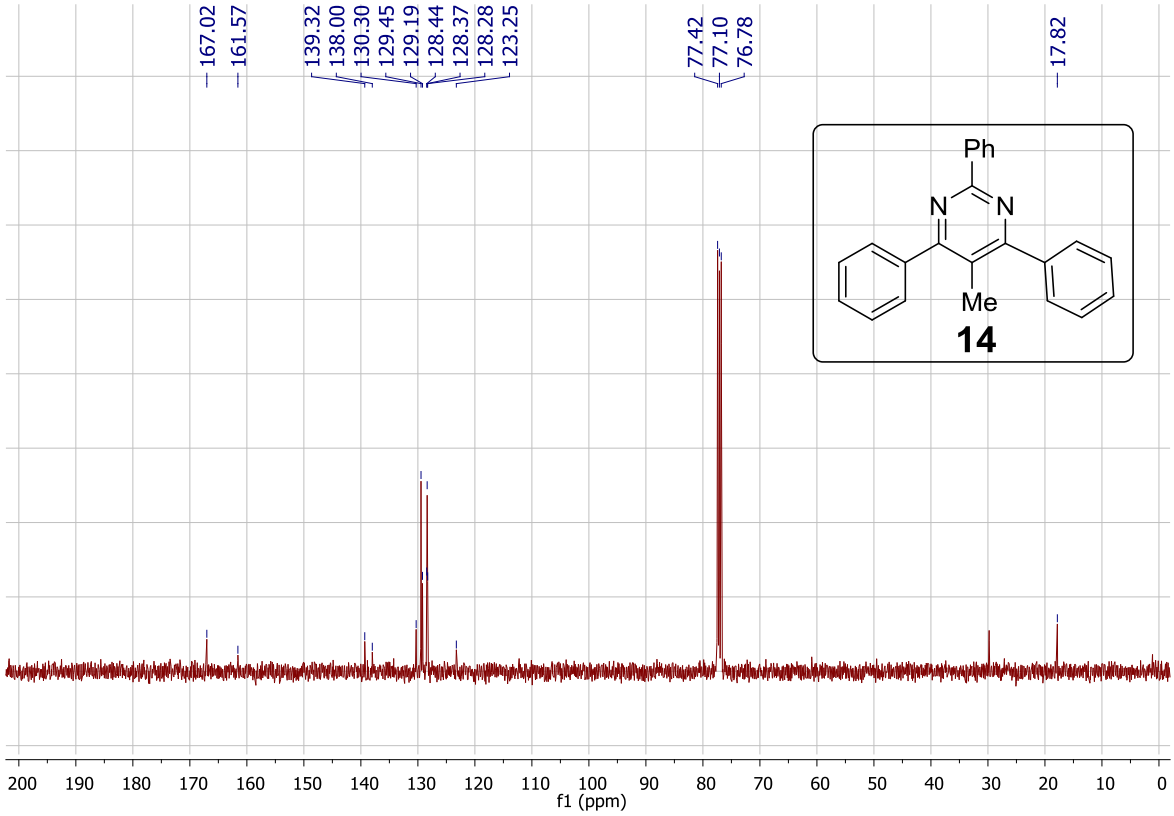
N
Me
14
2.06
4.00
9.25
3.00
f1 (ppm)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128.37
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123.25
77.42
77.10
76.78
17.82
Ph
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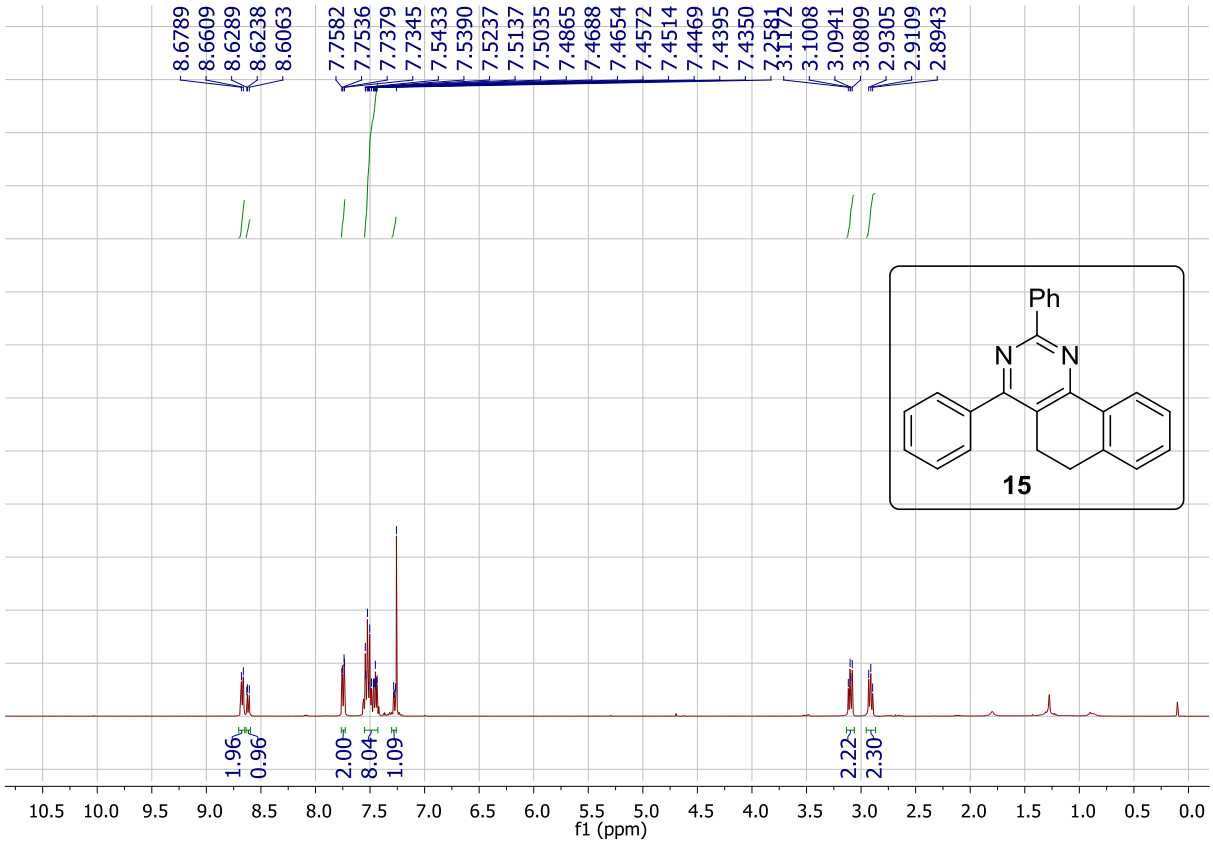
N
Me
14
f1 (ppm)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7.5237
7.5137
7.5035
7.4865
7.4688
7.4654
7.4572
7.4514
7.4469
7.4395
7.4350
3.1008
3.0941
3.0809
2.9305
2.9109
2.8943
Ph
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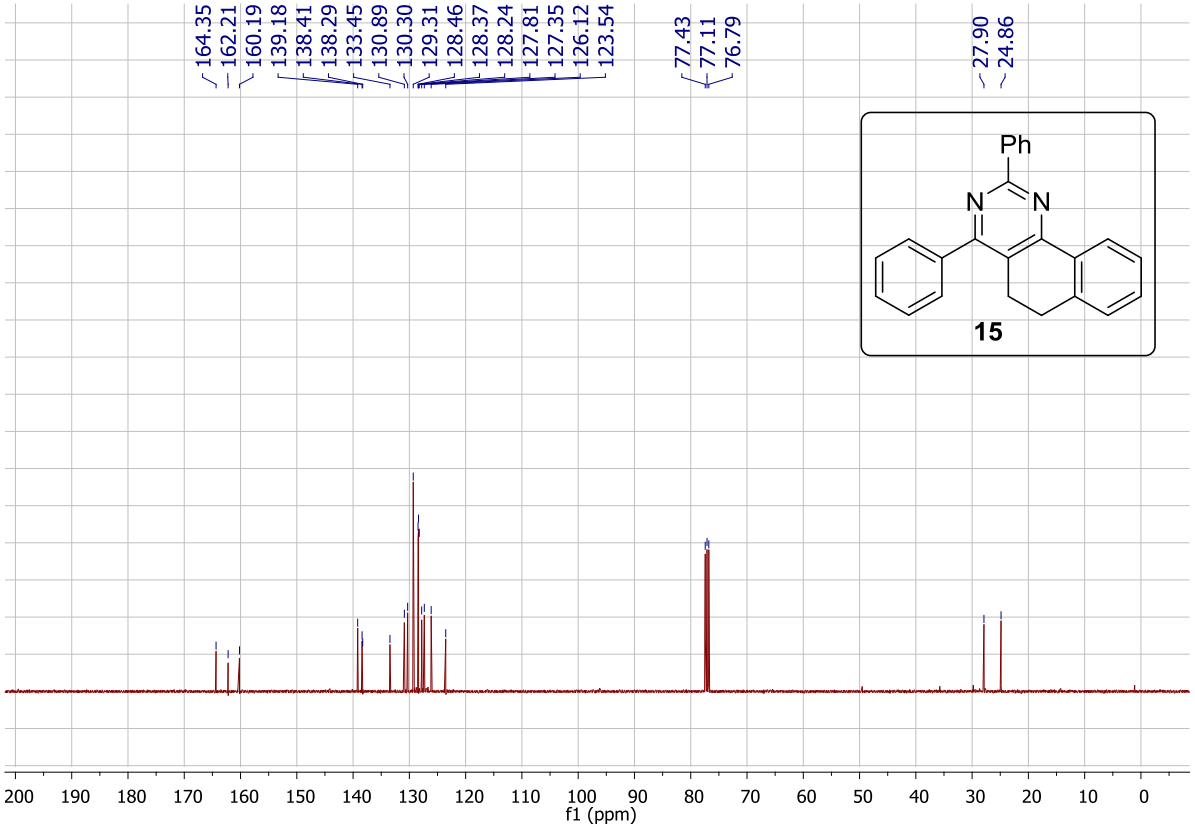
1.96
0.96
2.00
8.04
1.09
2.22
2.30
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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162.21
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139.18
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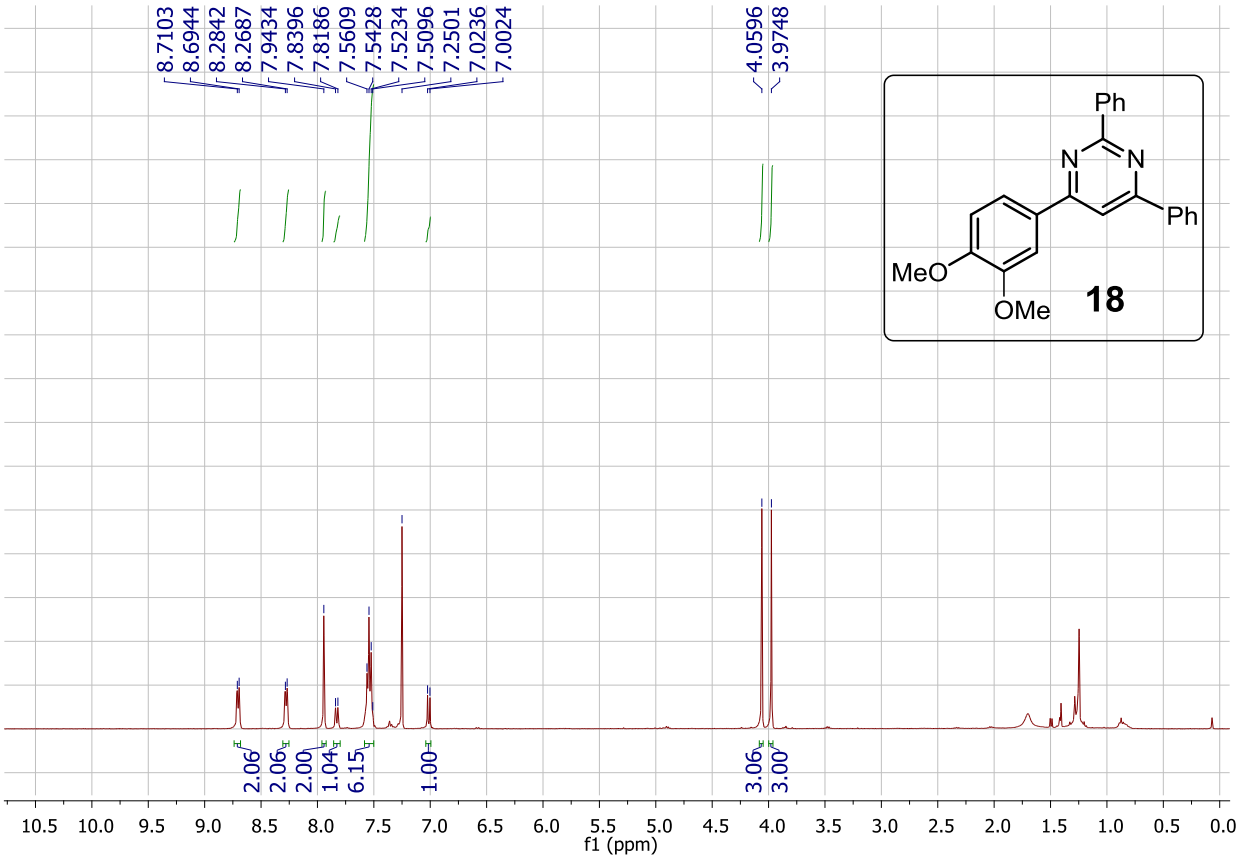
138.29
133.45
130.89
130.30
129.31
128.46
128.37
128.24
127.81
127.35
126.12
123.54
77.43
77.11
76.79
27.90
24.86
Ph
N
N
15
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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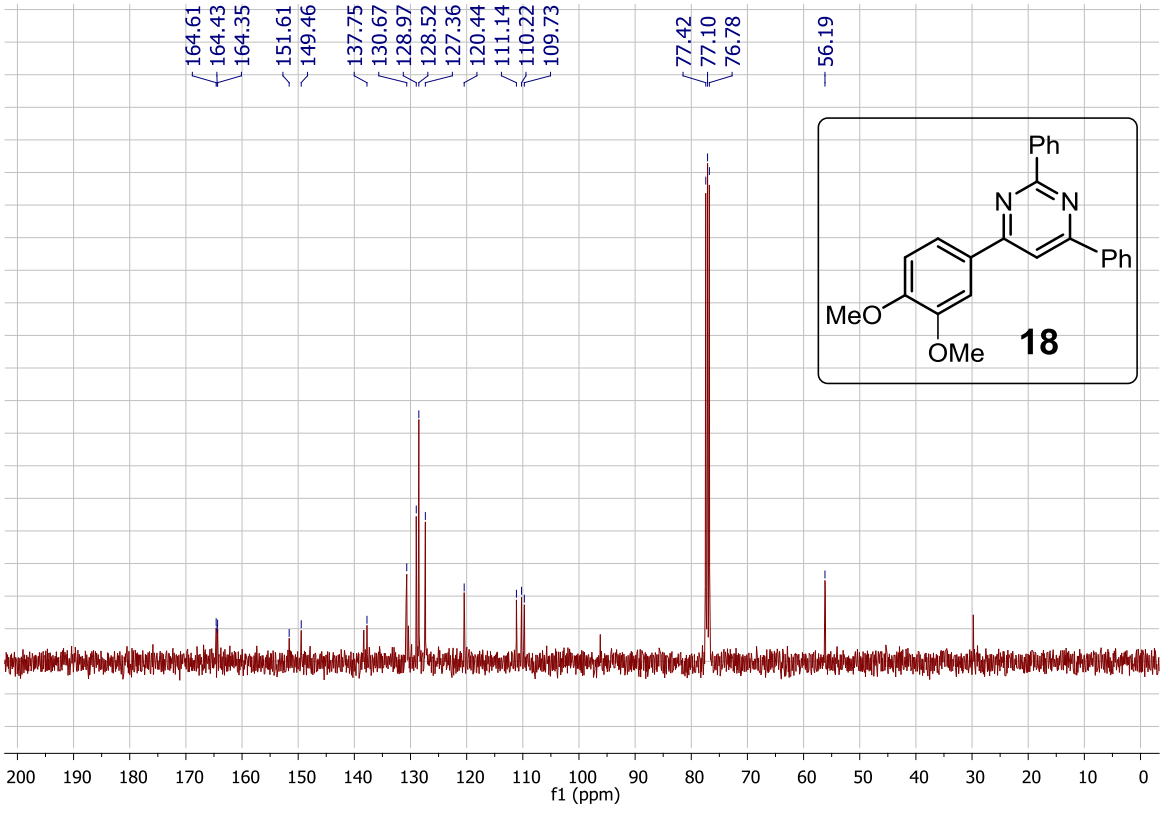
7.2501
7.0236
7.0024
4.0596
3.9748
Ph
N
N
Ph
MeO
OMe
18
2.06
2.06
2.00
1.04
6.15
1.00
3.06
3.00
f1 (ppm)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127.36
120.44
111.14
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77.42
77.10
76.78
56.19
Ph
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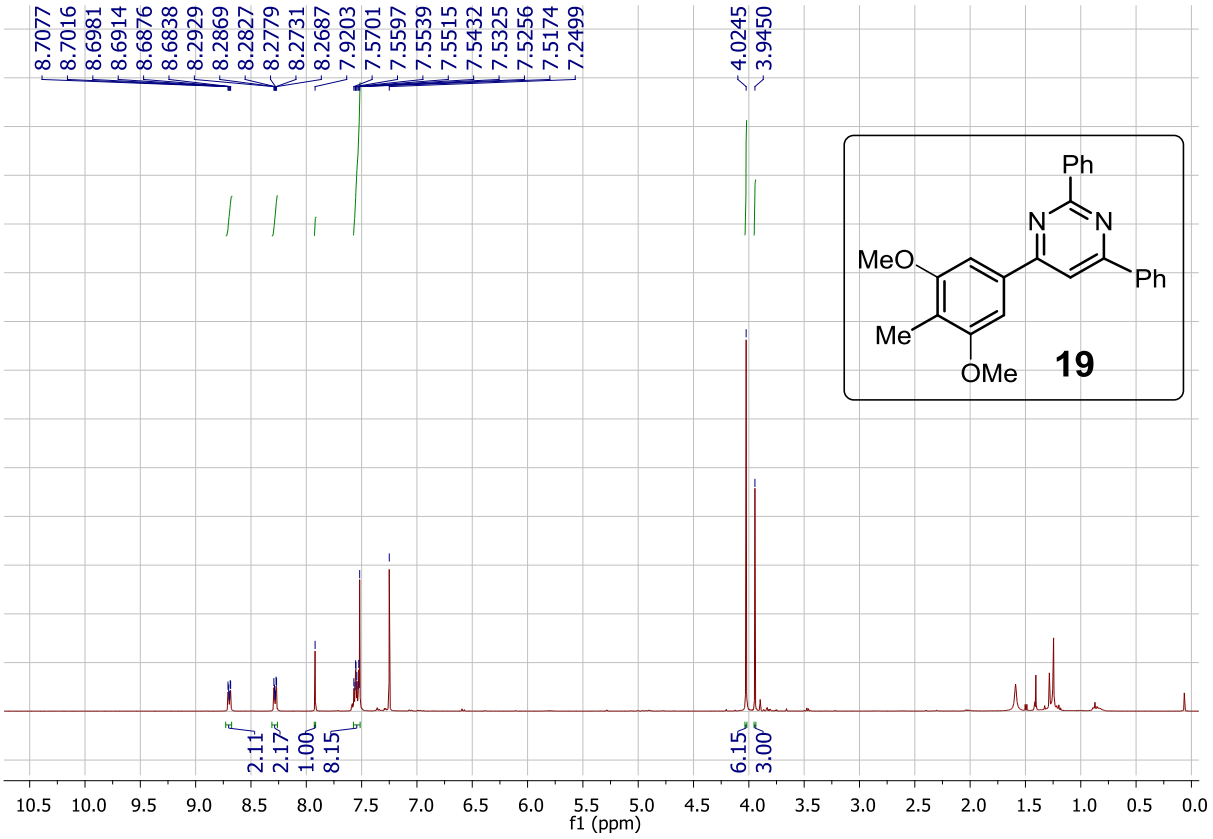
N
Ph
MeO
OMe
18
f1 (ppm)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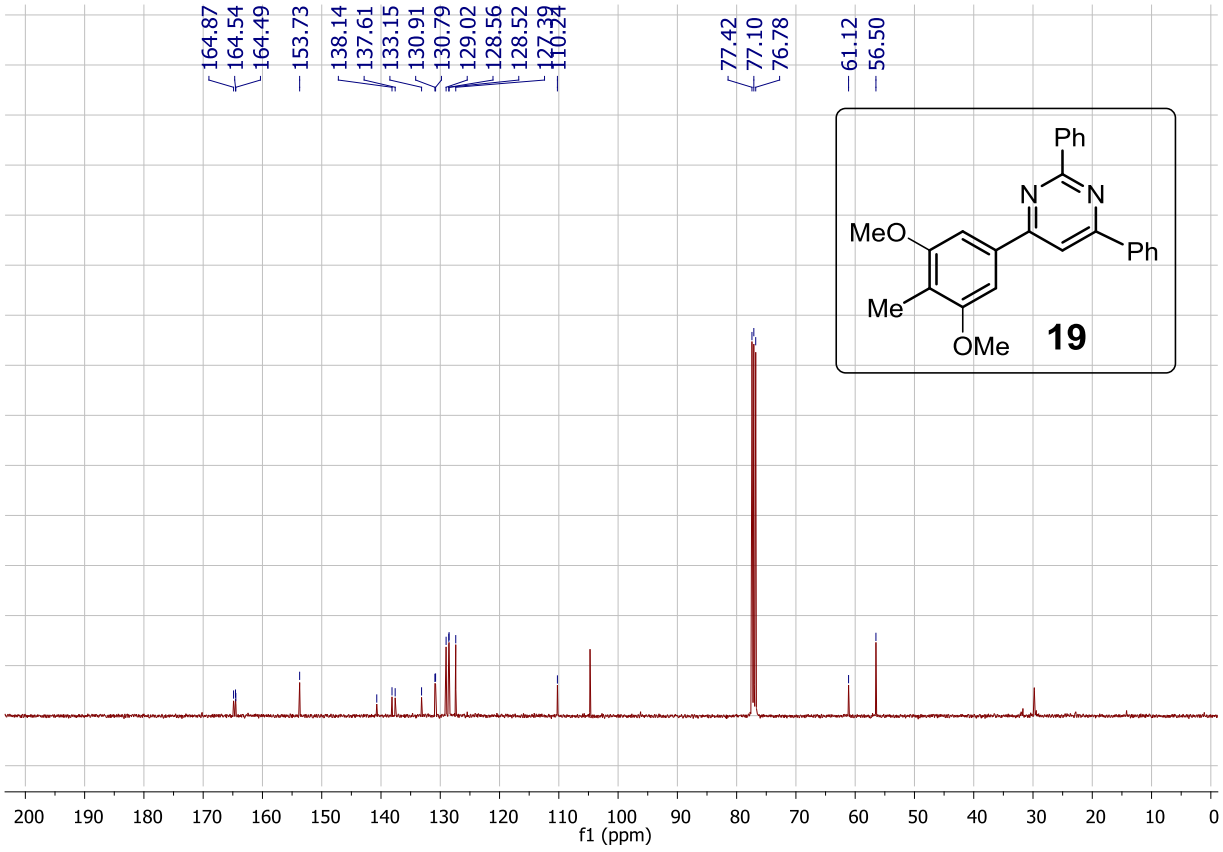
8.2731
8.2687
7.9203
7.5701
7.5597
7.5539
7.5515
7.5432
7.5325
7.5256
7.5174
7.2499
4.0245
3.9450
2.11
2.17
1.00
8.15
6.15
3.00
f1 (ppm)
Ph
N
N
MeO
Ph
Me
OMe
19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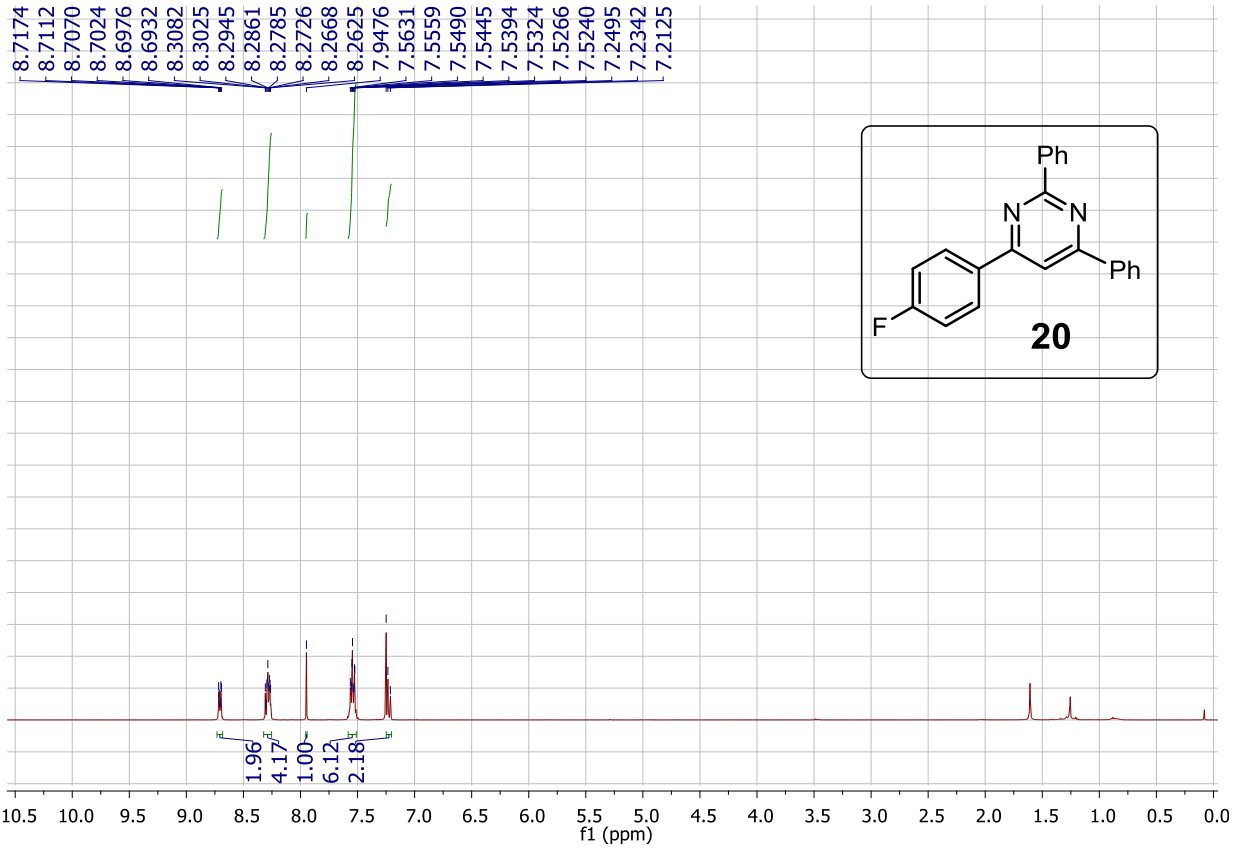
133.15
130.91
130.79
129.02
128.56
128.52
127.39
110.24
77.42
77.10
76.78
61.12
56.50
f1 (ppm)
Ph
N
N
MeO
Ph
Me
OMe
19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8.2861
8.2785
8.2726
8.2668
8.2625
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7.5631
7.5559
7.5490
7.5445
7.5394
7.5324
7.5266
7.5240
7.2495
7.2342
7.2125
1.96
4.17
1.00
6.12
2.18
10.5 10.0 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
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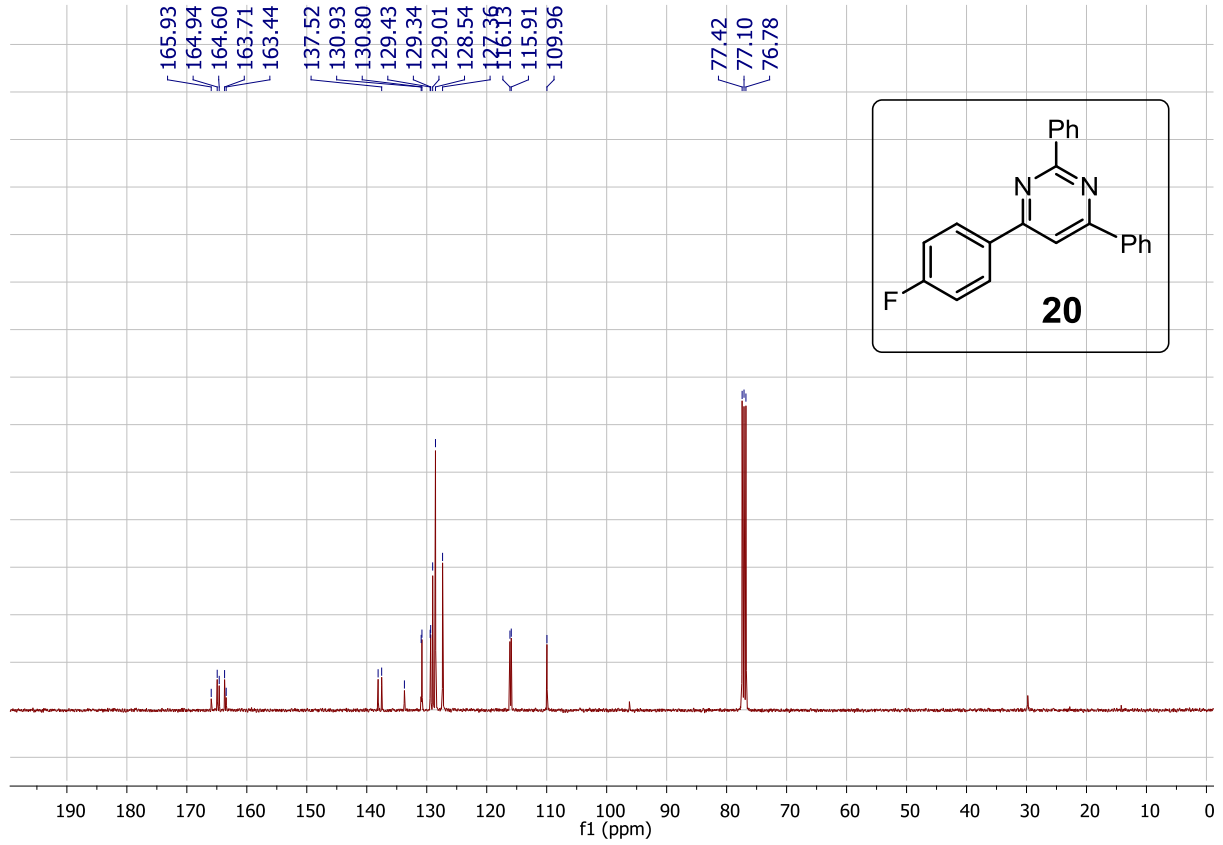
N
Ph
F
20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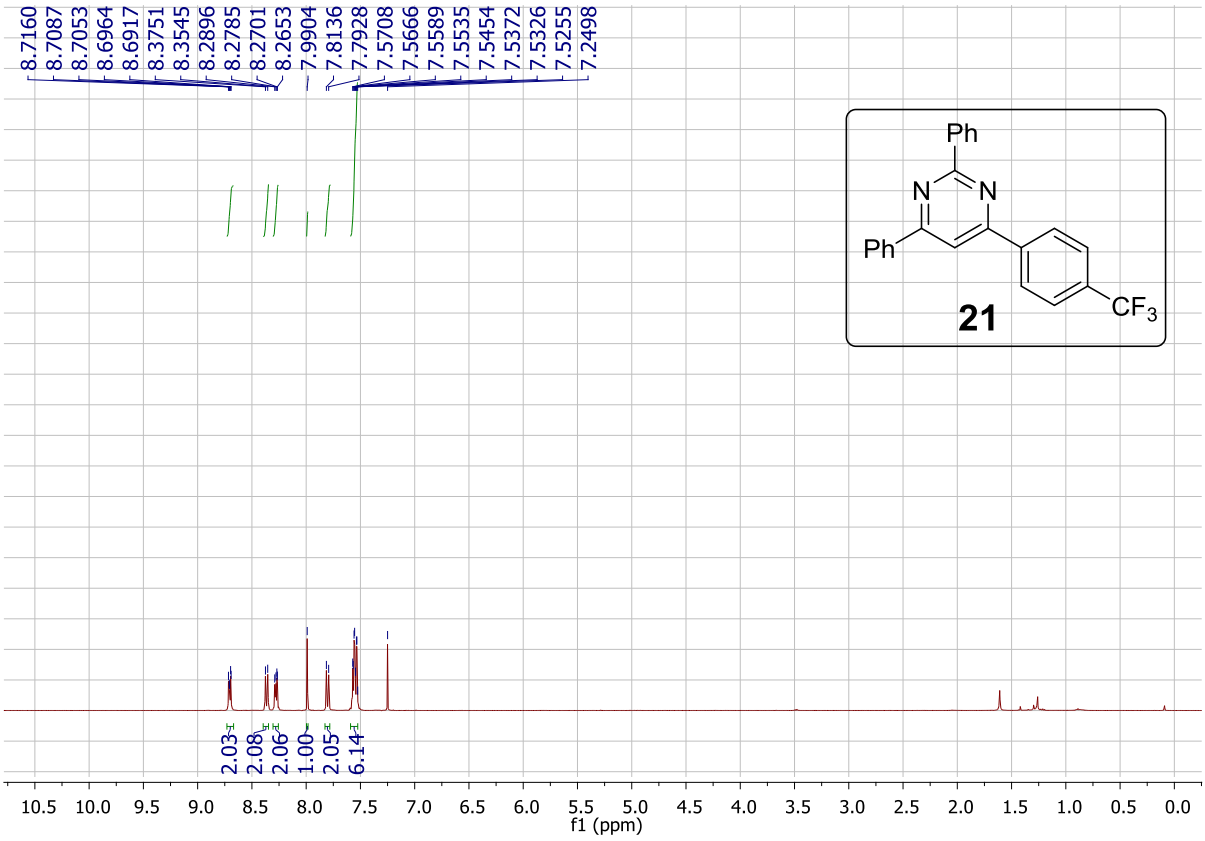
129.34
129.01
128.54
127.36
116.13
115.91
109.96
77.42
77.10
76.78
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Ph
N
N
Ph
F
20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7.8136
7.7928
7.5708
7.5666
7.5589
7.5535
7.5454
7.5372
7.5326
7.5255
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2.06
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2.05
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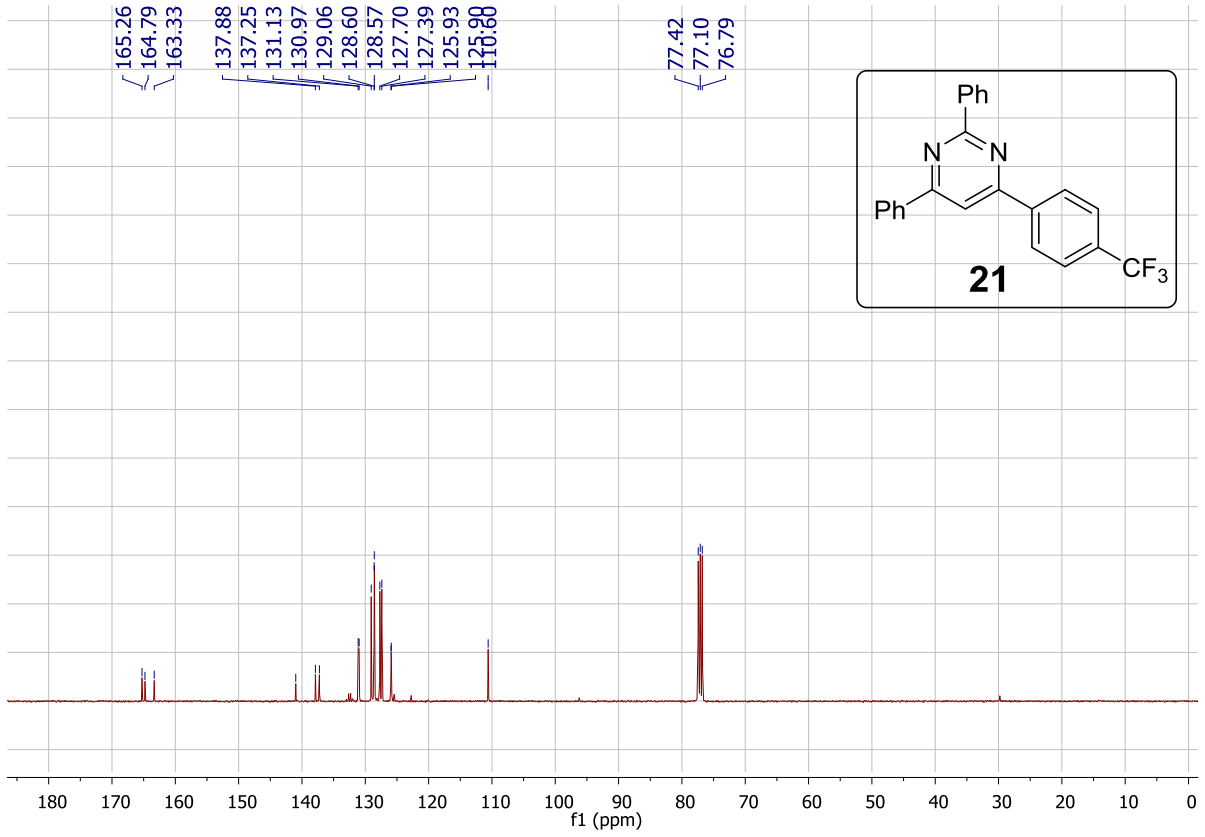
Ph
CF3
21
f1 (ppm)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125.93
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77.10
76.79
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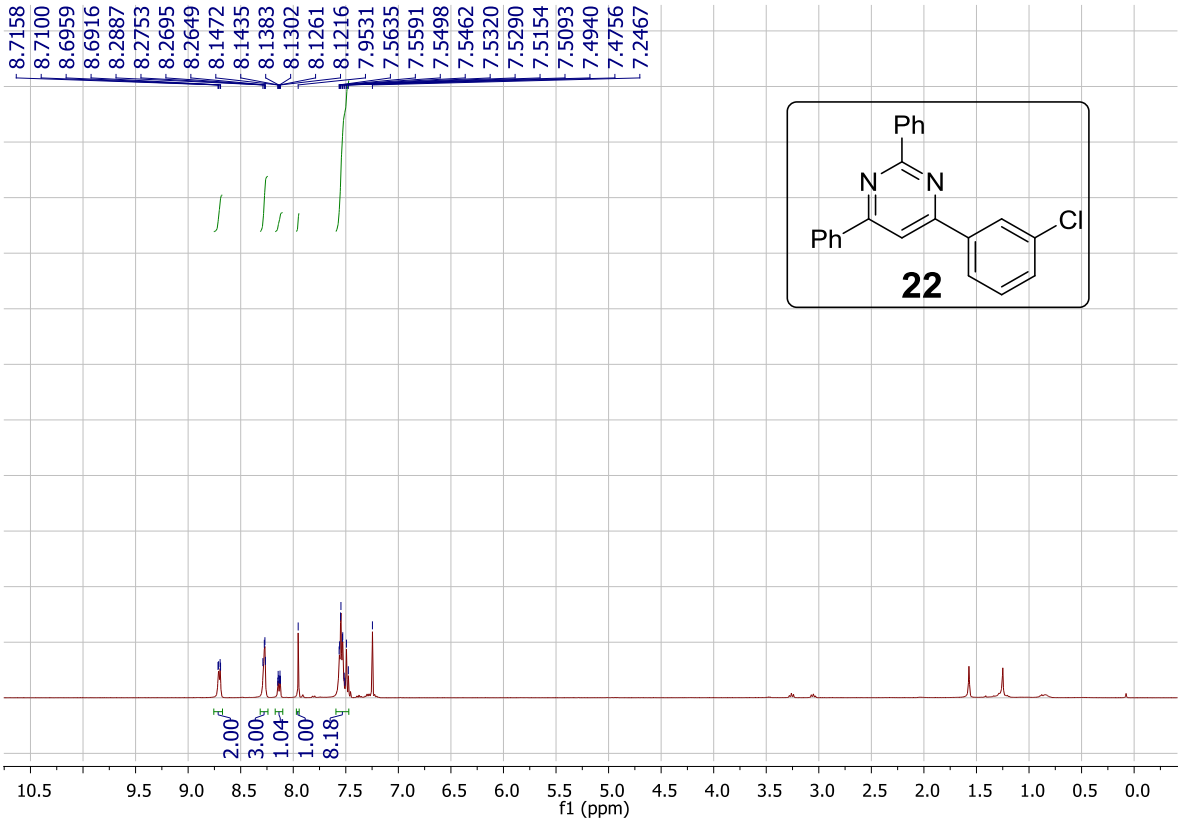
N
N
Ph
CF3
21
f1 (ppm)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8.1472
8.1435
8.1383
8.1302
8.1261
8.1216
7.9531
7.5635
7.5591
7.5498
7.5462
7.5320
7.5290
7.5154
7.5093
7.4940
7.4756
7.2467
Ph
N
N
Ph
Cl
22
2.00
3.00
1.04
1.00
8.18
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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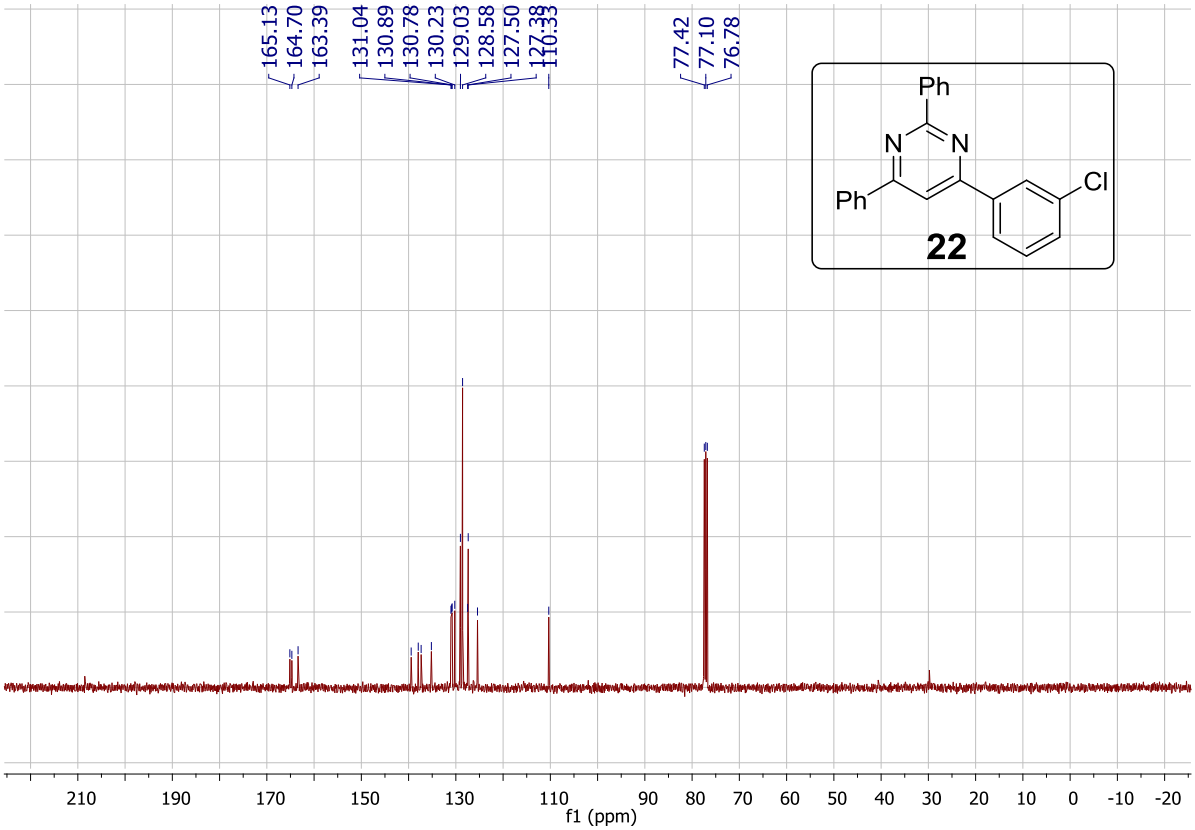
0.0
f1 (ppm)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130.89
130.78
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129.03
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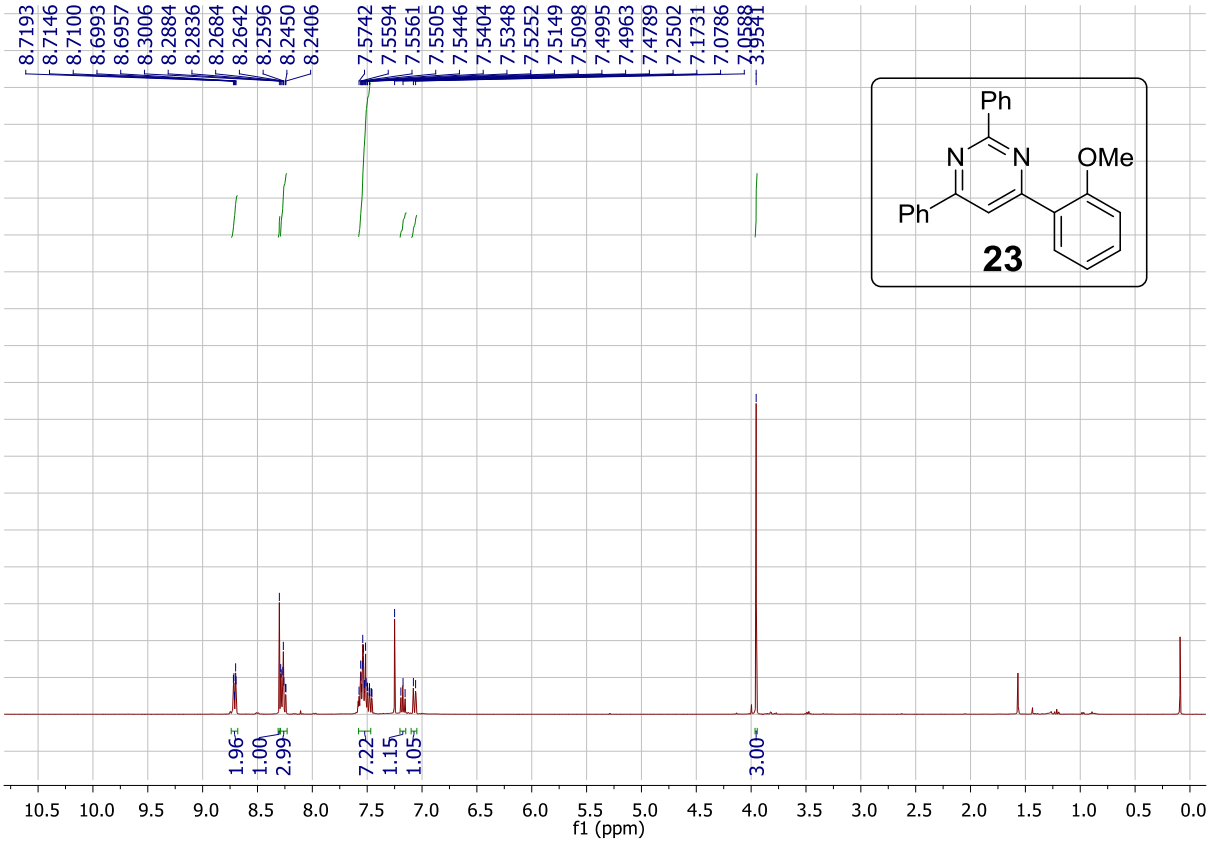
127.50
127.38
110.33
77.42
77.10
76.78
Ph
N
N
Ph
Cl
22
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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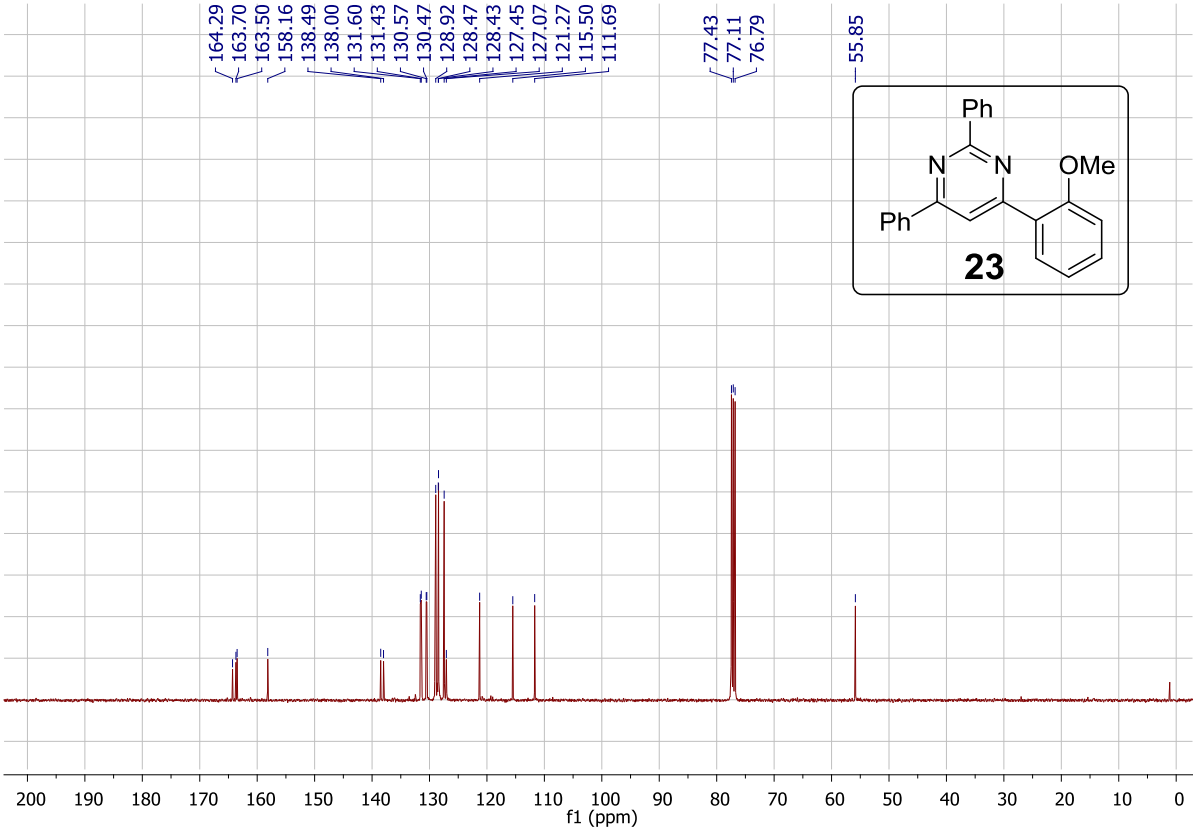
8.2450
8.2406
7.5742
7.5594
7.5561
7.5505
7.5446
7.5404
7.5348
7.5252
7.5149
7.5098
7.4995
7.4963
7.4789
7.2502
7.1731
7.0786
3.9541
Ph
N
N
OMe
Ph
23
1.96
1.00
2.99
7.22
1.15
1.05
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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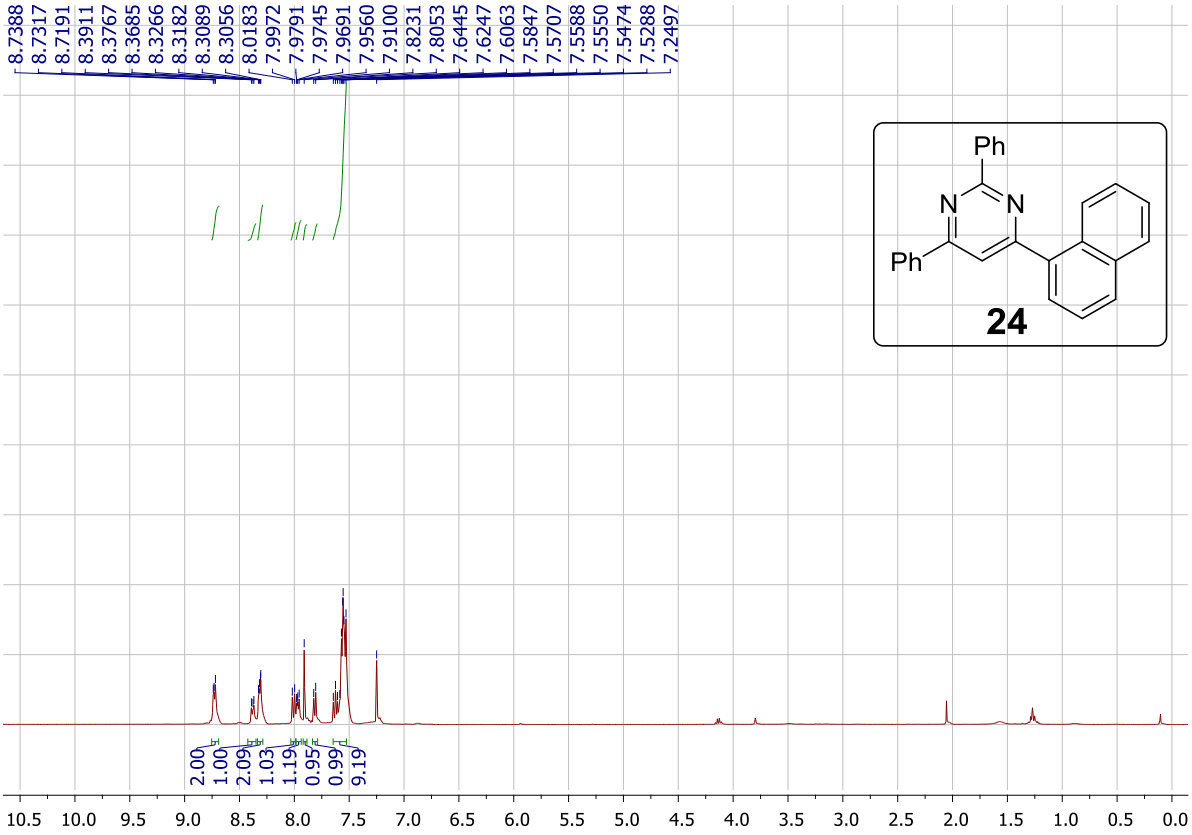
130.47
128.92
128.47
128.43
127.45
127.07
121.27
115.50
111.69
77.43
77.11
76.79
55.85
Ph
N
N
OMe
Ph
23
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.3056
8.0183
7.9972
7.9791
7.9745
7.9691
7.9560
7.9100
7.8231
7.8053
7.6445
7.6247
7.6063
7.5847
7.5707
7.5588
7.5550
7.5474
7.5288
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Ph
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N
Ph
24
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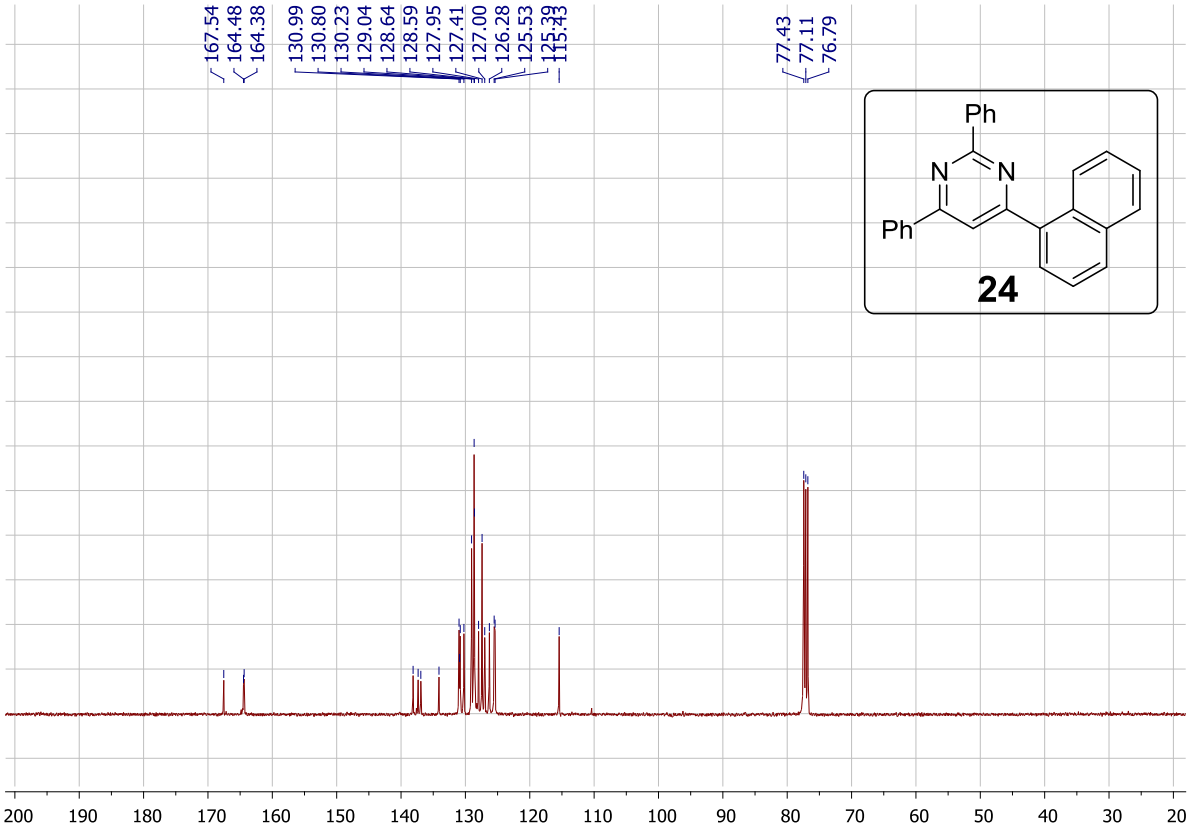
1.00
2.09
1.03
1.19
0.95
0.99
9.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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128.64
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127.41
127.00
126.28
125.53
125.39
125.43
115.43
77.43
77.11
76.79
Ph
N
N
Ph
24
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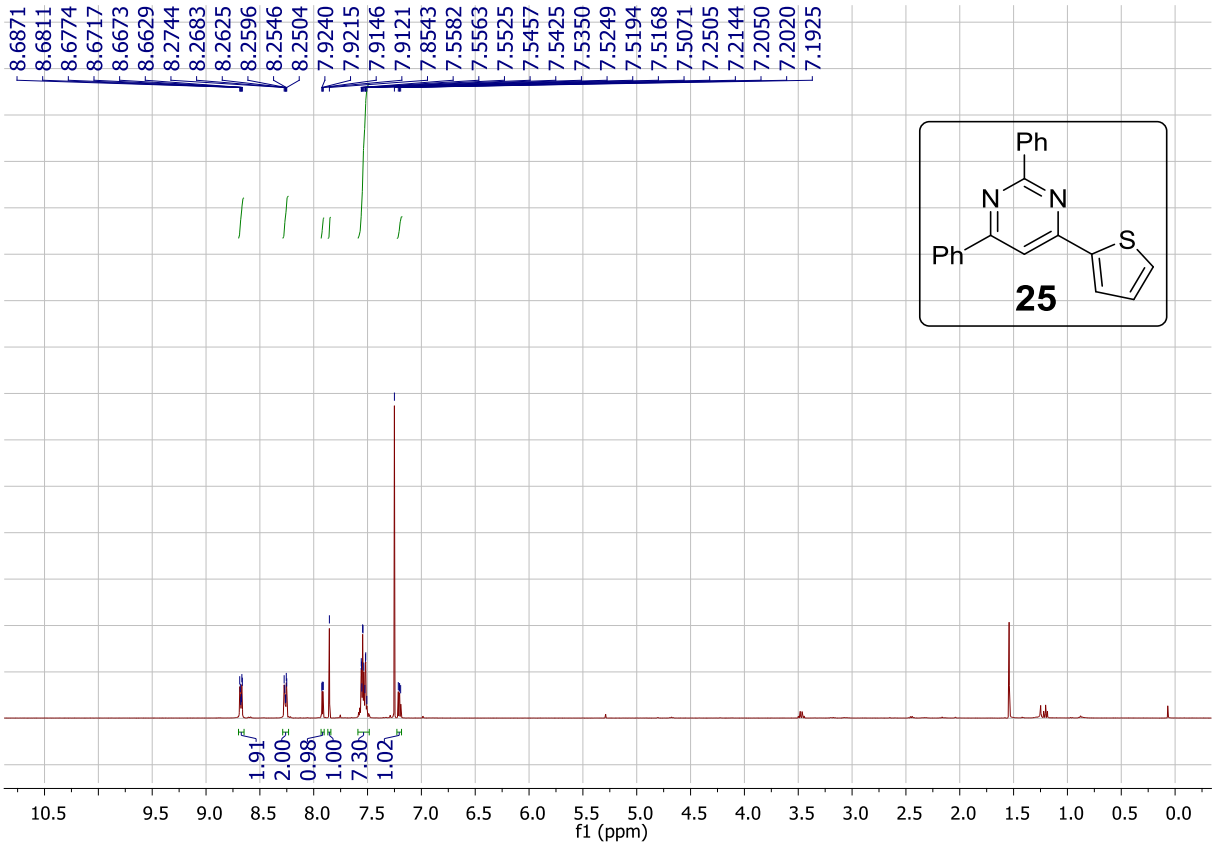
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8.2546
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7.9215
7.9146
7.9121
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7.5582
7.5563
7.5525
7.5457
7.5425
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7.5194
7.5168
7.5071
7.2505
7.2144
7.2050
7.2020
7.1925
Ph
N
N
Ph
S
25
1.91
2.00
0.98
1.00
7.30
1.02
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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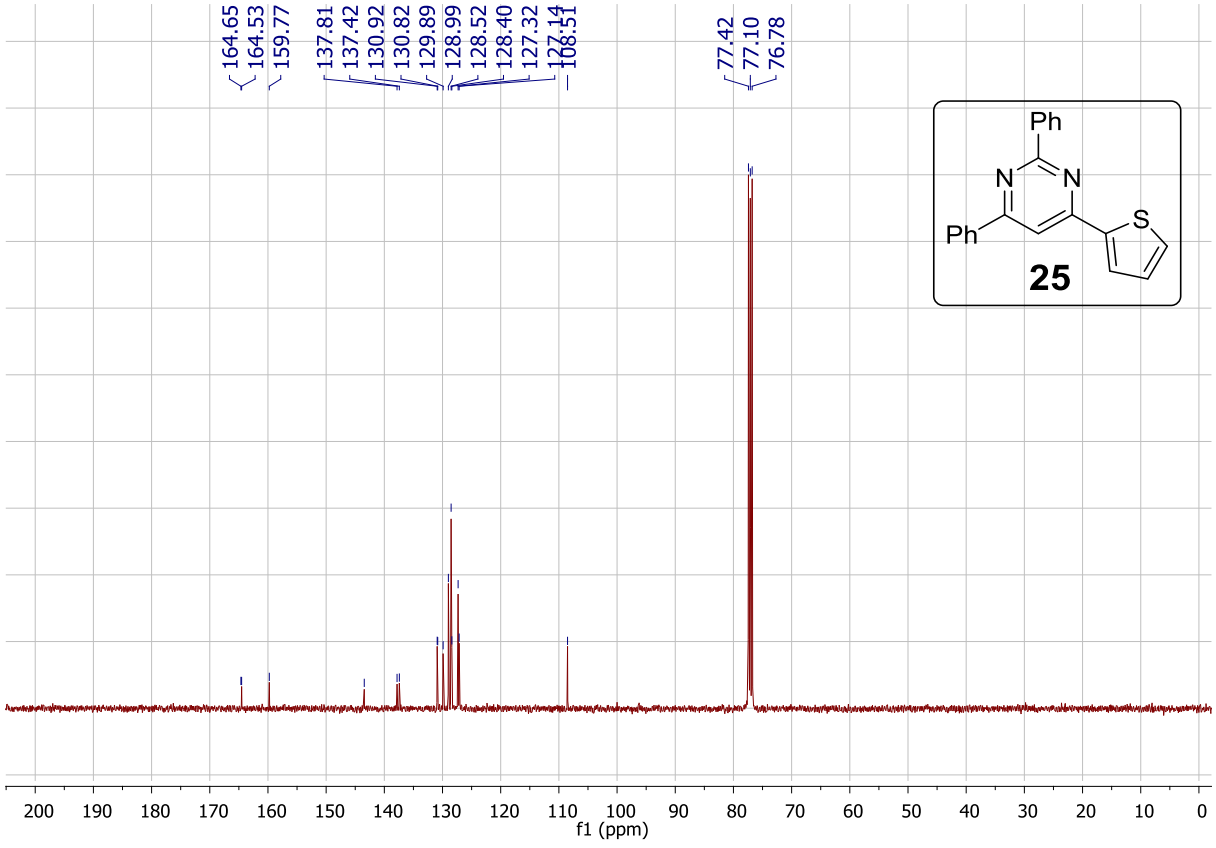
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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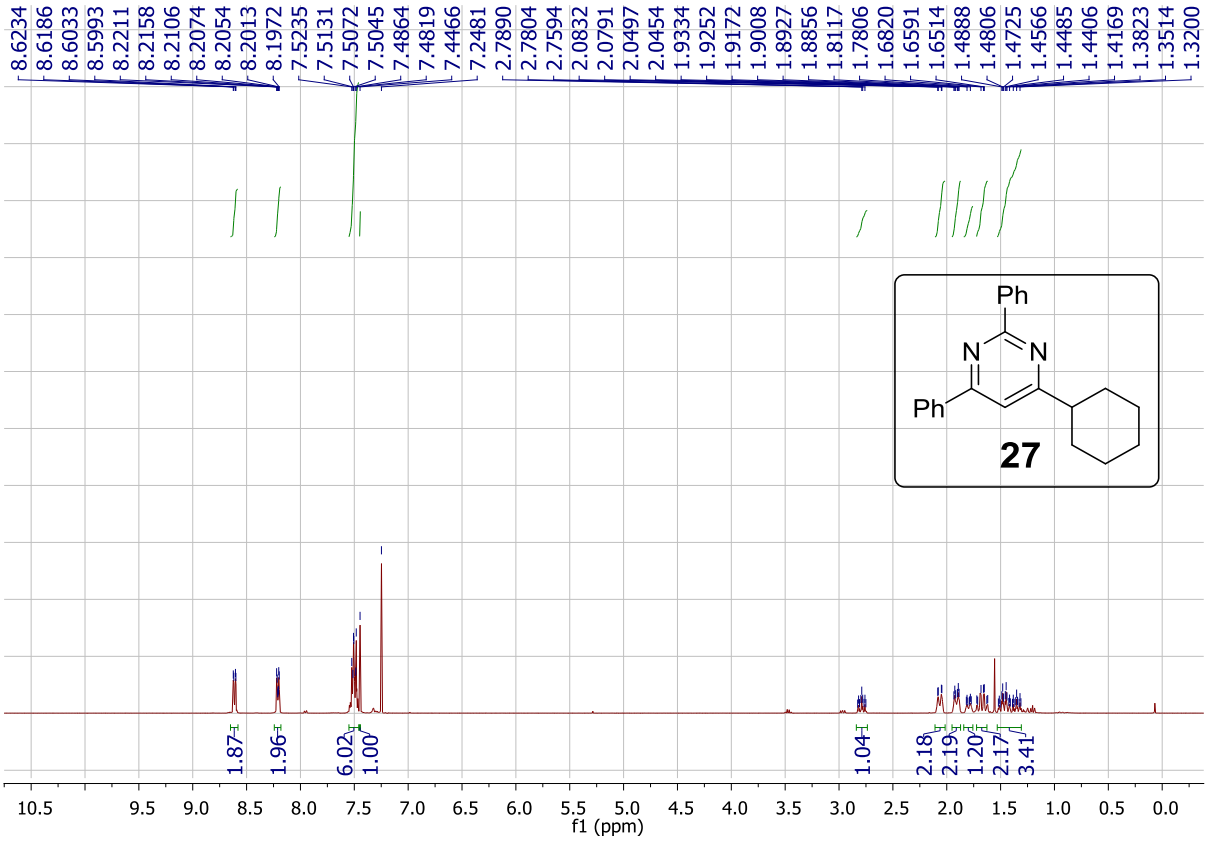
129.89
128.99
128.52
128.40
127.32
77.42
77.10
76.78
Ph
N
N
Ph
S
25
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4466
7.2481
2.7890
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2.0832
2.0791
2.0497
2.0454
1.9334
1.9252
1.9172
1.9008
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1.8856
1.8117
1.7806
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1.6514
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1.4806
1.4725
1.4566
1.4485
1.4406
1.4169
1.3823
1.3514
1.3200
Ph
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N
Ph
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1.87
1.96
6.02
1.00
1.04
2.18
2.19
1.20
2.17
3.41
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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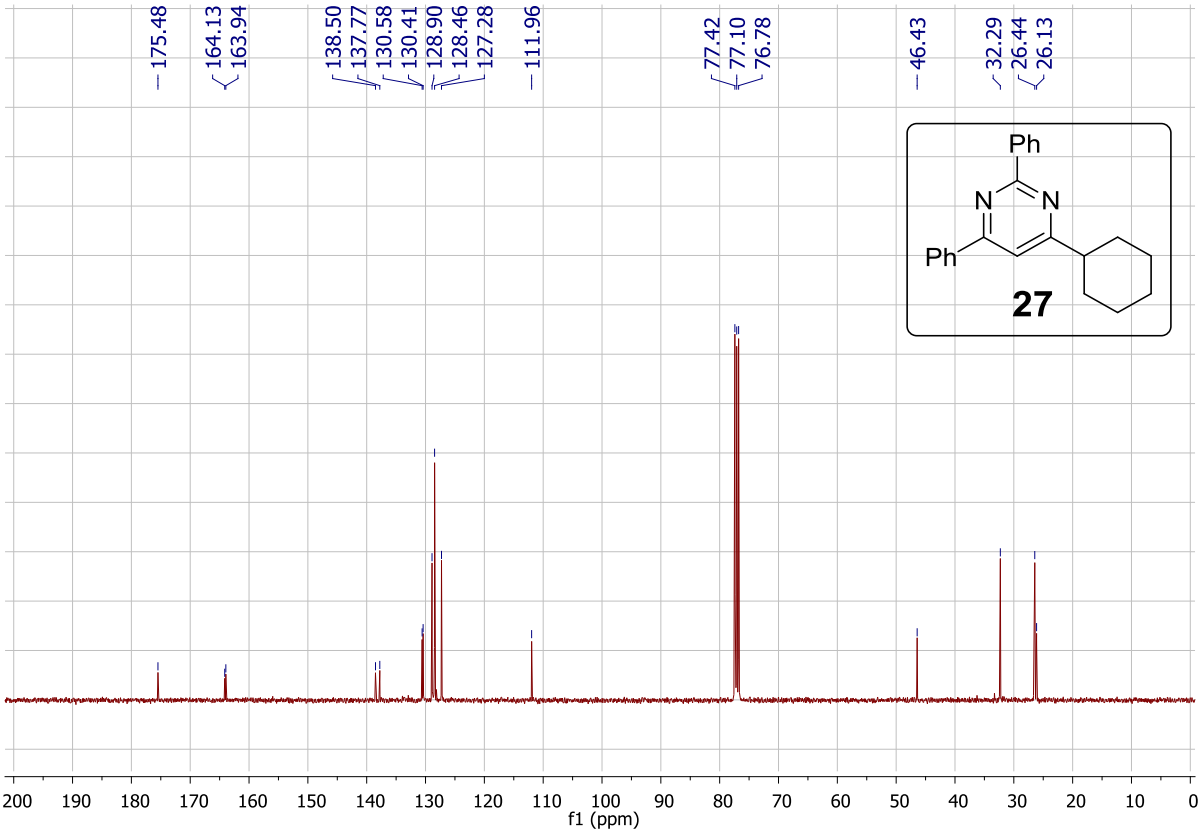
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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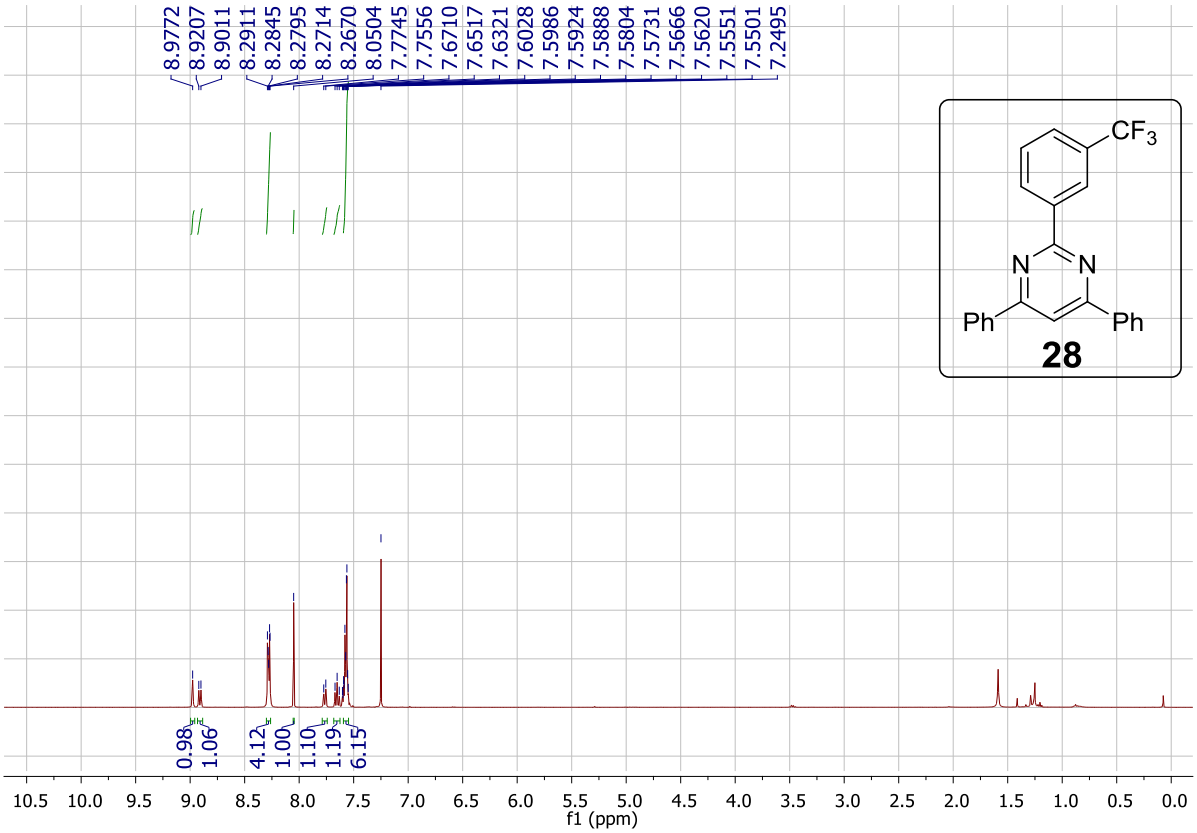
128.90
128.46
127.28
111.96
77.42
77.10
76.78
46.43
32.29
26.44
26.13
Ph
N
N
Ph
27
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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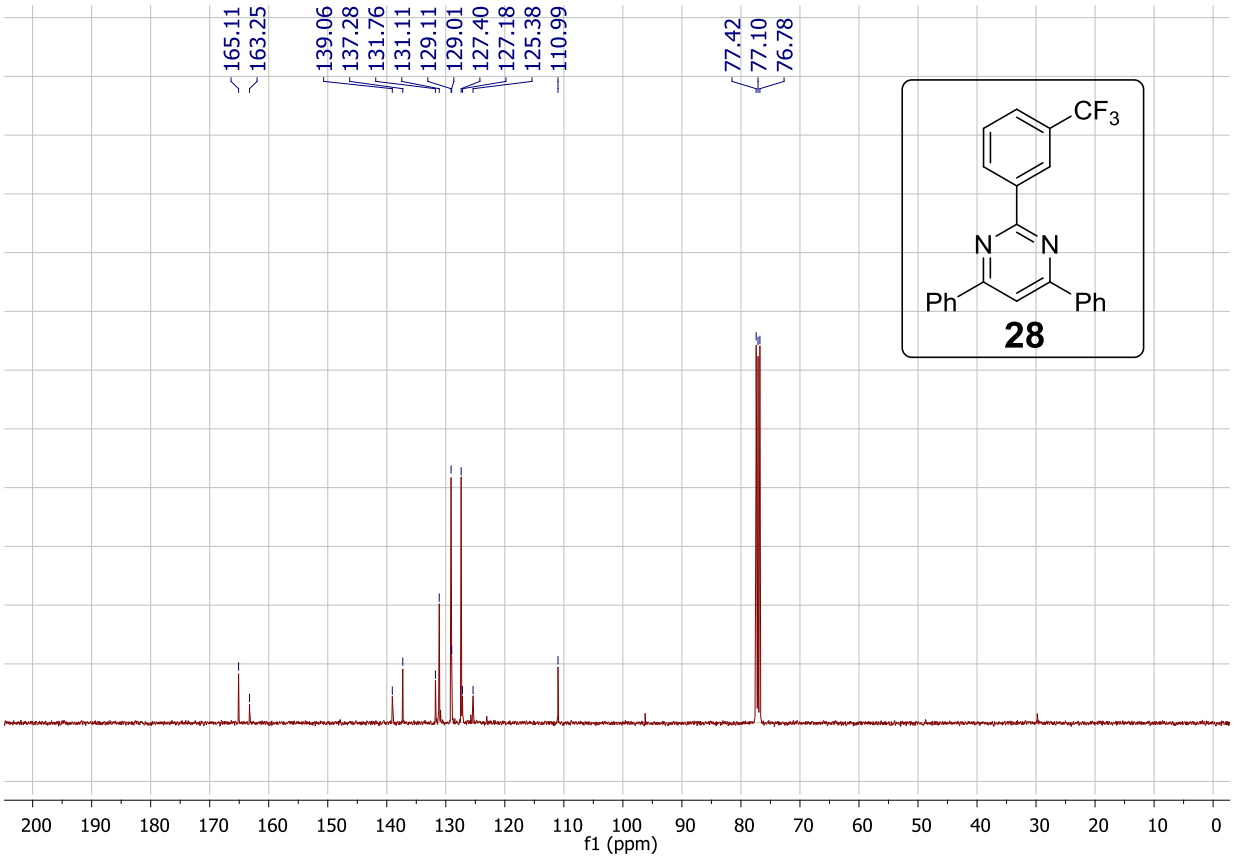
7.7556
7.6710
7.6517
7.6321
7.6028
7.5986
7.5924
7.5888
7.5804
7.5731
7.5666
7.5620
7.5551
7.5501
7.2495
0.98
1.06
4.12
1.00
1.10
1.19
6.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
CF3
N
N
Ph
Ph
28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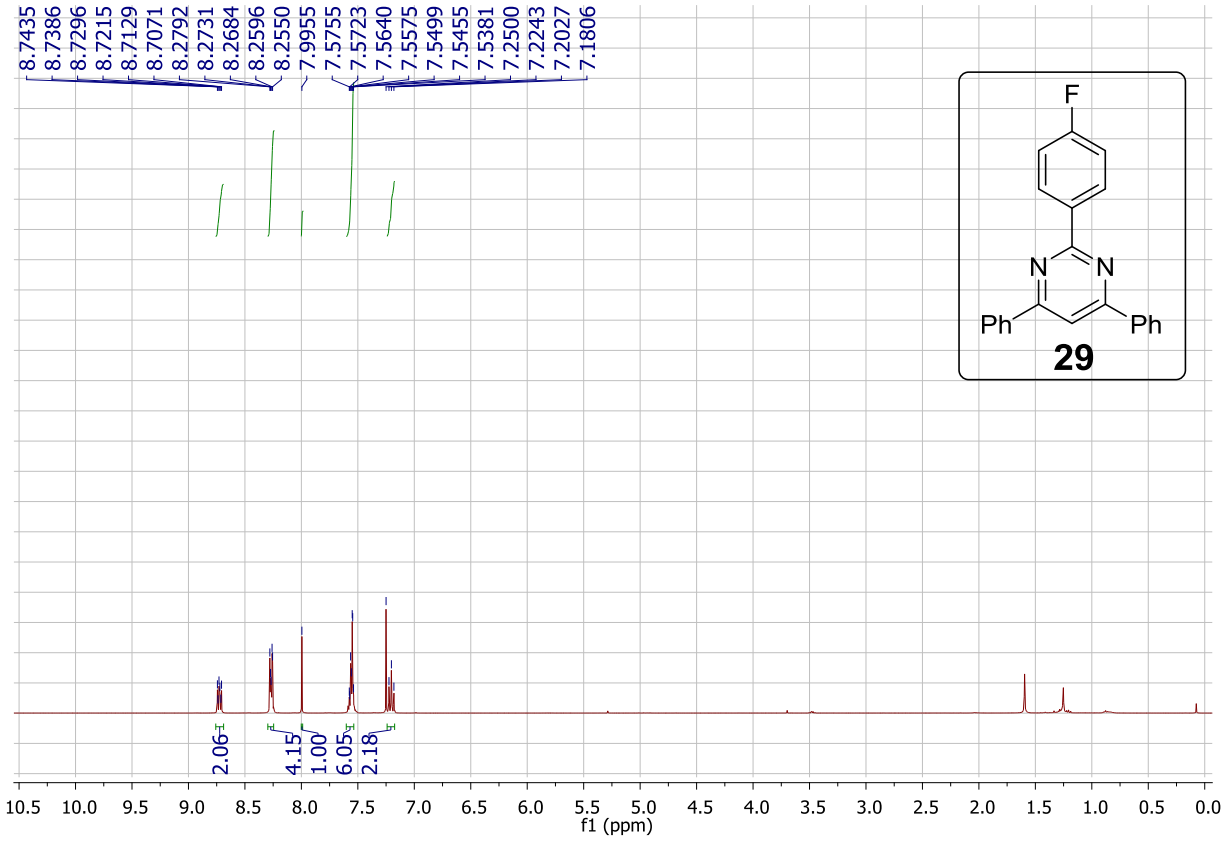
127.40
127.18
125.38
110.99
77.42
77.10
76.78
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
CF3
N
N
Ph
Ph
28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8.2550
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7.5755
7.5723
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7.5575
7.5499
7.5455
7.5381
7.2500
7.2243
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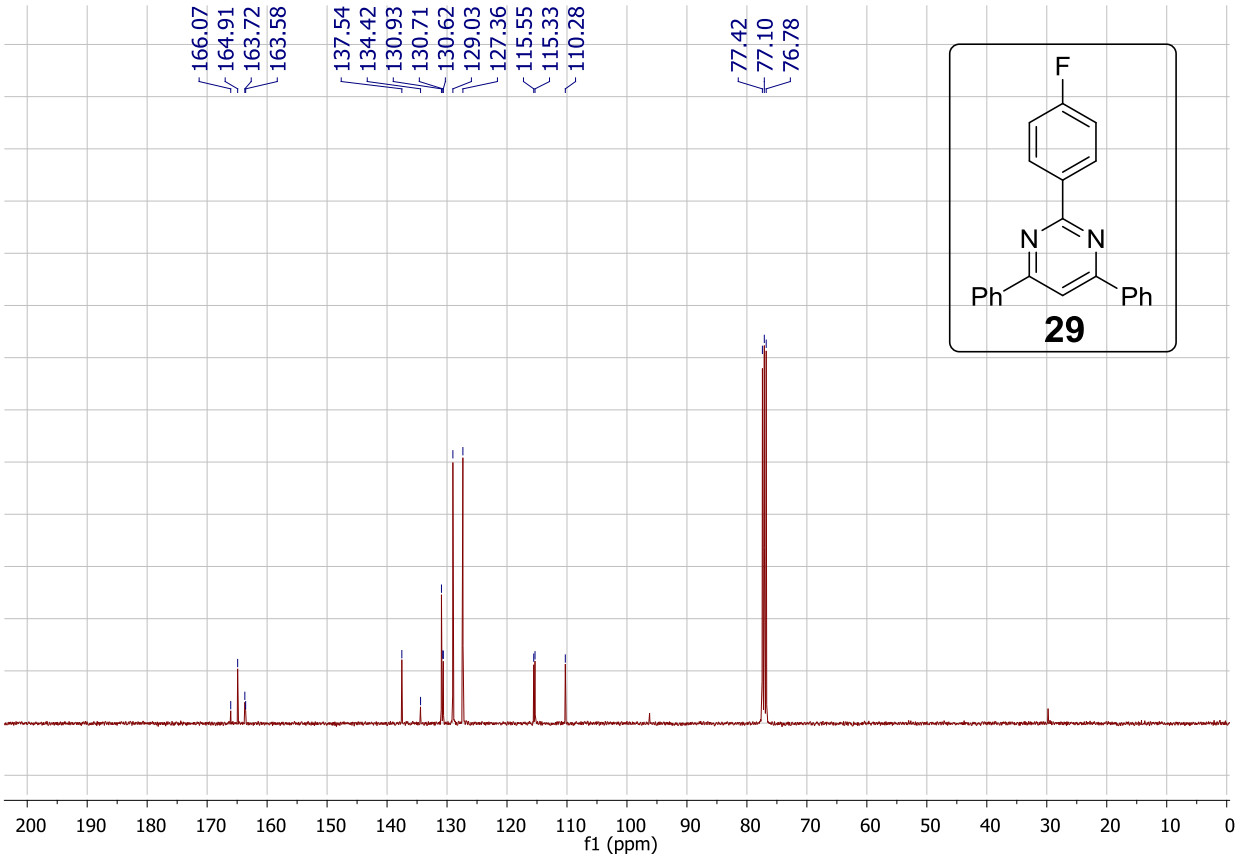
4.15
1.00
6.05
2.18
F
N
N
Ph
Ph
29
f1 (ppm)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130.71
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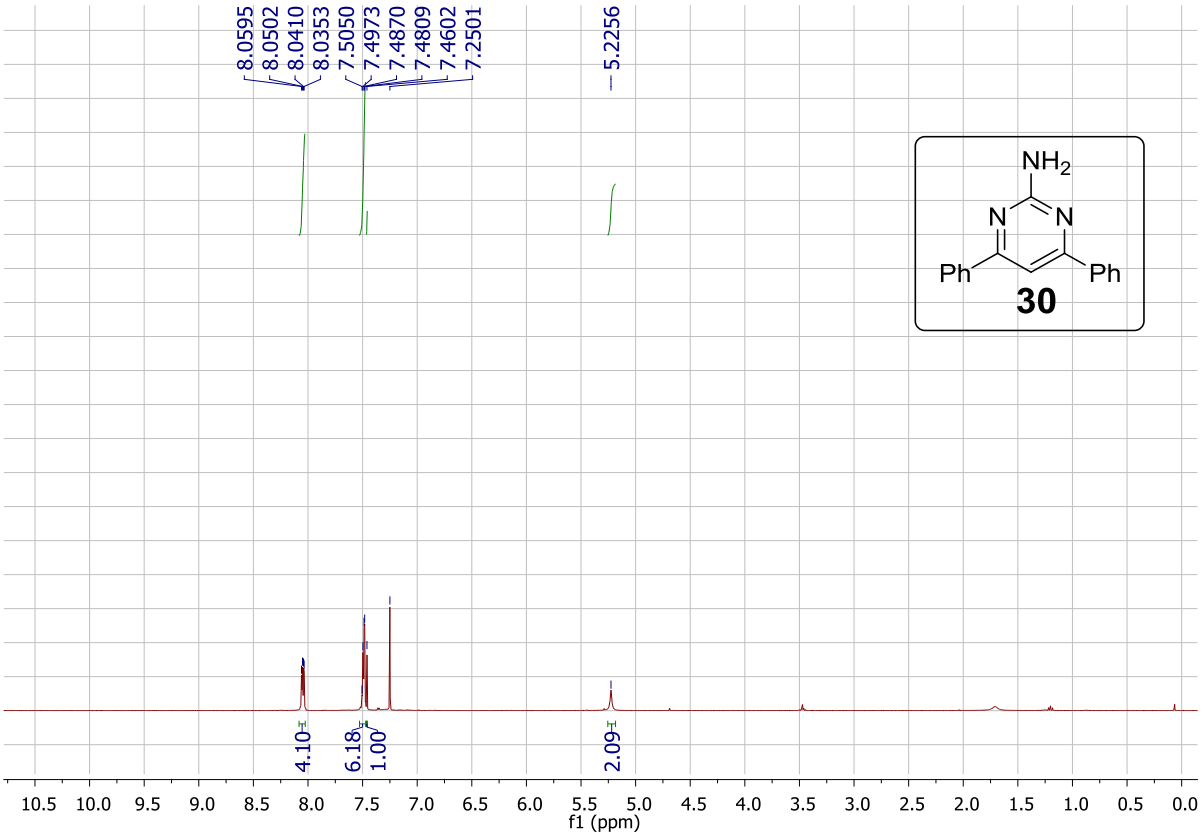
129.03
127.36
115.55
115.33
110.28
77.42
77.10
76.78
F
N
N
Ph
Ph
29
f1 (ppm)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7.4870
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7.4602
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NH2
N
N
Ph
Ph
30
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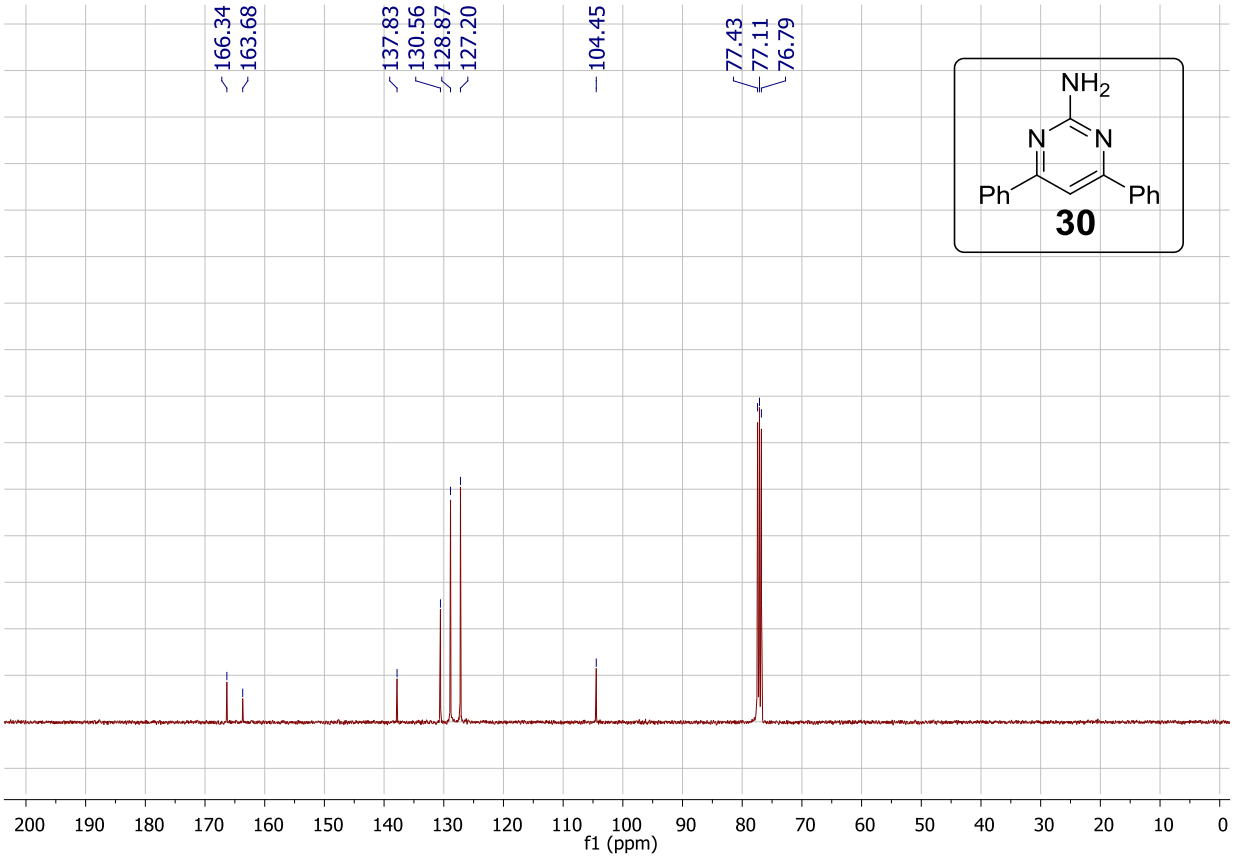
6.18
1.00
2.09
f1 (ppm)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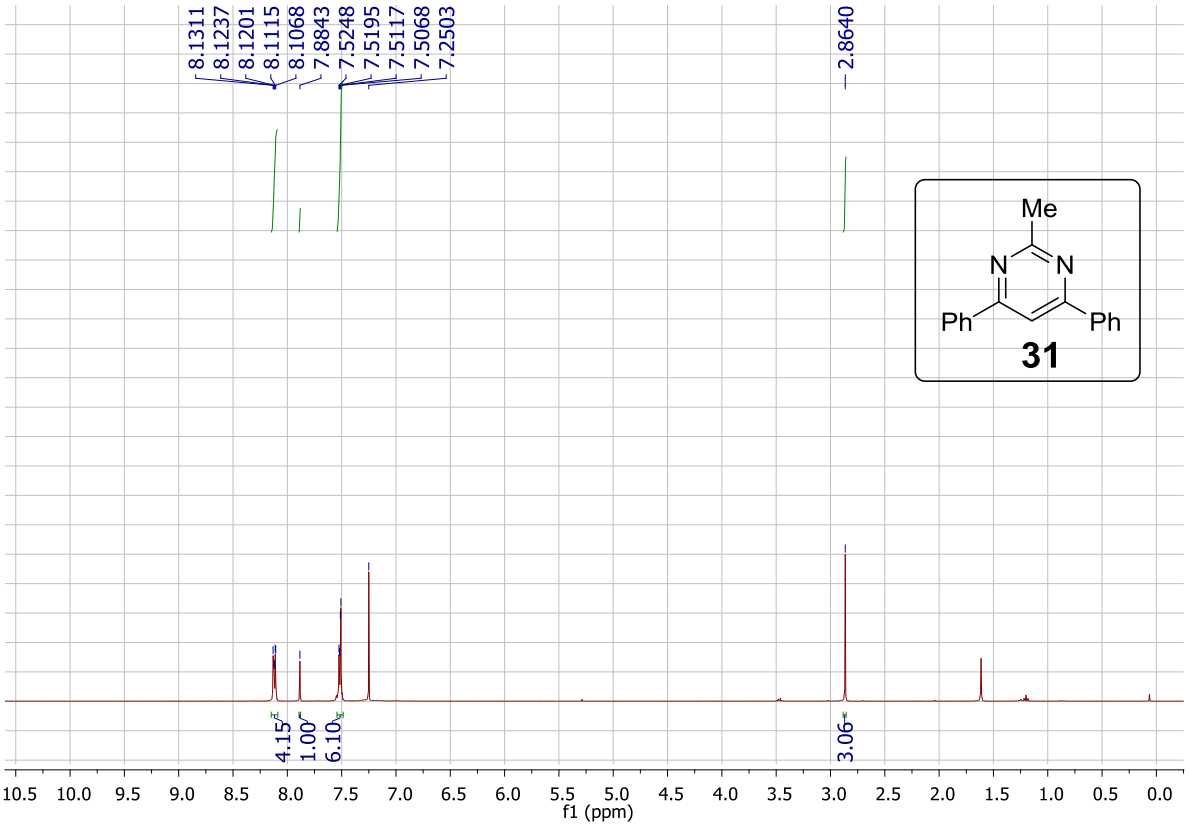
77.11
76.79
NH2
N
N
Ph
Ph
30
f1 (ppm)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7.5117
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Me
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Ph
Ph
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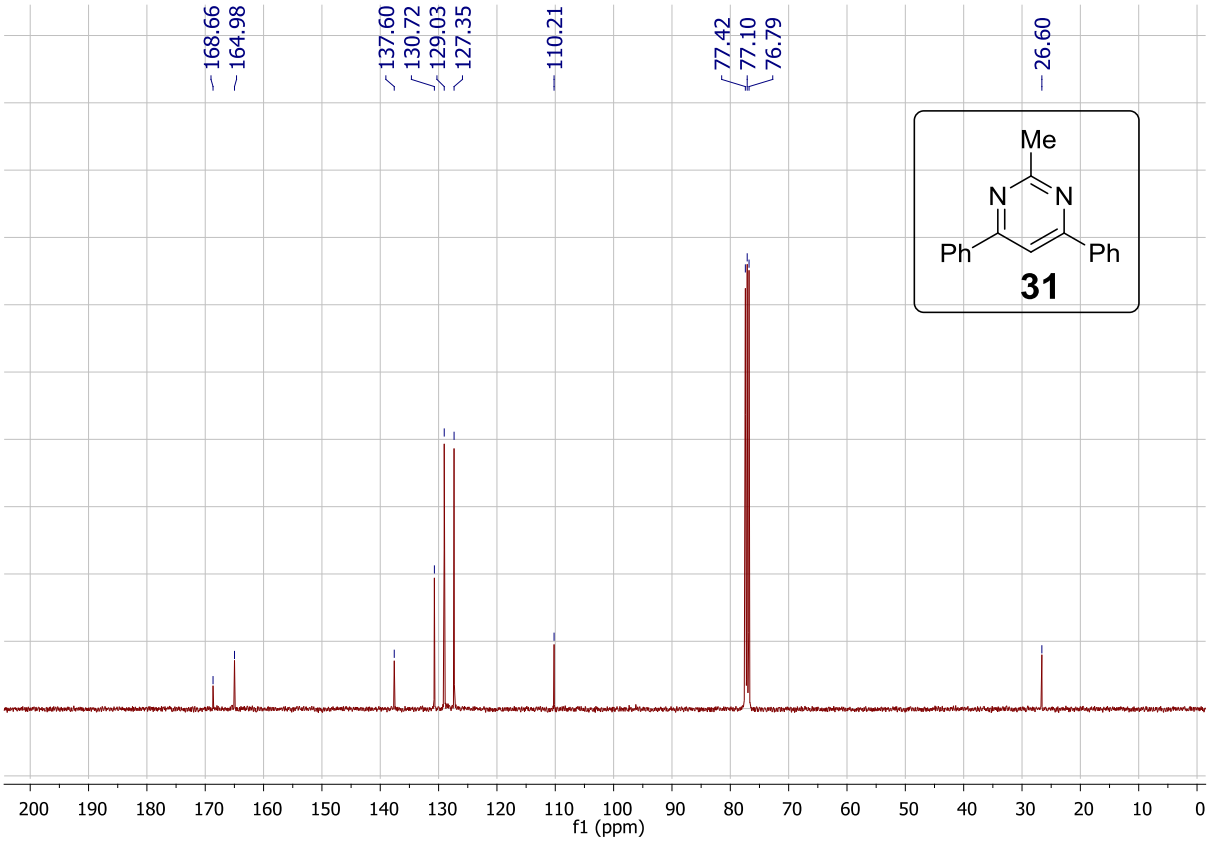
1.00
6.10
3.06
f1 (ppm)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129.03
127.35
110.21
77.42
77.10
76.79
26.60
Me
N
N
Ph
Ph
31
f1 (ppm)

8. References

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