Supporting Information

Ruthenaelectro-Catalyzed C–H Phosphorylation: ortho to para Position-Selectivity Switch

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1. General Experimental Details

Platinum electrodes (10 mm × 25 mm × 0.25 mm, 99.9%, obtained from ChemPur® Karlsruhe, Germany) and graphite felt (GF) electrodes (10 mm × 25 mm × 6 mm, SIGRACELL® GFA 6 EA, obtained from SGL Carbon, Wiesbaden, Germany) were connected using stainless steel adapters. Electrocatalysis was performed using a ROHDE&SCHWARZ HMP4040 potentiostat.

Solvents for column chromatography and extraction (EtOAc, *n*-hexane, MeOH, DCM) were distilled prior to their use. Routine TLC analysis was carried out on aluminium sheets coated with silica gel 60 F254, 0.2 mm thickness. Plates were analyzed using a 254 nm UV lamp. Chromatography was carried out on Merck silica gel 60 (40–63 μm). All starting materials, reagents and solvents were purchased from commercial suppliers (Aldrich, Alfa, TCI, Daicel, etc.) and used as supplied unless otherwise stated.

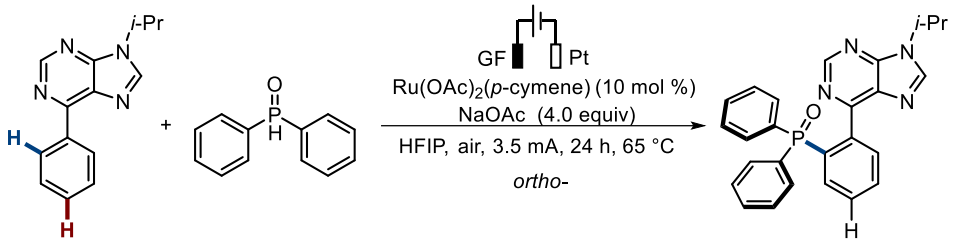
NMR spectra were recorded on Bruker-300 MHz spectrometer or Bruker-400 MHz spectrometer. Chemical shifts (δ) are given in ppm relative to TMS. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δH = 7.26 ppm, δC = 77.00 ppm). Data for ^1H NMR are reported as follows: chemical shift (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, dd =doublet of doublets, ddd = doublet of double doublets, dt = doublet of triplets), coupling constants *J* are reported in Hertz (Hz).

MS: EI-MS were recorded with Finnigan MAT 95, 70 eV and Finnigan LCQ; High resolution mass spectrometry (HR-MS) with APEX IV 7T FTICR; ESI-MS were recorded with Bruker *Daltonics maXis* (ESI-QTOF-MS), Bruker Daltonics *micrOTOF* (ESI-TOF-MS) or Thermo Scientific *LTQ Orbitrap XL* (ESI-Orbitrap-MS). All IR spectra were recorded on a Bruker FT-IR Alpha-P device or on a Thermo Scientific Nicolet iS5 device equipped with an iD7 ATR detector and were recorded in the range from 4000 to 400 cm^{-1}. CV studies were performed using a Metrohm Autolab PGSTAT204 workstation and Nova 2.1 software.

Headspace analysis was performed on an Agilent 7890B GC System using a Thermal Conductivity Detector and a 5Å MS column. The gas evolution study was conducted using the GasMess-System (LIKAT Rostock and MesSen Nord GmbH).

2. Optimization of the Reaction Conditions

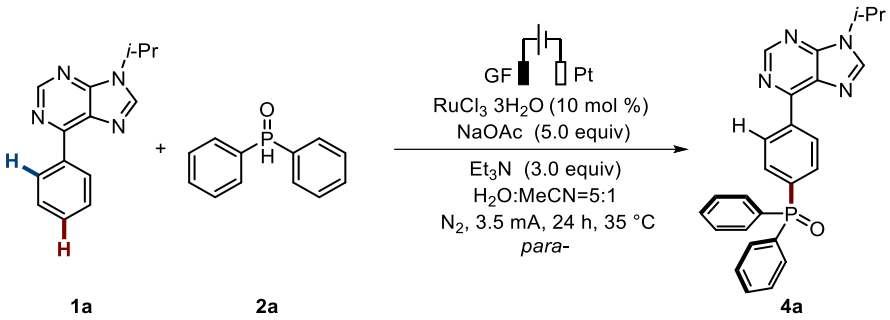
Table S1. Reaction optimization for *ortho*-C–H phosphorylation.[a]



Entry	Deviation from standard conditions	Yield [b]
1	None	73
2	TEF / CH_3CN / MeOH / DMA as solvent	65/-/-/-
3	35°C /45° C	19/35
4	GF(+) / GF(-), Pt(+) / GF(-), RVC(+) / Pt(-) as electrode	32/23/63
5	*n*-Bu_4NOAc, $NaPF_6$, *n*-Bu_4NBF_4, $LiClO_4$ as electrolyte	70/55/34/65
6	1 mA 72 h, 2 mA 36 h, 4 mA 18 h	49/65/61
7	No [$Ru(OAc)_2$(*p*-cymene)]	0
8	No electricity	0

[a]**Reaction conditions A**: Undivided cell, GF anode, Pt cathode, **1a** (0.3 mmol, 1.0 equiv), **2a** (4.0 equiv), [$Ru(OAc)_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), HFIP (3.0 mL), electrolyte (0.1 M), air, 65 °C, 3.5 mA, 24 h. [b]Isolated yields.

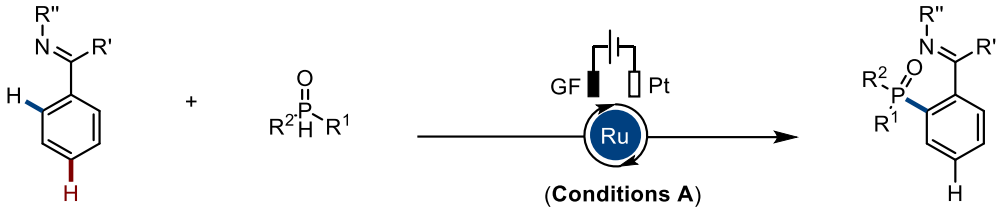
Table S2. Reaction optimization for *para*-C–H phosphorylation.[a]



Entry	Deviation from standard conditions	Yield [b]
1	None	82
2	H_2O / CH_3CN / PhMe / MeOH as solvent	25/12/-/-
3	55°C / 25°C	72/67
4	GF(+) / GF(-), Pt(+) / GF(-), RVC(+) / Pt(-) as electrode	5/8/77
5	*n*-Bu_4NOAc, $NaPF_6$, *n*-Bu_4NBF_4, Et_4NCl, *n*-Bu_4NClO_4 as electrolyte	80/61/39/79/21
6	2 mA 36 h, 4 mA 18 h, 6 mA 12 h	65/76/59
7	No [$RuCl_3 \cdot 3H_2O$]	58
8	No electricity	0

[a]**Reaction conditions B**: Undivided cell, GF anode, Pt cathode, **1a** (0.3 mmol, 1.0 equiv), **2a** (4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), MeCN:H_2O = (0.5:2.5 mL), electrolyte (0.1 M), N_2, 35 °C, 3.5 mA, 24 h. [b]Isolated yields.

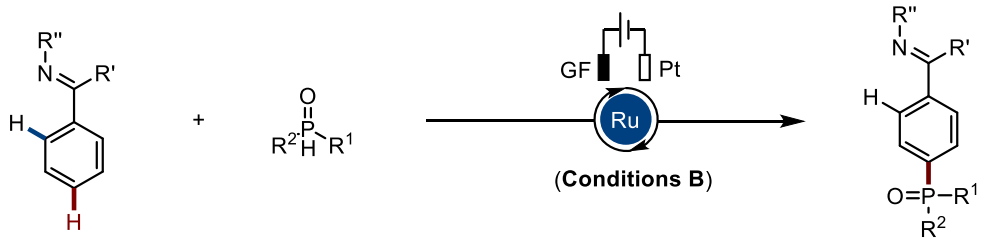
3. General Procedure



1 2 3

Conditions A:

Under air atmosphere, an undivided cell was charged with **1** (0.3 mmol, 1.0 equiv), **2** (1.2 mmol, 4.0 equiv), [$Ru(OAc)_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), HFIP (3.0 mL), and equipped with a graphite felt (GF) anode (10 mm × 25 mm × 6 mm) and a platinum (Pt) cathode (10 mm × 25 mm × 0.25 mm). The resulting light-red suspension was stirred vigorously at room temperature for 10 minutes, and then placed in a pre-heated oil bath at 65 °C for electrolysis under a constant current of 3.5 mA for 24 hours. After the reaction was completed, the electrodes were carefully washed with DCM (3 × 10 mL) and MeOH (3 × 10 mL). The combined mixture was initially purified by flash column chromatography on silica gel (DCM/MeOH = 30/1-10/1) to afford the crude product, which was further purified by chromatography on silica gel to afford the corresponding product **3**.



1 2 4

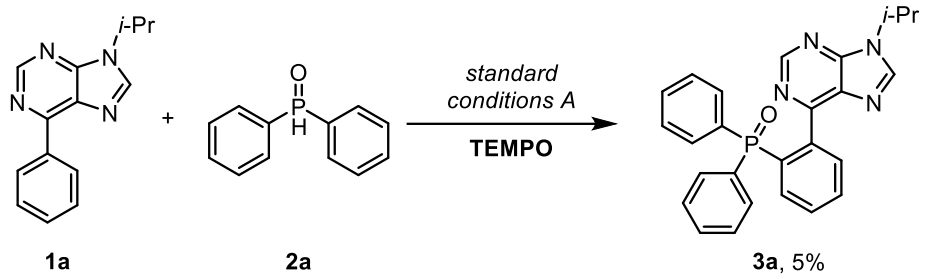
Conditions B:

Under N_2 atmosphere, an undivided cell was charged with **1** (0.3 mmol, 1.0 equiv), **2** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL), and equipped with a graphite felt (GF) anode (10 mm × 25 mm × 6 mm) and a platinum (Pt) cathode (10 mm × 25 mm × 0.25 mm). The resulting black suspension was stirred vigorously at room temperature for 10 minutes, and then placed in a pre-heated oil bath at 35 °C for electrolysis under a constant current of 3.5 mA for 24 hours. After the reaction was completed, the electrodes were carefully washed with DCM (3 × 10 mL) and MeOH (3 × 10 mL). The combined mixture was initially purified by flash column chromatography on silica gel (DCM/MeOH = 30/1-10/1) to afford the crude product, which was further purified by chromatography on silica gel to afford the corresponding product **4**.

Figure S1. Picture of the electrochemical cell, stirring bar, and teflon cap with a graphite felt (GF) anode and a platinum (Pt) cathode

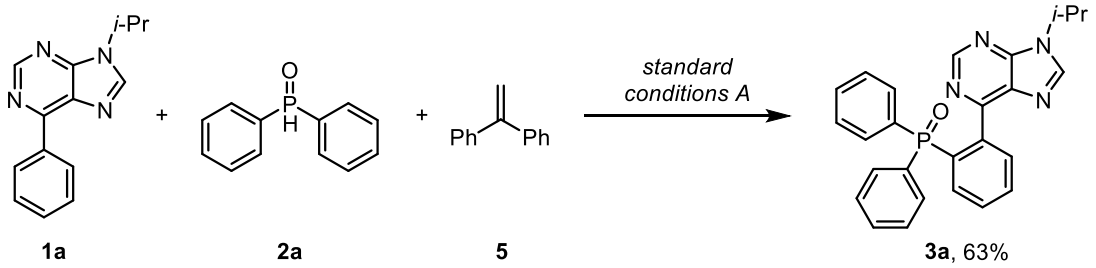
4. Mechanistic Studies

1) Radical trapping experiments for the *ortho*-C–H phosphorylation



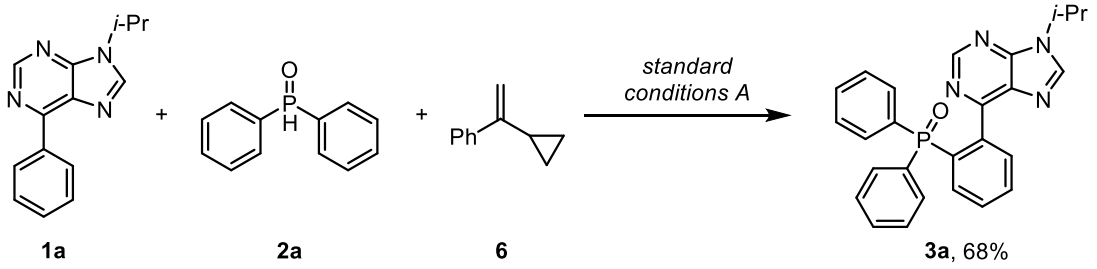
1a **2a** **3a**, 5%

Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [Ru(OAc)$_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), **TEMPO** (1.2 mmol, 4.0 equiv), HFIP (3.0 mL). After the reaction was completed, the residue was purified with column chromatography on silica gel to give the compound **3a** (6.5 mg, 5%).



1a **2a** **5** **3a**, 63%

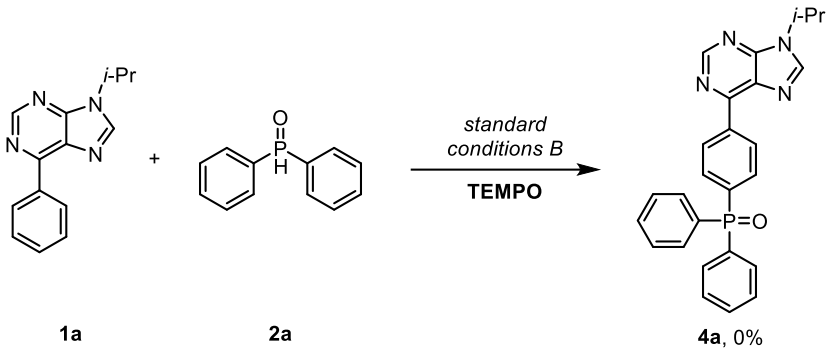
Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [Ru(OAc)$_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), **5** (1.2 mmol, 4.0 equiv), HFIP (3.0 mL). After the reaction was completed, the residue was purified with column chromatography on silica gel to give the compound **3a** (82.8 mg, 63%).



1a **2a** **6** **3a**, 68%

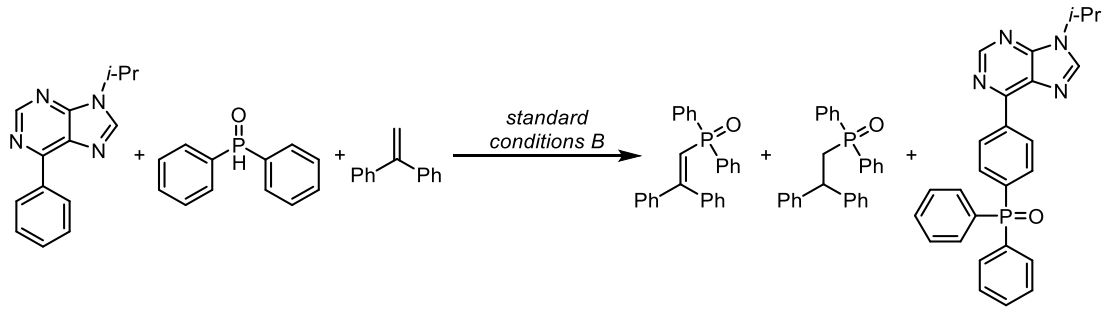
Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [Ru(OAc)$_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), **6** (1.2 mmol, 4.0 equiv), HFIP (3.0 mL). After the reaction was completed, the residue was purified with column chromatography on silica gel to give the compound **3a** (89.5 mg, 68%).

2) Radical trapping experiments for the *para*-C–H phosphorylation



1a **2a** **4a**, 0%

Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), **TEMPO** (1.2 mmol, 4.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL). After the reaction was completed, the TLC and GC-MS were employed to observe the result, no desired product had been observed.

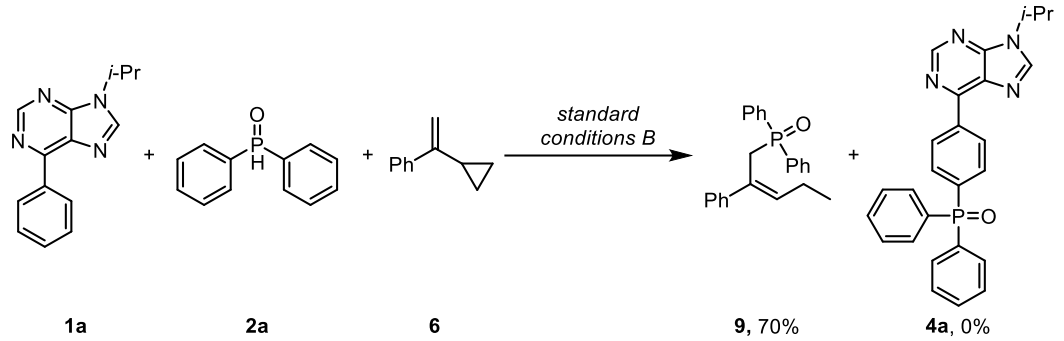


1a **2a** **5** **7**,52% **8**,10% **4a**, 0%

Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), **5** (1.2 mmol, 4.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL). After the reaction was completed, the residue was purified with chromatography column on silica gel to give the mixed compounds **7** and **8** (71.5 mg, **7**:**8** = 5:1).[1]

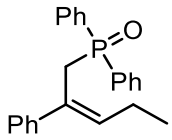
^{31}P NMR (121 MHz, $CDCl_3$) δ 29.45, 18.67.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{22}OP$ 381.1403; Found 381.1408; $[M+H]^+$ Calcd for $C_{26}H_{24}OP$ 383.1559; Found 383.1551.



Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), **6** (1.2 mmol, 4.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL). After the reaction was completed, the residue was purified with chromatography column on silica gel to give the compound **9** (72.7 mg, 70%).

(Z)-Diphenyl(2-phenylpent-2-en-1-yl)phosphine oxide (**9**)



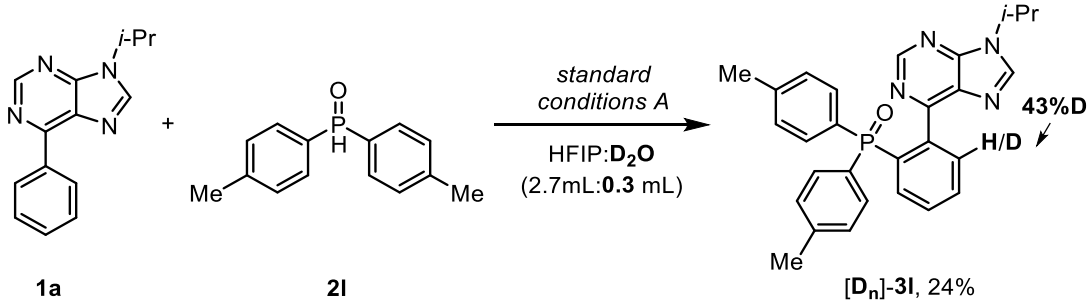
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 – 7.53 (m, 4H), 7.36 – 7.30 (m, 2H), 7.27 – 7.21 (m, 4H), 7.06 – 7.00 (m, 5H), 5.71 – 5.60 (m, 1H), 3.54 (d, J = 14.8 Hz, 2H), 2.11 – 2.02 (m, 2H), 0.87 (t, J = 7.5 Hz, 3H).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.63.

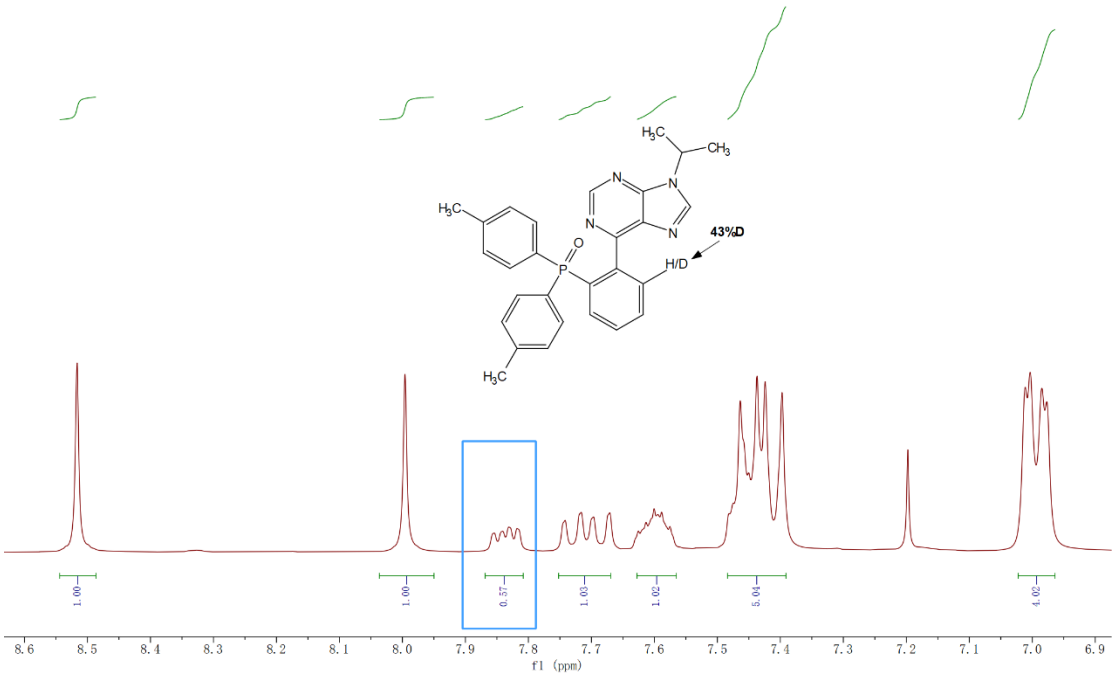
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{24}OP$ 347.1559; Found 347.1563.

IR (ATR): 3055, 2961, 1591, 1436, 1182, 909, 712, 506 cm^{-1}.

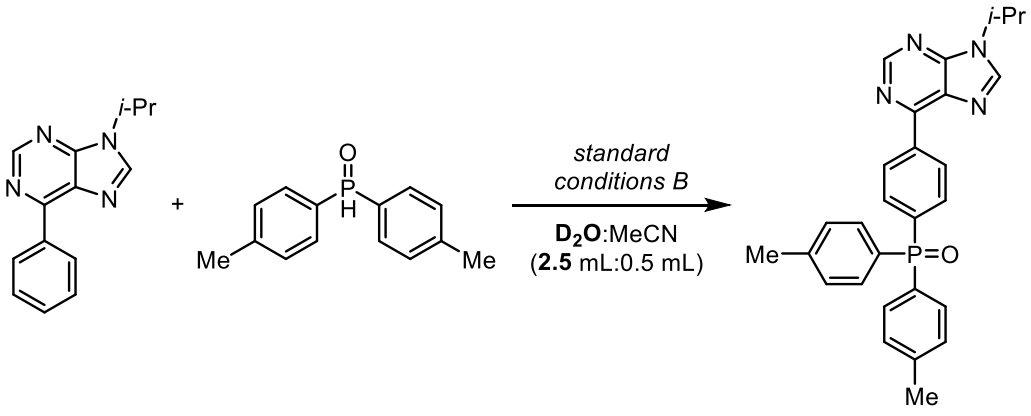
3) H/D-Exchange study for the *ortho*-C–H phosphorylation



Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2l** (1.2 mmol, 4.0 equiv), [$Ru(OAc)_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), HFIP:$\mathbf{D_2O}$ = (2.7 mL:**0.3** mL). After the reaction was completed, the residue was purified with column chromatography on silica gel to give the product **[D]$_n$–3l** in a 24% isolated yield. The H incorporation was determined by ^{1}H-NMR spectroscopy.

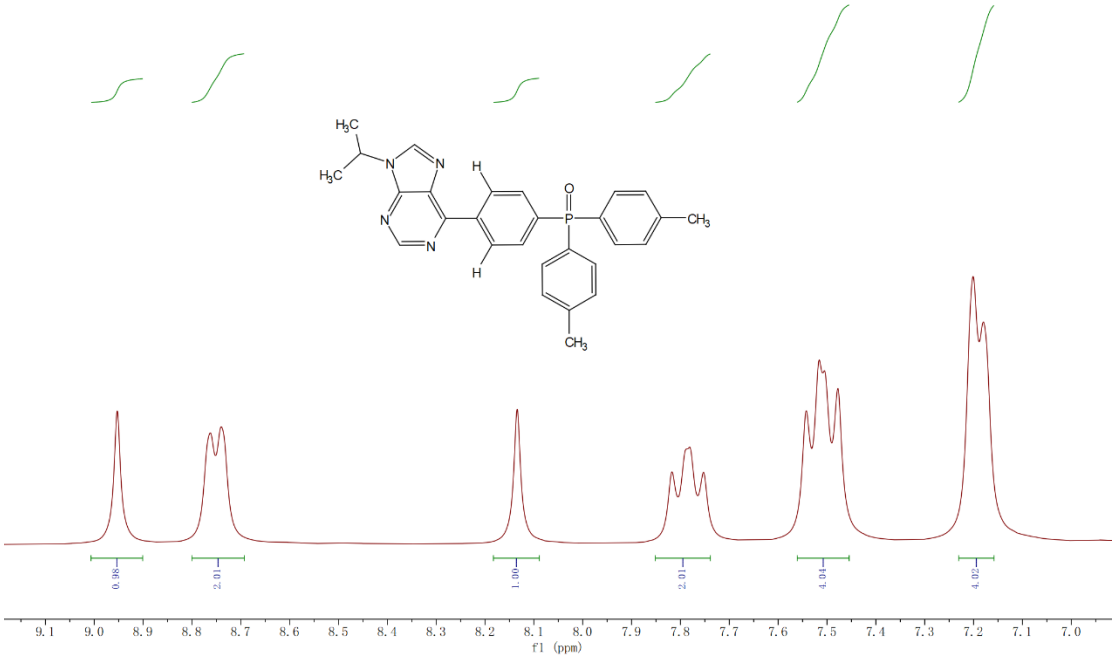


4) H/D-Exchange study for the *para*-C–H phosphorylation



1a **2l** **4g**, 75%

Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2l** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), **D_2O**:MeCN = (**2.5** mL:0.5 mL). After the reaction was completed, the residue was purified with column chromatography on silica gel to give the product **4g** in a 75% isolated yield. No H/D exchange was detected by ^{1}H-NMR spectroscopy.



5) Hydrogen detection for the *ortho*-C–H phosphorylation

Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [Ru(OAc)$_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), HFIP (3.0 mL). After the reaction was completed, 1.0 mL of the headspace volume was removed for GC analysis.

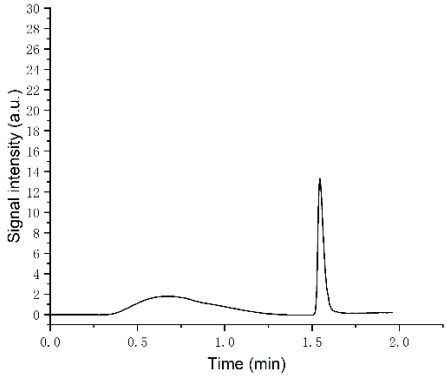


Figure S2. GC-TCD chromatogram obtained for the headspace analysis of the *ortho*-C–H phosphorylation.

6) Gas evolution measurement for the *ortho*-C–H phosphorylation:

Following standard procedure A using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [Ru(OAc)$_2$(*p*-cymene)] (10 mol %), NaOAc (4.0 equiv), HFIP (3.0 mL) at **55 °C** under air atmosphere according to the general procedure.

The change in volume of the headspace was recorded under isobaric conditions.

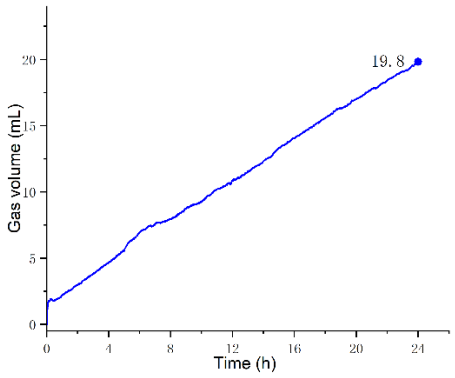


Figure S3. Measurement of the hydrogen volume generated during catalysis.

Calculation of cathode hydrogen generation efficiency:

Current: I = 3.5 mA, Time: t = 24 h = 86400 s, Faraday constant: F = 96485.3321 C/mol

Therefore, the number of electrons passing through the electron cathode is:

$$n_e = \frac{I \times t}{F} = 0.0035\ A \times 86400\ s \div 96485.3321\ C/mol = 0.003134\ mol = 3.134\ mmol$$

Theoretical hydrogen production:

$$n_{H_2} = \frac{n_e}{2} = 1.567\ mmol$$

Measured amount of hydrogen:

$$V_{mH_2} = 19.8\ mL = 0.0000198\ m^3$$

$$n_{mH_2} = \frac{P \times V_{mH_2}}{RT} = \frac{99270\ Pa \times 0.0000198\ m^3}{8.3145\ J/(K \cdot mol) \times 298.15\ K} = 0.000793\ mol = 0.793\ mmol$$

Hydrogen generation efficiency:

$$efficiency = \frac{0.793\ mmol}{1.567\ mmol} = 50\%$$

7) Hydrogen detection for the *para*-C–H phosphorylation

Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL). After the reaction was completed, 1.0 mL of the headspace volume was removed for GC analysis.

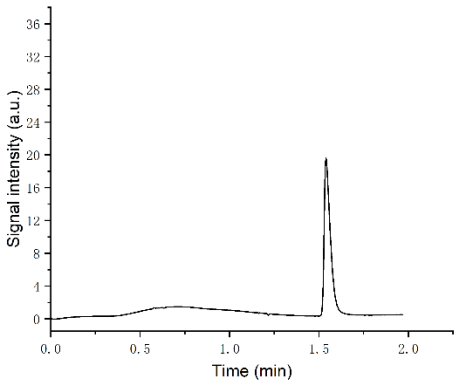


Figure S4. GC-TCD chromatogram obtained for the headspace analysis of the *para*-C–H phosphorylation.

8) Gas evolution measurement for the *para*-C–H phosphorylation:

Following standard procedure B using **1a** (0.3 mmol, 1.0 equiv), **2a** (1.2 mmol, 4.0 equiv), [$RuCl_3 \cdot 3H_2O$] (10 mol %), NaOAc (5.0 equiv), Et_3N (3.0 equiv), MeCN: H_2O = (0.5 mL: 2.5 mL) at 35 °C under N_2 atmosphere according to the general procedure.

The change in volume of the headspace was recorded under isobaric conditions.

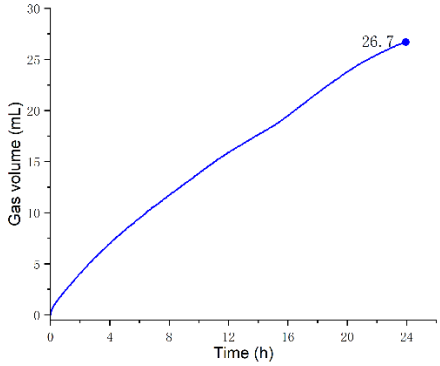


Figure S5. Measurement of the hydrogen volume generated during catalysis.

Calculation of cathode hydrogen generation efficiency:

Current: I = 3.5 mA, Time: t = 24 h = 86400 s, Faraday constant: F = 96485.3321 C/mol

Therefore, the number of electrons passing through the electron cathode is:

$$n_e = \frac{I \times t}{F} = 0.0035\ A \times 86400\ s \div 96485.3321\ C/mol = 0.003134\ mol = 3.134\ mmol$$

Theoretical hydrogen production:

$$n_{H_2} = \frac{n_e}{2} = 1.567\ mmol$$

Measured amount of hydrogen:

$$V_{mH_2} = 26.7\ mL = 0.0000267\ \mathrm{m}^3$$

$$n_{mH_2} = \frac{P \times V_{mH_2}}{RT} = \frac{99270\ Pa \times 0.0000267\ m^3}{8.3145\ J/(K \cdot mol) \times 298.15\ K} = 0.001069\ mol = 1.069\ mmol$$

Hydrogen generation efficiency:

$$efficiency = \frac{1.069\ mmol}{1.567\ mmol} = 68\%$$

9) Cyclic Voltammetry Studies

CV measurements were conducted with a Metrohm Autolab PGSTAT204 potentiostat and Nova 2.1 software. A glassy carbon working electrode (disk, diameter: 3mm), a coiled platinum wire counter electrode and a saturated calomel reference electrode (SCE) were employed.

The voltammograms were recorded at room temperature in HFIP (3 mL) at a substrate concentration of 25.0 mmol/L and with 100 mmol/L *n*-Bu_4NPF_6 as supporting electrolyte. The scan rate is 100 mV/s.

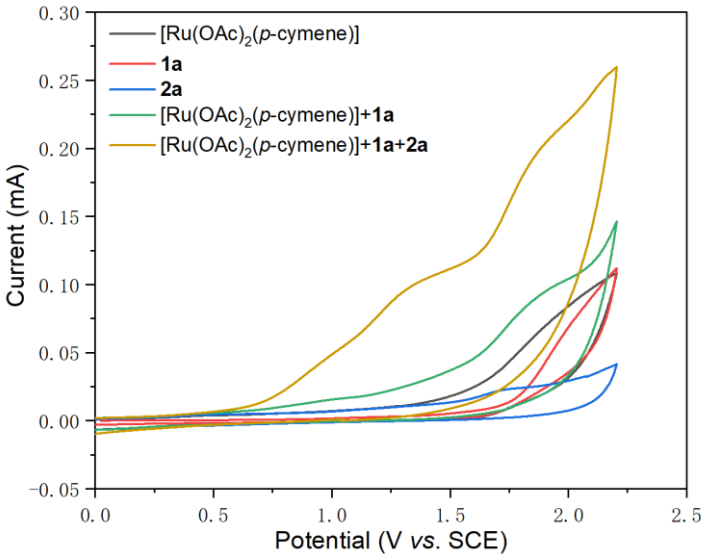


Figure S6. Cyclic voltammetry studies for *ortho*-C–H phosphorylation.

The voltammograms were recorded at room temperature in 5 mL H_2O/MeCN (1:1) at a substrate concentration of 15.0 mmol/L and with 60 mmol/L *n*-Bu_4NPF_6 as supporting electrolyte. The scan rate is 100 mV/s.

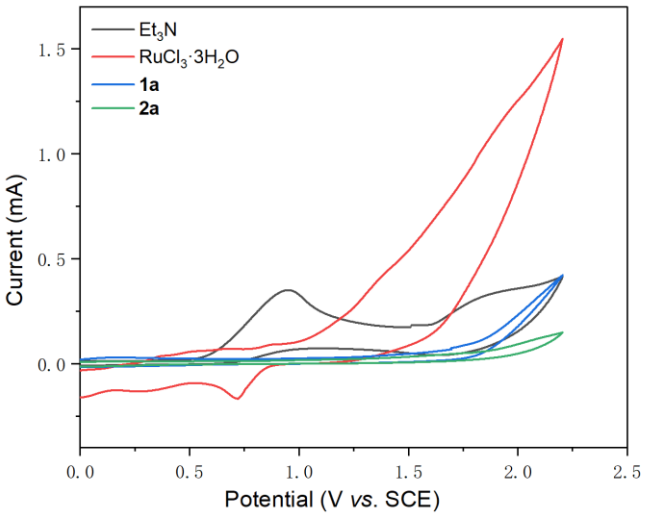
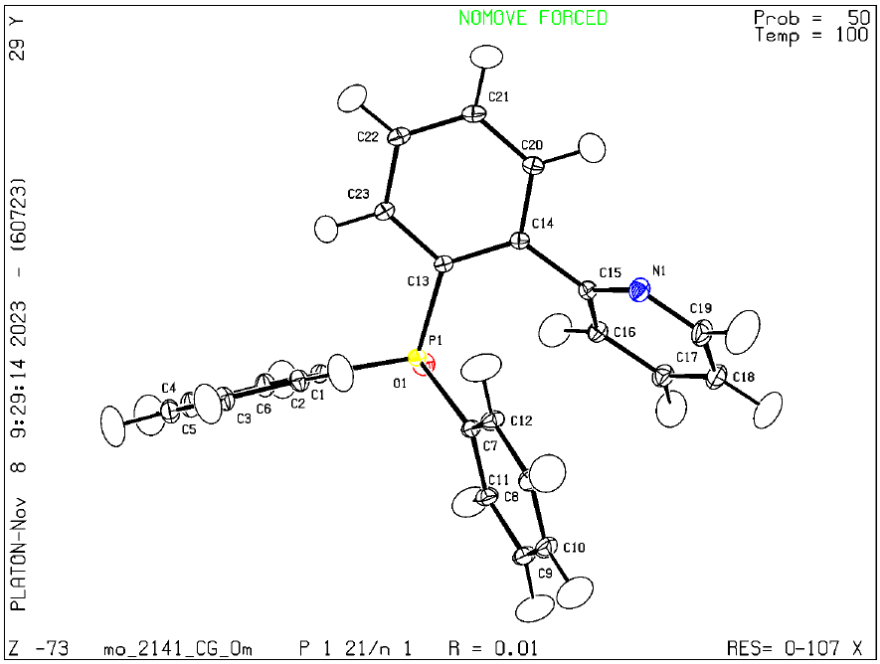


Figure S7. Cyclic voltammetry studies for *para*-C–H phosphorylation.

5. X-ray Crystallographic Data

X-ray crystallographic data of **3i**. (CCDC: 2360253)



Bond precision:	C-C = 0.0004 A	Wavelength=0.71073	
Cell:	a=8.8853(7)	b=21.2925(17)	c=9.3998(7)
	alpha=90	beta=102.203 (3)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	1738.2(2)	1738.2(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H18 N O P	C23 H18 N O P
Sum formula	C23 H18 N O P	C23 H18 N O P
Mr	355.35	355.38
Dx,g cm-3	1.358	1.358
Z	4	4
Mu (mm-1)	0.170	0.170
F000	744.0	744.8
F000’	744.68	
h,k,lmax	13,33,14	13,33,14
Nref	6942	6932
Tmin,Tmax	0.924,0.932	0.912,0.976
Tmin’	0.924	

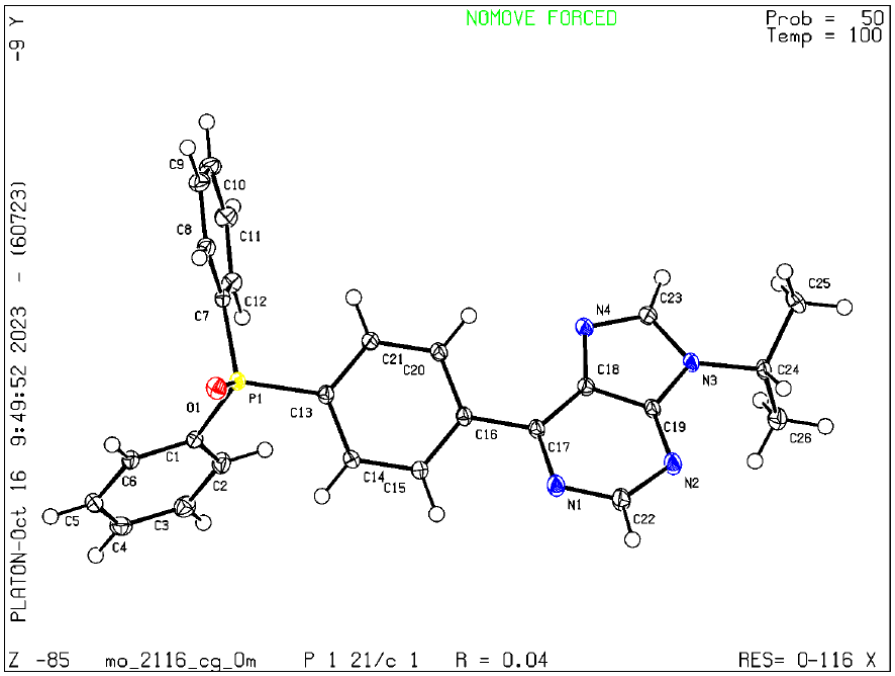
Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.976
AbsCorr = NUMERICAL

Data completeness= 0.999 Theta(max)= 33.740

R(reflections)= 0.0113(6753) wR2(reflections)= 0.0275(6932)

S = 1.091 Npar= 397

X-ray crystallographic data of **4a**. (CCDC: 2360254)



Bond precision:	C-C = 0.0016 A		Wavelength=0.71073
Cell:	a=9.7051(6)	b=22.4271(11)	c=10.9067(7)
	alpha=90	beta=113.919(2)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	2170.1(2)	2170.0(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H23 N4 O P	C26 H23 N4 O P
Sum formula	C26 H23 N4 O P	C26 H23 N4 O P
Mr	438.45	438.45
Dx,g cm-3	1.342	1.342
Z	4	4
Mu (mm-1)	0.154	0.154
F000	920.0	920.0
F000’	920.71	
h,k,lmax	14,33,16	14,33,16
Nref	7253	6973
Tmin,Tmax	0.930,0.981	0.784,1.000
Tmin’	0.930	

Correction method= # Reported T Limits: Tmin=0.784 Tmax=1.000

AbsCorr = NUMERICAL

Data completeness= 0.961	Theta(max)= 33.551
R(reflections)= 0.0402(6320)	wR2(reflections)= 0.1088(6973)
S = 1.024	Npar= 291

6. Computational Studies

All calculations were performed using the Gaussian 16, Revision A.03 package.[2] All structures were optimized at the PBE0[3, 4] level of theory in combination with D3 dispersion corrections with the Becke-Johnson damping scheme (D3BJ).[5, 6] Analytical frequency calculations were carried out at the same level of theory in order to identify each stationary point as either an intermediate (no imaginary frequencies) or a transition state (only one imaginary frequency) and to provided thermal and non-thermal corrections to the Gibbs free energy at 338.15 K and 1 atm. All atoms were described with the def2-SVP basis set, while ruthenium was in addition described with a SSD pseudopotential.[7-11] The electronic energy was then refined through PBE0 single-point calculations on the optimized geometries in combination with a standalone version of Grimme's most recent dispersion correction D4[12, 13] with a def2-TZVPP basis set combined with a SSD pseudopotential for ruthenium.[7-11] Solvent effects were included implicitly through the use of the SMD[14] model for HFIP the parameters were taken from Liu, Engle and coworkers.[15] Energies reported herein are based on gas-phase Gibbs free energies with a def2-SVP basis set for which the electronic energies were corrected to PBE0-D4 with a def2-TZVPP basis set and solvent effects.

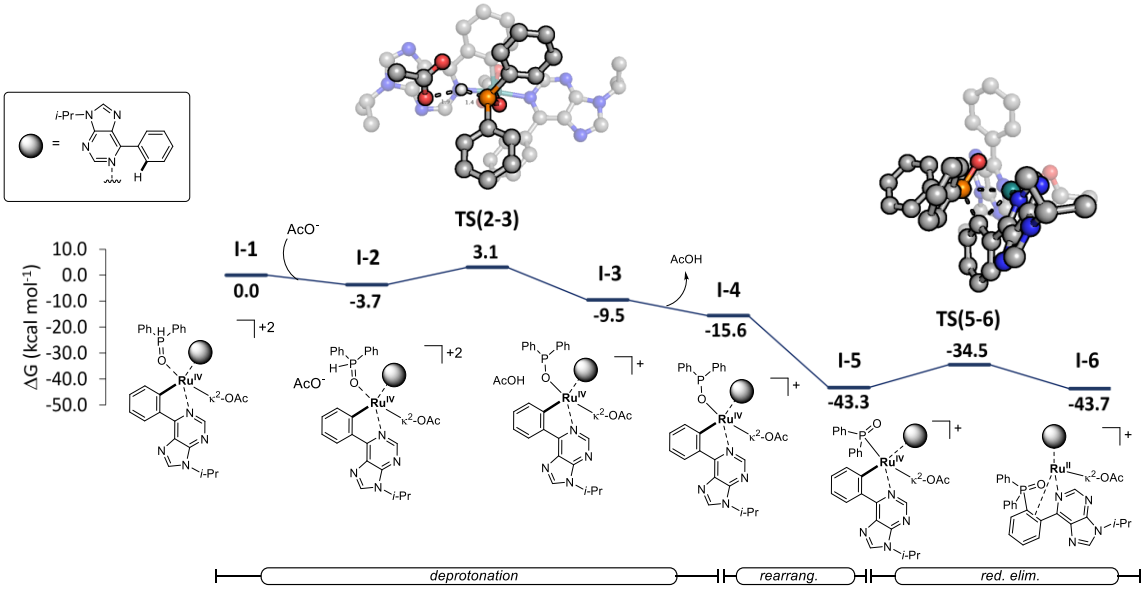


Figure S8. Computed relative Gibbs free energies ($\Delta G_{338.15}$) in kcal mol^{-1} for the ruthenium-catalyzed ortho-C–H phosphorylation at the PBE0-D4/def2-TZVPP-SMD(HFIP)//PBE0-D3BJ/def2-SVP level of theory.

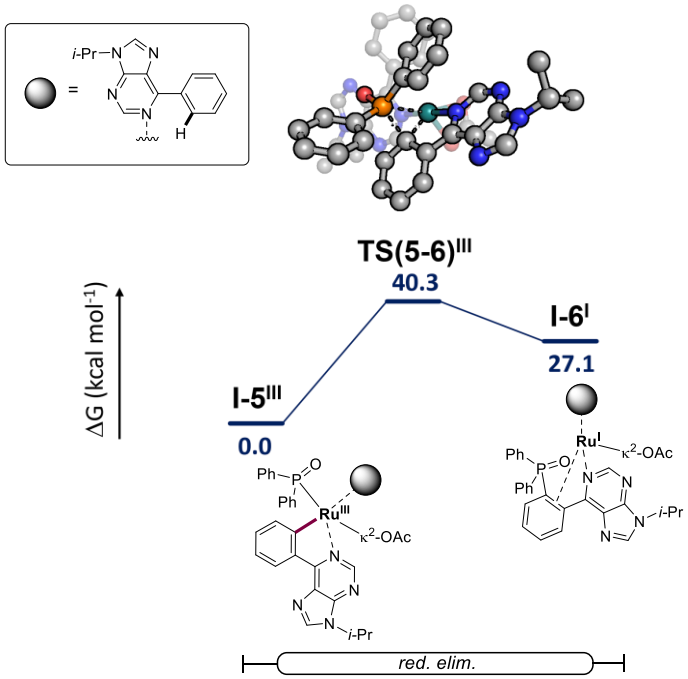


Figure S9. Computed relative Gibbs free energies ($\Delta G_{338.15}$) in kcal mol^{-1} for the ruthenium-catalyzed ortho-C–H phosphorylation reductive elimination step through a ruthenium(III) pathway at the PBE0-D4/def2-TZVPP-SMD(HFIP)//PBE0-D3BJ/def2-SVP level of theory.

Table S3. Calculated electronic energies at the PBE0-D4/def2-TZVPP-SMD(HFIP) level of theory and Gibbs free energies with dispersion corrections for all structures in the present work (all in Hartree).

Structure	Electronic Energy	Total Gibbs Free Energy
I-1	-2723.228119	-2722.561087
I-2	-2951.725394	-2951.014093
TS(2-3)	-2951.710840	-2951.003381
I-3	-2951.731412	-2951.023461
I-4	-2722.780299	-2722.124228
I-5	-2722.827029	-2722.168375
TS(5-6)	-2722.812487	-2722.154319
I-6	-2722.827574	-2722.169027
I-5^{III}	-2722.989976	-2722.335678
TS(5-6)^{III}	-2722.924999	-2722.271498
I-6^{I}	-2722.946189	-2722.292517
Acetate	-228.463443	-228.447157
Acetic Acid	-228.939683	-228.908851

Cartesian coordinates of the optimized structures

I-1

Lowest frequency = 12.4224 cm^{-1}

Charge = 2, Multiplicity = 1

96

Ru	-0.205080	-1.257346	-0.239294
O	0.230397	-2.725443	-1.613169
C	-0.161583	-3.673466	-0.860006
O	-0.575914	-3.246258	0.256475
C	-0.106264	-5.097317	-1.235002
H	-0.812539	-5.680260	-0.631052
H	-0.312404	-5.215244	-2.307144
H	0.912223	-5.471228	-1.041852
N	-2.317288	-1.177931	-0.400698
C	-2.836154	-0.167919	-1.150216
C	-3.135128	-1.953855	0.354580
C	-4.200131	0.093001	-1.014144
C	-1.948702	0.558364	-2.059765
N	-4.433024	-1.806357	0.494433
H	-2.652067	-2.776805	0.884110
C	-4.941895	-0.778895	-0.177219
N	-5.021468	1.030621	-1.571832
C	-0.918983	-0.143593	-2.713043
C	-2.070677	1.940121	-2.242434
N	-6.229266	-0.345323	-0.249887
C	-6.203975	0.739216	-1.094801
C	0.007529	0.543899	-3.501818
H	-0.925168	-1.236762	-2.722277
C	-1.131423	2.617317	-3.013123
H	-2.891285	2.478451	-1.768937
C	-7.418602	-0.917862	0.405876
H	-7.121351	1.284489	-1.325765
C	-0.085126	1.926549	-3.634248
H	0.774758	-0.008180	-4.049846
H	-1.220300	3.698472	-3.140661
C	-7.678195	-2.326999	-0.104164
C	-7.280883	-0.837333	1.918261
H	-8.245159	-0.263613	0.086391
H	0.632010	2.467340	-4.256013
H	-8.615099	-2.706352	0.327137

H	-7.777724	-2.343317	-1.199086
H	-6.866303	-3.007244	0.190744
H	-6.456669	-1.473813	2.271157
H	-8.208920	-1.188846	2.390302
H	-7.103152	0.196376	2.249126
N	1.858002	-1.130799	-0.259718
C	2.482043	-1.081952	0.943695
C	2.564725	-1.057433	-1.410477
C	3.867838	-0.929220	0.942134
C	1.583131	-1.189711	2.066103
N	3.869042	-0.930666	-1.499123
H	1.986522	-1.123496	-2.332914
C	4.495154	-0.868102	-0.327101
N	4.794629	-0.838405	1.939300
C	1.973851	-1.134438	3.411945
C	0.225448	-1.337492	1.719885
N	5.827051	-0.749017	-0.066016
C	5.934847	-0.738194	1.303886
C	1.002208	-1.221039	4.402698
H	3.034278	-1.026920	3.651950
C	-0.740888	-1.423957	2.716515
C	6.940744	-0.727090	-1.030765
H	6.911514	-0.654714	1.784558
C	-0.344973	-1.360700	4.055884
H	1.292050	-1.185111	5.454736
H	-1.799287	-1.530831	2.478596
C	7.015592	-2.050207	-1.777806
C	6.832973	0.477063	-1.952727
H	7.840767	-0.618485	-0.405106
H	-1.103403	-1.428553	4.839542
H	7.901996	-2.056823	-2.427389
H	7.099244	-2.896936	-1.081342
H	6.127470	-2.194312	-2.409914
H	5.926581	0.416180	-2.571978
H	7.703731	0.504511	-2.622408
H	6.817408	1.416436	-1.382058
O	-0.394283	0.676205	0.156247
P	0.204717	1.760071	1.115983
H	0.110763	1.307274	2.452821
C	-0.804564	3.215774	0.912144
C	-0.230382	4.465669	0.652660
C	-2.198224	3.071236	0.996152
C	-1.057505	5.572701	0.473254
H	0.854690	4.576243	0.589240

C	-3.012488	4.182446	0.815827
H	-2.644171	2.091682	1.188499
C	-2.441967	5.430765	0.553047
H	-0.617360	6.551346	0.271452
H	-4.097704	4.078267	0.876958
H	-3.085446	6.302238	0.412648
C	1.928003	2.105581	0.826463
C	2.803603	2.249288	1.909754
C	2.383723	2.246033	-0.493022
C	4.142292	2.548017	1.670898
H	2.448939	2.122999	2.936113
C	3.725701	2.533554	-0.718811
H	1.692849	2.128209	-1.332615
C	4.598272	2.691099	0.361006
H	4.829863	2.665550	2.510504
H	4.094421	2.641592	-1.740887
H	5.647045	2.935940	0.178385

I-2

Lowest frequency = 13.4853 cm^{-1}

Charge = 1, Multiplicity = 1

103

Ru	-0.246206	-0.986907	-1.079319
O	0.083199	-1.447083	-3.086147
C	-0.381522	-2.630916	-2.997549
O	-0.788305	-2.945796	-1.851608
C	-0.397540	-3.554556	-4.157843
H	-1.116730	-4.365094	-3.990454
H	-0.632850	-3.003676	-5.077908
H	0.606656	-3.991275	-4.273711
N	-2.347460	-0.604412	-1.177391
C	-2.813249	0.668100	-1.272808
C	-3.180637	-1.612680	-0.825597
C	-4.129267	0.886165	-0.842018
C	-1.979150	1.726650	-1.847496
N	-4.434005	-1.497902	-0.442557
H	-2.744739	-2.612406	-0.864940
C	-4.869435	-0.242606	-0.424350
N	-4.894506	2.017899	-0.734398
C	-1.097935	1.424809	-2.897080
C	-2.074949	3.047376	-1.388037

N	-6.092581	0.234154	-0.054798
C	-6.034602	1.592152	-0.262230
C	-0.299237	2.419278	-3.451012
H	-1.069176	0.417376	-3.315229
C	-1.269219	4.035051	-1.942485
H	-2.786098	3.296267	-0.600222
C	-7.232676	-0.528743	0.465365
H	-6.894963	2.225680	-0.038248
C	-0.376017	3.724491	-2.967055
H	0.372764	2.176591	-4.277425
H	-1.336348	5.058092	-1.568706
C	-7.735611	-1.517740	-0.575803
C	-6.867894	-1.185692	1.789050
H	-8.012766	0.228399	0.645411
H	0.252246	4.506669	-3.398108
H	-8.634772	-2.026607	-0.200529
H	-7.997635	-1.006270	-1.513291
H	-6.971047	-2.278146	-0.789624
H	-6.076188	-1.934873	1.644081
H	-7.748579	-1.691285	2.209729
H	-6.520406	-0.439803	2.519300
N	1.785562	-1.229364	-1.013962
C	2.277515	-1.995972	-0.007343
C	2.601040	-0.524422	-1.823521
C	3.661916	-1.999725	0.164108
C	1.258319	-2.552540	0.851498
N	3.907882	-0.436821	-1.700132
H	2.110204	0.028943	-2.628399
C	4.403523	-1.151290	-0.694877
N	4.478590	-2.557340	1.106173
C	1.525903	-3.348292	1.973019
C	-0.059418	-2.137308	0.552344
N	5.685243	-1.207859	-0.238472
C	5.656736	-2.057912	0.837894
C	0.474771	-3.731986	2.798171
H	2.557813	-3.634800	2.186322
C	-1.095142	-2.504617	1.406718
C	6.835612	-0.423108	-0.702049
H	6.567882	-2.272432	1.399105
C	-0.823871	-3.301536	2.520896
H	0.669163	-4.356483	3.672459
H	-2.114421	-2.153316	1.250785
C	7.195263	-0.792562	-2.132859
C	6.567900	1.063310	-0.509787

H	7.659366	-0.726832	-0.036072
H	-1.643285	-3.577012	3.188815
H	8.095199	-0.242451	-2.442578
H	7.401409	-1.868647	-2.227518
H	6.376980	-0.527350	-2.817705
H	5.794537	1.408507	-1.210649
H	7.488674	1.633208	-0.699263
H	6.214967	1.271643	0.509767
O	-0.172794	0.529482	-0.042539
P	0.843738	0.986719	1.320716
H	1.769303	-0.010959	1.031996
C	-0.534884	0.679820	2.459824
C	-1.833811	1.042575	2.079135
C	-0.325990	0.011838	3.669899
C	-2.912836	0.731076	2.900567
H	-1.994030	1.567369	1.137874
C	-1.413283	-0.318593	4.475387
H	0.685248	-0.257307	3.974632
C	-2.705718	0.038345	4.093856
H	-3.920788	1.031753	2.604060
H	-1.246763	-0.855217	5.411967
H	-3.553849	-0.216002	4.734015
C	1.089973	2.649427	0.658904
C	0.457179	3.737623	1.267541
C	1.983243	2.851087	-0.396227
C	0.712824	5.027163	0.808592
H	-0.222193	3.580867	2.108842
C	2.242819	4.145879	-0.839148
H	2.503817	2.007008	-0.851157
C	1.608314	5.233004	-0.240821
H	0.219262	5.878053	1.283648
H	2.952459	4.304883	-1.654185
H	1.817560	6.247281	-0.588678
O	3.755141	0.936614	1.560887
C	3.221917	1.293844	2.597059
O	1.914218	1.389975	2.745587
C	3.981090	1.691176	3.828588
H	3.539692	1.226558	4.720883
H	5.037303	1.416167	3.730197
H	3.897583	2.781322	3.956815

TS(2-3)

Lowest frequency = -173.7764 cm^{-1}

Charge = 1, Multiplicity = 1

103

Ru	-0.321971	-1.302334	-0.650503
O	0.067200	-2.583381	-2.226040
C	-0.379525	-3.615443	-1.629145
O	-0.807715	-3.373339	-0.470607
C	-0.354355	-4.963477	-2.238053
H	-1.099595	-5.611211	-1.760808
H	-0.524851	-4.895689	-3.320291
H	0.644253	-5.399546	-2.077431
N	-2.439617	-1.079412	-0.852263
C	-2.912984	0.025171	-1.488119
C	-3.274392	-1.857928	-0.122822
C	-4.242359	0.377952	-1.234236
C	-2.035550	0.763520	-2.398084
N	-4.541425	-1.616707	0.134922
H	-2.829890	-2.767867	0.284075
C	-4.991100	-0.486799	-0.402009
N	-5.017665	1.426921	-1.649198
C	-1.120653	0.058200	-3.196064
C	-2.058682	2.162712	-2.443864
N	-6.232489	0.069299	-0.319281
C	-6.174726	1.211131	-1.084304
C	-0.201248	0.747061	-3.983612
H	-1.164210	-1.031146	-3.245168
C	-1.129166	2.842584	-3.222103
H	-2.787716	2.711030	-1.846788
C	-7.393370	-0.430690	0.427889
H	-7.049721	1.856228	-1.184676
C	-0.190384	2.140497	-3.980079
H	0.497062	0.192293	-4.614671
H	-1.125098	3.934055	-3.226008
C	-7.842006	-1.777444	-0.119599
C	-7.089114	-0.459724	1.918773
H	-8.183639	0.313469	0.239012
H	0.539145	2.684612	-4.583639
H	-8.756548	-2.101223	0.397050
H	-8.060801	-1.714999	-1.195409
H	-7.066607	-2.540166	0.040504
H	-6.291479	-1.184282	2.137885
H	-7.987914	-0.759093	2.476092
H	-6.778480	0.532135	2.279390

N	1.723235	-1.319082	-0.591746
C	2.309733	-1.583911	0.603860
C	2.460433	-1.028235	-1.684552
C	3.699745	-1.588404	0.641001
C	1.361477	-1.739389	1.678644
N	3.770537	-0.960218	-1.720899
H	1.899264	-0.836053	-2.601761
C	4.357782	-1.215626	-0.557597
N	4.601920	-1.750321	1.651759
C	1.706340	-1.878005	3.027073
C	0.008519	-1.656583	1.285387
N	5.677526	-1.149353	-0.238403
C	5.751015	-1.470621	1.094493
C	0.693863	-1.957337	3.975835
H	2.762158	-1.892286	3.302344
C	-0.997564	-1.746902	2.244683
C	6.777842	-0.675945	-1.085401
H	6.712710	-1.480042	1.610263
C	-0.646348	-1.891066	3.587049
H	0.948857	-2.058505	5.032514
H	-2.050848	-1.668674	1.980932
C	7.053364	-1.665684	-2.206961
C	6.491675	0.734502	-1.583341
H	7.648131	-0.647007	-0.410034
H	-1.435704	-1.935962	4.340562
H	7.913847	-1.325478	-2.800709
H	7.282764	-2.665910	-1.811306
H	6.183302	-1.740295	-2.875571
H	5.704875	0.718222	-2.350208
H	7.403125	1.163747	-2.023239
H	6.138543	1.376315	-0.764453
O	-0.328178	0.578444	-0.287175
P	0.536118	1.481558	0.729519
H	1.892620	1.053751	0.925600
C	-0.446858	1.503675	2.229162
C	-1.844864	1.434199	2.122756
C	0.178284	1.566041	3.479557
C	-2.620408	1.436001	3.276286
H	-2.316730	1.358589	1.139908
C	-0.615920	1.565203	4.626595
H	1.272439	1.585008	3.533105
C	-2.004517	1.501965	4.528515
H	-3.709213	1.381873	3.201745
H	-0.138739	1.609478	5.608143

H	-2.615203	1.502370	5.434616
C	0.622400	3.106408	-0.013519
C	-0.446931	4.008203	0.061068
C	1.791788	3.434290	-0.714760
C	-0.355307	5.234279	-0.588504
H	-1.341510	3.758440	0.636645
C	1.867258	4.664110	-1.366366
H	2.642597	2.743266	-0.702555
C	0.798042	5.557179	-1.307757
H	-1.180785	5.946937	-0.527278
H	2.776334	4.932973	-1.908810
H	0.868704	6.523884	-1.812318
O	3.742535	1.296887	0.515865
C	3.891856	1.390508	1.767210
O	2.989333	1.132492	2.593148
C	5.233484	1.851087	2.310558
H	5.123165	2.867283	2.719676
H	5.533645	1.201843	3.145114
H	6.013710	1.866654	1.538264

I-3

Lowest frequency = 9.3613 cm^{-1}

Charge = 1, Multiplicity = 1

103

Ru	0.292215	0.976236	-1.024824
O	-0.063138	1.628059	-2.961923
C	0.324822	2.824916	-2.750411
O	0.700793	3.042815	-1.572984
C	0.291661	3.858375	-3.812643
H	0.950261	4.694965	-3.550818
H	0.577421	3.419994	-4.777854
H	-0.739061	4.234648	-3.905242
N	2.422785	0.792940	-1.104400
C	2.985007	-0.426230	-1.315710
C	3.176038	1.822067	-0.646949
C	4.314162	-0.584873	-0.904934
C	2.221889	-1.486777	-1.977287
N	4.435437	1.764991	-0.271269
H	2.664723	2.784266	-0.587295
C	4.968365	0.552110	-0.377909
N	5.164554	-1.658581	-0.913559

C	1.334824	-1.160308	-3.014221
C	2.365018	-2.824222	-1.585061
N	6.227504	0.137482	-0.060394
C	6.272160	-1.193918	-0.403122
C	0.566922	-2.152085	-3.617220
H	1.274139	-0.133583	-3.379786
C	1.590870	-3.808002	-2.187698
H	3.072212	-3.084812	-0.797666
C	7.312042	0.930933	0.529062
H	7.181266	-1.777256	-0.244868
C	0.684003	-3.475300	-3.194376
H	-0.111451	-1.891996	-4.433247
H	1.685326	-4.844172	-1.858692
C	7.730611	2.049323	-0.413876
C	6.911269	1.429384	1.910130
H	8.147764	0.220583	0.634463
H	0.077515	-4.255113	-3.660251
H	8.592308	2.586494	0.007051
H	8.022267	1.650615	-1.396300
H	6.909770	2.767288	-0.552973
H	6.066730	2.129995	1.839175
H	7.756556	1.954951	2.376436
H	6.624981	0.593389	2.565445
N	-1.750304	0.990473	-0.995440
C	-2.344321	1.631948	0.042038
C	-2.472273	0.339271	-1.929913
C	-3.740508	1.629880	0.065352
C	-1.412289	2.150156	1.010540
N	-3.783616	0.243856	-1.949102
H	-1.898947	-0.148729	-2.722192
C	-4.385247	0.889127	-0.953232
N	-4.659145	2.136660	0.941236
C	-1.782783	2.747817	2.220993
C	-0.052418	1.925692	0.697182
N	-5.716218	0.961786	-0.666117
C	-5.807084	1.720094	0.474006
C	-0.791039	3.122863	3.119427
H	-2.841973	2.884583	2.445532
C	0.928587	2.301585	1.610380
C	-6.820692	0.297435	-1.367199
H	-6.778681	1.936316	0.921770
C	0.552535	2.893501	2.817687
H	-1.066118	3.581602	4.070999
H	1.984468	2.108579	1.428222

C	-6.950915	0.827118	-2.787060
C	-6.650229	-1.214022	-1.302772
H	-7.719298	0.581245	-0.795815
H	1.326544	3.165300	3.538780
H	-7.822803	0.369460	-3.275614
H	-7.087931	1.918187	-2.793144
H	-6.056048	0.579174	-3.375740
H	-5.775569	-1.528508	-1.889593
H	-7.541578	-1.707132	-1.715738
H	-6.508571	-1.554390	-0.266994
O	0.326695	-0.669141	-0.165553
P	-0.695936	-1.252055	1.043093
H	-2.991228	-1.008455	1.344273
C	0.403761	-0.871668	2.447052
C	1.800130	-0.900523	2.304327
C	-0.167463	-0.459665	3.654963
C	2.615202	-0.528697	3.368098
H	2.240228	-1.202219	1.351328
C	0.658428	-0.098808	4.720647
H	-1.255179	-0.393437	3.749386
C	2.044033	-0.129427	4.579244
H	3.702355	-0.550699	3.255703
H	0.210832	0.221381	5.664331
H	2.685218	0.161017	5.415089
C	-0.488406	-3.039183	0.742437
C	0.455886	-3.854743	1.377210
C	-1.382417	-3.610293	-0.174544
C	0.513047	-5.215786	1.084488
H	1.140766	-3.427880	2.112815
C	-1.317956	-4.968502	-0.472829
H	-2.141517	-2.984441	-0.654621
C	-0.369573	-5.772881	0.158678
H	1.246598	-5.848666	1.589458
H	-2.018510	-5.404362	-1.188841
H	-0.326034	-6.842165	-0.061900
O	-3.968989	-1.063553	1.487800
C	-4.235758	-0.559602	2.693535
O	-3.385104	-0.105603	3.418968
C	-5.686756	-0.655871	3.059872
H	-5.838832	-1.585055	3.631109
H	-5.954245	0.187236	3.707851
H	-6.332998	-0.692876	2.174405

I-4

Lowest frequency = 12.8958 cm^{-1}

Charge = 1, Multiplicity = 1

95

Ru	-0.121660	-1.211113	-0.350593
O	0.285972	-2.398653	-2.085163
C	-0.062310	-3.470609	-1.504592
O	-0.434379	-3.324712	-0.307920
C	-0.004017	-4.794136	-2.173235
H	-0.628919	-5.521859	-1.642135
H	-0.315096	-4.700968	-3.222050
H	1.038578	-5.148084	-2.162168
N	-2.244277	-1.114633	-0.577193
C	-2.779307	-0.003920	-1.147925
C	-3.036476	-2.004449	0.063147
C	-4.143126	0.220327	-0.931685
C	-1.943001	0.869885	-1.979181
N	-4.330152	-1.888688	0.276894
H	-2.530585	-2.900553	0.428633
C	-4.851141	-0.764930	-0.204621
N	-4.988452	1.227876	-1.312894
C	-0.963588	0.302874	-2.808812
C	-2.090729	2.261396	-1.936402
N	-6.140895	-0.324623	-0.151474
C	-6.147617	0.871824	-0.829509
C	-0.109422	1.119562	-3.546545
H	-0.901103	-0.781348	-2.920792
C	-1.225399	3.070650	-2.665311
H	-2.863898	2.706642	-1.311530
C	-7.291016	-0.984323	0.477663
H	-7.071294	1.444393	-0.933721
C	-0.228304	2.506137	-3.462886
H	0.637881	0.669232	-4.204270
H	-1.330638	4.155697	-2.605037
C	-7.585492	-2.310722	-0.207511
C	-7.071065	-1.120599	1.977136
H	-8.133536	-0.296327	0.301429
H	0.442822	3.149697	-4.036383
H	-8.494008	-2.756556	0.221566
H	-7.748453	-2.172218	-1.286176
H	-6.753727	-3.014976	-0.062882
H	-6.224706	-1.790947	2.185104

H	-7.969628	-1.544209	2.447602
H	-6.871173	-0.142924	2.439554
N	1.918631	-1.093934	-0.309012
C	2.506314	-1.179070	0.909611
C	2.646048	-0.853071	-1.421447
C	3.888681	-0.979441	0.962871
C	1.582413	-1.463934	1.977811
N	3.949226	-0.684505	-1.461467
H	2.084405	-0.811556	-2.356405
C	4.538748	-0.744269	-0.269989
N	4.792176	-0.975864	1.988771
C	1.947190	-1.603434	3.324716
C	0.235245	-1.596371	1.570144
N	5.862626	-0.610702	0.038306
C	5.939646	-0.756613	1.401729
C	0.963522	-1.877353	4.265259
H	2.997136	-1.493449	3.604148
C	-0.738887	-1.864286	2.528597
C	6.988546	-0.447145	-0.888748
H	6.901275	-0.691213	1.913857
C	-0.370332	-2.004763	3.867122
H	1.231146	-1.989028	5.317799
H	-1.790837	-1.949260	2.256259
C	7.114059	-1.671028	-1.785194
C	6.867103	0.851403	-1.670690
H	7.875911	-0.389652	-0.237980
H	-1.141171	-2.210251	4.613887
H	8.008617	-1.579610	-2.417407
H	7.207803	-2.590793	-1.189694
H	6.236124	-1.762051	-2.440932
H	5.962683	0.844127	-2.295561
H	7.741406	0.971229	-2.325914
H	6.823767	1.716526	-0.995117
O	-0.357419	0.546559	0.253186
P	0.143756	1.455476	1.531087
C	-0.914077	2.914842	1.228792
C	-0.449801	4.155523	0.782305
C	-2.283655	2.739523	1.475756
C	-1.349716	5.197538	0.558522
H	0.615967	4.308411	0.599215
C	-3.180785	3.776123	1.238837
H	-2.648350	1.776323	1.845540
C	-2.713487	5.007802	0.776371
H	-0.981621	6.164910	0.208539

H	-4.247893	3.626873	1.418046
H	-3.414795	5.825798	0.596378
C	1.811845	2.006077	1.043495
C	2.771674	2.176972	2.047039
C	2.155657	2.234075	-0.296859
C	4.058868	2.600297	1.720202
H	2.510397	1.970774	3.088636
C	3.446186	2.643200	-0.620495
H	1.406944	2.092400	-1.081261
C	4.393408	2.835436	0.388028
H	4.801785	2.741569	2.508184
H	3.715160	2.819506	-1.664628
H	5.398334	3.178522	0.132041

I-5

Lowest frequency = 15.4997 cm^{-1}

Charge = 1, Multiplicity = 1

95

Ru	0.166255	0.496813	-0.842323
O	0.448816	2.209553	-2.142399
C	0.358342	1.453764	-3.149902
O	0.157929	0.222000	-2.910127
C	0.508236	1.956687	-4.540536
H	0.070829	1.250657	-5.256231
H	0.046385	2.948028	-4.633451
H	1.581724	2.063078	-4.761058
N	-1.993025	0.680639	-0.959993
C	-2.808022	1.406223	-0.141234
C	-2.518438	-0.293151	-1.742632
C	-4.129816	0.940054	-0.016006
C	-2.361178	2.642348	0.513845
N	-3.746728	-0.763059	-1.712159
H	-1.827079	-0.725920	-2.467236
C	-4.513732	-0.163582	-0.807957
N	-5.191376	1.353769	0.748299
C	-1.395261	3.457537	-0.091969
C	-2.957636	3.073394	1.712078
N	-5.817023	-0.415706	-0.493396
C	-6.154378	0.527056	0.446556
C	-0.999166	4.647276	0.506987
H	-0.961225	3.170728	-1.047597

C	-2.547627	4.257212	2.313612
H	-3.755925	2.482499	2.157979
C	-6.682751	-1.466913	-1.035613
H	-7.156762	0.548924	0.878224
C	-1.561435	5.044409	1.718845
H	-0.248998	5.272085	0.017313
H	-3.011265	4.575199	3.250033
C	-6.907484	-1.262552	-2.526656
C	-6.120331	-2.840345	-0.697600
H	-7.641481	-1.335296	-0.508443
H	-1.245853	5.977297	2.191857
H	-7.614792	-2.015161	-2.903112
H	-7.326365	-0.266450	-2.730150
H	-5.962487	-1.367151	-3.078480
H	-5.157011	-2.997425	-1.204117
H	-6.817242	-3.622391	-1.030767
H	-5.971729	-2.949353	0.386861
N	2.196264	0.395496	-0.745461
C	2.760474	-0.827313	-0.894926
C	2.935890	1.486709	-0.458287
C	4.149773	-0.900454	-0.754825
C	1.817716	-1.903962	-1.102353
N	4.240783	1.497216	-0.284357
H	2.379829	2.421908	-0.357320
C	4.813977	0.306330	-0.434648
N	5.042068	-1.936281	-0.809234
C	2.214420	-3.220899	-1.371835
C	0.452483	-1.555289	-0.970392
N	6.130824	-0.030640	-0.297651
C	6.193314	-1.381345	-0.535648
C	1.251084	-4.211909	-1.512168
H	3.279860	-3.444286	-1.455771
C	-0.494900	-2.570386	-1.104382
C	7.248418	0.850261	0.058409
H	7.147238	-1.909968	-0.490784
C	-0.098078	-3.882904	-1.379377
H	1.548882	-5.240418	-1.724882
H	-1.559822	-2.362606	-1.001695
C	7.430281	1.936727	-0.990969
C	7.059179	1.401055	1.464723
H	8.132829	0.192989	0.048377
H	-0.861357	-4.657574	-1.489263
H	8.316925	2.540309	-0.750572
H	7.573066	1.501137	-1.990507

H	6.555305	2.601738	-1.016504
H	6.168594	2.044358	1.511152
H	7.933931	2.001448	1.752008
H	6.948452	0.586526	2.195799
P	0.040427	-0.281621	1.250908
O	0.216527	1.263825	1.182722
C	-1.493156	-0.811746	2.020181
C	-2.140042	0.124990	2.836470
C	-2.049485	-2.082497	1.822352
C	-3.354123	-0.204663	3.432200
H	-1.697250	1.111179	2.987345
C	-3.266808	-2.398039	2.419466
H	-1.543822	-2.823446	1.202943
C	-3.921584	-1.459492	3.217593
H	-3.861647	0.526937	4.064315
H	-3.703901	-3.386736	2.263308
H	-4.876554	-1.712170	3.684002
C	1.469792	-1.073617	1.994513
C	2.499474	-0.243008	2.454711
C	1.604376	-2.466341	2.040516
C	3.667913	-0.812801	2.953221
H	2.378269	0.841370	2.411969
C	2.778823	-3.024267	2.534443
H	0.811890	-3.117689	1.665387
C	3.810189	-2.199717	2.985761
H	4.470747	-0.167525	3.316851
H	2.893984	-4.109636	2.558420
H	4.731169	-2.644787	3.369055

TS(5-6)

Lowest frequency = -127.7435 cm^{-1}

Charge = 1, Multiplicity = 1

95

scf done: -2720.126539

Ru	-0.001914	-1.066800	-0.009383
O	-0.106245	-3.056401	0.660761
C	-0.078348	-3.479472	-0.536405
O	-0.018087	-2.594559	-1.440050
C	-0.085423	-4.934297	-0.848852
H	-0.410273	-5.104607	-1.882083
H	0.937569	-5.324539	-0.731401
H	-0.729879	-5.471248	-0.140988

N	2.123810	-1.101716	-0.013966
C	2.979046	-0.836558	1.009266
C	2.600091	-1.216092	-1.281288
C	4.319505	-0.589537	0.655302
C	2.550589	-0.839543	2.415368
N	3.836532	-1.025991	-1.689335
H	1.855484	-1.494503	-2.029792
C	4.668928	-0.698051	-0.707280
N	5.429226	-0.272160	1.396642
C	1.579118	-1.740075	2.872658
C	3.161023	0.031802	3.333974
N	6.007265	-0.434488	-0.773042
C	6.393235	-0.186740	0.521346
C	1.200573	-1.741747	4.210270
H	1.130114	-2.452472	2.182581
C	2.764046	0.037148	4.666450
H	3.956651	0.697373	2.999480
C	6.864208	-0.438989	-1.961702
H	7.431687	0.055179	0.755509
C	1.778555	-0.845342	5.107803
H	0.447845	-2.454363	4.554674
H	3.236369	0.727781	5.368531
C	6.931241	-1.833724	-2.567194
C	6.404863	0.620266	-2.953412
H	7.862860	-0.164848	-1.584897
H	1.473313	-0.844628	6.156869
H	7.633859	-1.840289	-3.412669
H	7.278027	-2.569507	-1.827216
H	5.942475	-2.143028	-2.935272
H	5.402076	0.379993	-3.335198
H	7.098932	0.660329	-3.804950
H	6.377815	1.615201	-2.485212
N	-2.036753	-0.986442	-0.154677
C	-2.524579	-0.275298	-1.198110
C	-2.872634	-1.574812	0.726600
C	-3.908014	-0.196148	-1.345296
C	-1.512877	0.384064	-2.021279
N	-4.190734	-1.515531	0.688747
H	-2.388643	-2.136953	1.529035
C	-4.675949	-0.830276	-0.337292
N	-4.720646	0.431894	-2.246349
C	-1.681172	0.574350	-3.388708
C	-0.279489	0.729882	-1.386376
N	-5.978552	-0.561991	-0.658021

C	-5.928677	0.188730	-1.804393
C	-0.615533	1.052190	-4.155200
H	-2.635814	0.316769	-3.850390
C	0.773864	1.204218	-2.189423
C	-7.182814	-0.966098	0.076459
H	-6.847800	0.537006	-2.279383
C	0.615520	1.339516	-3.565038
H	-0.745989	1.185618	-5.231574
H	1.721825	1.481472	-1.724426
C	-7.299908	-2.482363	0.119233
C	-7.199681	-0.324803	1.456621
H	-8.017920	-0.559794	-0.516723
H	1.450745	1.686599	-4.176568
H	-8.243601	-2.767904	0.605130
H	-7.293633	-2.908970	-0.894261
H	-6.469946	-2.919611	0.692367
H	-6.363326	-0.696723	2.065917
H	-8.138960	-0.572141	1.971142
H	-7.124782	0.770000	1.383980
P	-0.328454	1.387341	0.416633
O	-0.068772	0.409009	1.580728
C	0.890325	2.713799	0.472263
C	1.827517	2.646918	1.507893
C	0.894508	3.796346	-0.417897
C	2.783181	3.653328	1.638313
H	1.794733	1.807521	2.205006
C	1.846601	4.799033	-0.275239
H	0.165603	3.858651	-1.228680
C	2.793936	4.725338	0.749435
H	3.518386	3.597236	2.444189
H	1.851741	5.644876	-0.965996
H	3.540984	5.515394	0.855156
C	-2.001616	2.058187	0.558264
C	-2.727250	1.693899	1.697490
C	-2.582434	2.875198	-0.419122
C	-4.040302	2.136535	1.846982
H	-2.256928	1.053969	2.447355
C	-3.891361	3.316652	-0.260117
H	-2.032866	3.141244	-1.324598
C	-4.621253	2.943329	0.869925
H	-4.611298	1.846062	2.731556
H	-4.348726	3.943824	-1.027727
H	-5.650848	3.289144	0.989639

I-6

Lowest frequency = 14.1755 cm^{-1}

Charge = 1, Multiplicity = 1

95

Ru	0.014496	-0.854164	0.750671
O	0.053725	-1.731913	2.651348
C	0.087356	-2.891870	2.137066
O	0.063246	-2.941787	0.870074
C	0.182983	-4.117107	2.974042
H	-0.165172	-4.993719	2.414937
H	1.237936	-4.271577	3.249790
H	-0.389766	-3.989448	3.901475
N	2.139221	-0.927546	0.543620
C	3.076972	-0.033124	0.953705
C	2.493337	-1.937310	-0.293960
C	4.363568	-0.173588	0.399034
C	2.798092	0.999210	1.961473
N	3.675265	-2.156014	-0.828977
H	1.695199	-2.639577	-0.537327
C	4.583690	-1.253336	-0.481980
N	5.526147	0.536582	0.563647
C	1.922407	0.748051	3.026967
C	3.480954	2.226719	1.912235
N	5.895927	-1.175199	-0.850887
C	6.395233	-0.080340	-0.188807
C	1.711619	1.714122	4.003981
H	1.416948	-0.213877	3.103339
C	3.263757	3.189178	2.892125
H	4.188349	2.420383	1.107042
C	6.628074	-2.072889	-1.748405
H	7.439823	0.213500	-0.308201
C	2.374181	2.939126	3.937179
H	1.028406	1.503250	4.829309
H	3.799601	4.139993	2.843193
C	6.698430	-3.475463	-1.161827
C	6.021148	-2.039865	-3.143989
H	7.645761	-1.652449	-1.792464
H	2.208852	3.695004	4.708627
H	7.311426	-4.119879	-1.807951
H	7.152404	-3.462672	-0.160353
H	5.692998	-3.914134	-1.087833

H	4.996493	-2.438747	-3.126538
H	6.621215	-2.657521	-3.827214
H	5.997291	-1.014130	-3.540589
N	-2.020384	-0.917973	0.714148
C	-2.247348	-1.046029	-0.601972
C	-3.014901	-0.910761	1.612738
C	-3.554933	-1.218679	-1.031356
C	-0.960818	-0.984785	-1.338917
N	-4.294177	-1.036888	1.301306
H	-2.726232	-0.797016	2.660545
C	-4.530488	-1.186139	0.005254
N	-4.149236	-1.372924	-2.251055
C	-0.649982	-2.011301	-2.277730
C	-0.121279	0.186894	-1.285410
N	-5.729298	-1.331690	-0.636236
C	-5.424924	-1.438001	-1.971096
C	0.467688	-1.924951	-3.067786
H	-1.325523	-2.864412	-2.354709
C	1.023820	0.236558	-2.138075
C	-7.065660	-1.402954	-0.033376
H	-6.218743	-1.566873	-2.709546
C	1.320607	-0.797471	-2.989065
H	0.695312	-2.726291	-3.773841
H	1.660782	1.123516	-2.109276
C	-7.175940	-2.622317	0.870419
C	-7.404208	-0.101057	0.676989
H	-7.747906	-1.530496	-0.889313
H	2.205923	-0.741461	-3.625336
H	-8.203110	-2.710292	1.251709
H	-6.933522	-3.544912	0.323273
H	-6.495870	-2.530953	1.729402
H	-6.717945	0.070730	1.518516
H	-8.429721	-0.148888	1.069599
H	-7.338301	0.752803	-0.011827
P	-0.580975	1.648181	-0.319688
O	-0.240192	1.273540	1.135332
C	0.343128	3.091395	-0.852296
C	1.107897	3.746786	0.116916
C	0.286028	3.577291	-2.165999
C	1.825055	4.889172	-0.233717
H	1.137149	3.355203	1.135272
C	1.010449	4.714082	-2.506602
H	-0.317345	3.072360	-2.924561
C	1.778725	5.369293	-1.540549

H	2.423809	5.402221	0.521975
H	0.974542	5.095748	-3.529162
H	2.342914	6.264220	-1.812999
C	-2.335158	1.979003	-0.571328
C	-3.115699	2.302051	0.543504
C	-2.908333	1.921732	-1.847415
C	-4.471623	2.573957	0.376029
H	-2.655837	2.326752	1.534540
C	-4.262355	2.199447	-2.007026
H	-2.311273	1.627736	-2.714740
C	-5.041084	2.527553	-0.896518
H	-5.086604	2.823189	1.243450
H	-4.712334	2.149694	-3.000605
H	-6.102388	2.752686	-1.025538

I-5^{III}

Lowest frequency = 15.0030 cm^{-1}

Charge = 0, Multiplicity = 2

95

Ru	0.197771	-0.234424	0.766573
O	-0.129269	0.824985	2.663644
C	0.056370	-0.218190	3.372358
O	0.342742	-1.300951	2.815929
C	-0.102127	-0.122027	4.861173
H	0.247603	-1.038834	5.349711
H	0.445893	0.751533	5.240680
H	-1.166224	0.032688	5.096315
N	2.311835	-0.287560	0.774182
C	3.168038	0.635266	0.274511
C	2.751411	-1.541607	1.062905
C	4.452892	0.183236	-0.064369
C	2.818252	2.055489	0.230151
N	3.952950	-2.026093	0.832765
H	2.011890	-2.193722	1.530143
C	4.763661	-1.157852	0.236056
N	5.545398	0.810685	-0.610729
C	2.139146	2.623591	1.314297
C	3.259627	2.870873	-0.822511
N	6.060442	-1.334729	-0.156989
C	6.459212	-0.116996	-0.658365
C	1.914039	3.997530	1.351499

H	1.787794	1.990785	2.130761
C	3.014013	4.235204	-0.784725
H	3.769294	2.418169	-1.671177
C	6.856130	-2.557683	-0.068989
H	7.468694	0.015509	-1.052391
C	2.348438	4.803432	0.304525
H	1.381902	4.434102	2.198771
H	3.336147	4.865512	-1.616527
C	7.061978	-2.958827	1.385360
C	6.225337	-3.663192	-0.904858
H	7.831502	-2.290189	-0.507888
H	2.155211	5.878276	0.326222
H	7.714411	-3.842179	1.442949
H	7.531603	-2.144238	1.955949
H	6.097988	-3.204967	1.853260
H	5.237466	-3.930735	-0.502611
H	6.863227	-4.558739	-0.887231
H	6.103712	-3.345190	-1.950675
N	-1.849839	-0.575934	0.787888
C	-2.242874	-1.695170	0.121851
C	-2.746266	0.206745	1.418082
C	-3.617998	-1.972158	0.115216
C	-1.191618	-2.398961	-0.570947
N	-4.053014	0.030347	1.441391
H	-2.326650	1.051684	1.965894
C	-4.452657	-1.048703	0.774772
N	-4.370564	-2.962968	-0.463106
C	-1.420648	-3.538859	-1.357331
C	0.082235	-1.779960	-0.498456
N	-5.729843	-1.500553	0.575645
C	-5.602265	-2.645099	-0.172339
C	-0.383344	-4.057344	-2.118320
H	-2.419981	-3.976764	-1.381370
C	1.095993	-2.300461	-1.318550
C	-6.972251	-0.876661	1.024638
H	-6.484805	-3.210999	-0.476088
C	0.862987	-3.420376	-2.112519
H	-0.547187	-4.940001	-2.740363
H	2.057395	-1.791116	-1.391450
C	-7.022044	-0.812862	2.544870
C	-7.149314	0.485943	0.367948
H	-7.769825	-1.550060	0.669682
H	1.667335	-3.799512	-2.749204
H	-7.987560	-0.400938	2.872532

H	-6.905798	-1.814253	2.984534
H	-6.218027	-0.167078	2.925783
H	-6.345517	1.167998	0.680741
H	-8.113911	0.924788	0.661568
H	-7.128058	0.398996	-0.728255
P	0.008694	1.004494	-1.171050
C	-1.520781	0.519122	-2.079644
C	-2.795258	0.999372	-1.757842
C	-1.384979	-0.420255	-3.106297
C	-3.920516	0.510686	-2.419007
H	-2.911551	1.765259	-0.987095
C	-2.510111	-0.908818	-3.767202
H	-0.382052	-0.767110	-3.366554
C	-3.781051	-0.454480	-3.416830
H	-4.911165	0.891385	-2.156226
H	-2.393716	-1.656056	-4.556047
H	-4.663610	-0.845618	-3.929209
C	-0.386692	2.769536	-0.847121
C	-0.112280	3.674827	-1.877300
C	-1.005503	3.223182	0.320116
C	-0.484370	5.011251	-1.752435
H	0.399431	3.308897	-2.771342
C	-1.383591	4.559770	0.442346
H	-1.159535	2.534102	1.152444
C	-1.128833	5.453865	-0.596575
H	-0.269820	5.714030	-2.561812
H	-1.868436	4.906615	1.358563
H	-1.424947	6.501839	-0.502133
O	1.200486	0.873056	-2.109889

TS(5-6)^{III}

Lowest frequency = -218.7340 cm^{-1}

Charge = 0, Multiplicity = 2

95

Ru	-0.133946	0.861876	-0.595572
O	0.024512	3.028834	-1.361911
C	-0.056321	2.556861	-2.522273
O	-0.209180	1.306626	-2.673464
C	0.067553	3.435000	-3.731584
H	-0.263036	4.454913	-3.499236
H	1.127227	3.474091	-4.028294

H	-0.504547	3.019929	-4.570931
N	-2.231007	0.945780	-0.553539
C	-2.931668	1.257655	0.557779
C	-2.866880	0.456246	-1.643662
C	-4.301439	0.957431	0.554864
C	-2.279801	1.944291	1.682381
N	-4.150315	0.166388	-1.743161
H	-2.224879	0.283331	-2.509987
C	-4.830930	0.404344	-0.627782
N	-5.292077	1.104709	1.494788
C	-1.350575	2.964661	1.433829
C	-2.622092	1.625416	3.004011
N	-6.163622	0.209663	-0.379761
C	-6.363109	0.647743	0.907424
C	-0.769134	3.652878	2.497947
H	-1.100895	3.239456	0.406839
C	-2.028473	2.309280	4.059133
H	-3.338354	0.826898	3.191773
C	-7.163681	-0.346931	-1.287278
H	-7.355087	0.599309	1.360858
C	-1.103407	3.326061	3.810258
H	-0.051781	4.450771	2.292710
H	-2.286787	2.044664	5.086980
C	-7.337395	0.548693	-2.506506
C	-6.810679	-1.782072	-1.654162
H	-8.101471	-0.347031	-0.707366
H	-0.645737	3.864237	4.644297
H	-8.135558	0.155153	-3.152647
H	-7.606938	1.572296	-2.207739
H	-6.404311	0.586991	-3.086836
H	-5.864512	-1.810781	-2.213632
H	-7.601727	-2.215950	-2.282962
H	-6.703714	-2.403687	-0.753198
N	1.887590	0.718034	-0.690454
C	2.368916	-0.471826	-1.161954
C	2.720761	1.722182	-0.353153
C	3.770868	-0.569085	-1.293506
C	1.374490	-1.459825	-1.437096
N	4.036876	1.700979	-0.421945
H	2.229669	2.631435	0.003273
C	4.520660	0.547786	-0.890583
N	4.602200	-1.587257	-1.683485
C	1.613522	-2.561599	-2.282936
C	0.043395	-1.178619	-0.910322

N	5.834395	0.183559	-1.050757
C	5.807477	-1.101712	-1.527161
C	0.570834	-3.373230	-2.683675
H	2.632484	-2.733194	-2.637272
C	-1.003348	-2.050083	-1.389198
C	7.014884	0.979456	-0.729029
H	6.734070	-1.636185	-1.743252
C	-0.745151	-3.092614	-2.244974
H	0.756439	-4.217498	-3.350511
H	-2.015168	-1.903385	-1.004710
C	7.051750	2.248698	-1.569170
C	7.072724	1.260435	0.767268
H	7.871246	0.342617	-1.006455
H	-1.570249	-3.727031	-2.579507
H	7.974647	2.810554	-1.363993
H	7.022815	2.009591	-2.642303
H	6.189902	2.887657	-1.329034
H	6.202789	1.858887	1.074586
H	7.988445	1.817564	1.013493
H	7.073913	0.322598	1.342383
P	-0.118568	-1.330872	1.056072
C	0.110563	-3.133630	1.279345
C	1.172553	-3.893387	0.776416
C	-0.902733	-3.763815	2.010771
C	1.222584	-5.265021	1.013459
H	1.952699	-3.428614	0.172927
C	-0.848110	-5.136112	2.244934
H	-1.727519	-3.151428	2.383272
C	0.214790	-5.888716	1.748164
H	2.052928	-5.851177	0.612476
H	-1.642035	-5.620250	2.819257
H	0.256985	-6.965522	1.930114
C	1.276244	-0.559760	1.938033
C	0.971834	0.572913	2.703228
C	2.602134	-1.005980	1.862002
C	1.987042	1.275495	3.347195
H	-0.068464	0.889360	2.792599
C	3.613849	-0.292501	2.499868
H	2.855241	-1.908219	1.305986
C	3.311204	0.852989	3.235851
H	1.734818	2.158655	3.938353
H	4.647586	-0.638016	2.422591
H	4.109485	1.411460	3.730655
O	-1.464203	-0.951319	1.632603

I-6[1]

Lowest frequency = 12.9615 cm^{-1}

Charge = 0, Multiplicity = 2

95

Ru	0.269156	-0.549960	-0.114819
O	-0.470508	-2.949014	-2.057053
C	-0.015783	-1.985820	-2.665984
O	0.492646	-0.933329	-2.114973
C	-0.013960	-1.936977	-4.179543
H	1.000041	-1.724699	-4.547958
H	-0.378638	-2.883602	-4.596059
H	-0.655846	-1.108121	-4.515534
N	2.363276	-0.370619	-0.167972
C	3.216852	-1.275957	0.356540
C	2.835115	0.720534	-0.811666
C	4.588052	-0.984681	0.271890
C	2.692967	-2.505087	0.967614
N	4.100333	1.054021	-0.968954
H	2.076539	1.376342	-1.236692
C	4.943916	0.200417	-0.402841
N	5.714924	-1.640966	0.704241
C	1.558738	-3.138588	0.434798
C	3.319190	-3.054675	2.096684
N	6.312157	0.249413	-0.364588
C	6.700158	-0.879134	0.314337
C	1.039593	-4.275570	1.047913
H	1.082386	-2.796360	-0.491724
C	2.787892	-4.186355	2.709060
H	4.220381	-2.584596	2.491795
C	7.177402	1.287282	-0.921069
H	7.757942	-1.083273	0.491113
C	1.642549	-4.794798	2.191913
H	0.162791	-4.755820	0.607513
H	3.272862	-4.596830	3.597807
C	7.033012	1.347403	-2.435729
C	6.904346	2.625351	-0.247486
H	8.201560	0.963256	-0.672151
H	1.230786	-5.684428	2.675018
H	7.733840	2.085997	-2.851323
H	7.249342	0.370032	-2.891403

H	6.009928	1.642988	-2.709083
H	5.875881	2.954708	-0.454441
H	7.599858	3.387254	-0.628491
H	7.034227	2.551670	0.842109
N	-1.734909	-0.766852	-0.421571
C	-2.399431	0.251360	-0.996192
C	-2.386385	-1.874912	-0.005074
C	-3.791561	0.126793	-1.099452
C	-1.643086	1.384935	-1.570887
N	-3.685575	-2.084683	-0.079069
H	-1.751457	-2.650424	0.425390
C	-4.355920	-1.070368	-0.611464
N	-4.773591	0.962147	-1.570603
C	-1.949253	1.692102	-2.904980
C	-0.603462	2.097147	-0.923674
N	-5.706879	-0.940429	-0.803514
C	-5.879949	0.295182	-1.376131
C	-1.218466	2.635657	-3.617238
H	-2.762120	1.151931	-3.392500
C	0.119840	3.048737	-1.661697
C	-6.747026	-1.907684	-0.458691
H	-6.879716	0.653175	-1.629320
C	-0.167251	3.306115	-2.997194
H	-1.466170	2.837335	-4.661682
H	0.920016	3.588346	-1.147453
C	-6.563461	-3.193946	-1.252361
C	-6.779336	-2.140112	1.045960
H	-7.690875	-1.428153	-0.766722
H	0.422606	4.041883	-3.548664
H	-7.384541	-3.891685	-1.032740
H	-6.560298	-2.992692	-2.333547
H	-5.612789	-3.676716	-0.983919
H	-5.836017	-2.594497	1.381711
H	-7.605278	-2.818535	1.304367
H	-6.926153	-1.194230	1.587827
P	-0.133843	2.156619	0.856779
C	-1.286878	3.403547	1.528277
C	-2.597117	3.572389	1.065948
C	-0.808043	4.205672	2.569559
C	-3.426836	4.522918	1.657972
H	-2.974964	2.975681	0.230557
C	-1.640453	5.155334	3.157470
H	0.227732	4.080695	2.895435
C	-2.950765	5.311546	2.705192

H	-4.447974	4.653864	1.291830
H	-1.263104	5.782220	3.969193
H	-3.602060	6.058901	3.165229
C	-0.526527	0.578542	1.618955
C	0.556010	-0.266832	2.048105
C	-1.848201	0.320257	2.131367
C	0.236662	-1.394127	2.874027
H	1.566749	0.145948	2.102044
C	-2.103109	-0.784995	2.894016
H	-2.653210	1.027391	1.919006
C	-1.049721	-1.674104	3.248363
H	1.055063	-2.024796	3.227701
H	-3.114448	-0.966212	3.266538
H	-1.260955	-2.547920	3.868986
O	1.297968	2.595056	1.031423

Acetate

Lowest frequency = 40.4371 cm^{-1}

Charge = -1, Multiplicity = 1

7

C	0.278887	-1.070415	0.000011
O	1.503675	-1.297973	0.000004
O	-0.331533	0.016875	-0.000015
C	-0.650467	-2.333331	0.000066
H	-1.312426	-2.307191	0.883529
H	-1.312534	-2.307188	-0.883315
H	-0.074836	-3.273163	0.000034

Acetic Acid

Lowest frequency = 79.7380 cm^{-1}

Charge = 0, Multiplicity = 1

8

C	0.297073	-1.163279	0.000013
O	1.496903	-1.233142	-0.000014
O	-0.355861	0.010101	0.000001
H	0.326101	0.699363	-0.000032
C	-0.650394	-2.324843	0.000066
H	-1.301893	-2.274652	0.884698

H	-1.301985	-2.274662	-0.884498
H	-0.083974	-3.262061	0.000045

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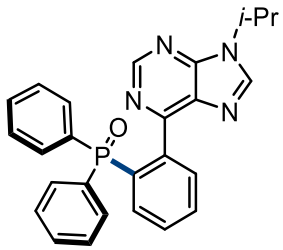
8. Characterization Data

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3a**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.13) yielded **3a** (95.9 mg, 73%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.93 (s, 1H), 7.85 – 7.73 (m, 2H), 7.58 – 7.49 (m, 5H), 7.45 – 7.39 (m, 1H), 7.19 – 7.08 (m, 6H), 4.68 (m, 6H), 1.46 (d, *J* = 6.8 Hz, 6H).

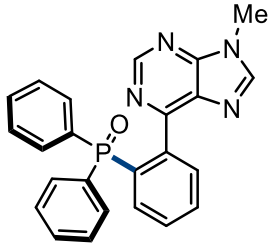
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.0 (d, *J* = 3.3 Hz) (C_q), 150.7 (C_q), 150.5 (CH), 141.9 (CH), 139.4 (d, *J* = 7.1 Hz) (C_q), 135.0 (d, *J* = 10.3 Hz) (CH), 133.4 (d, *J* = 106.4 Hz) (C_q), 132.1 (d, *J* = 101.0 Hz) (C_q), 131.3 (CH), 131.2 (CH), 131.2 (CH), 130.4 (d, *J* = 2.7 Hz) (CH), 128.6 (d, *J* = 12.0 Hz) (CH), 127.3 (d, *J* = 12.3 Hz) (CH), 46.9 (CH), 22.1 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 28.79.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{24}N_4OP$ 439.1682; Found 439.1686.

IR (ATR): 2977, 1577, 1331, 1178, 931, 719, 535 cm^{-1}.

(2-(9-Methyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3b**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.14) yielded **3b** (68.9 mg, 56%) as a colorless solid. M.p.: 210-211 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.94 – 7.86 (m, 2H), 7.72 (dd, *J* = 13.6, 7.7 Hz, 1H), 7.63 – 7.50 (m, 5H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.14 (m, 6H), 3.71 (s, 3H).

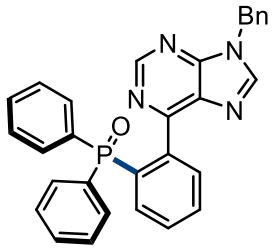
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2 (d, *J* = 3.1 Hz) (C_q), 151.7 (C_q), 151.1 (CH), 145.0 (CH), 139.6 (d, *J* = 6.7 Hz) (C_q), 135.2 (d, *J* = 10.6 Hz) (CH), 133.7 (d, *J* = 106.9 Hz) (C_q), 131.9 (d, *J* = 122.0 Hz) (C_q), 131.7 (CH), 131.5 (CH), 131.4 (CH), 130.8 (d, *J* = 2.8 Hz) (CH), 129.0 (d, *J* = 12.1 Hz) (CH), 127.7 (d, *J* = 12.3 Hz) (CH), 29.6 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.61.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{20}N_4OP$ 411.1369; Found 411.1376.

IR (ATR): 3058, 1715, 1581, 1397, 1115, 717, 640, 536 cm^{-1}.

(2-(9-Benzyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3c**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.3) yielded **3c** (103.1 mg, 71%) as a colorless solid. M.p.: 218-219 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.90 (s, 1H), 7.88 (dd, *J* = 7.7, 4.2 Hz, 1H), 7.79 – 7.71 (m, 1H), 7.61 – 7.50 (m, 5H), 7.47 – 7.40 (m, 1H), 7.28 – 7.20 (m, 5H), 7.13 – 7.08 (m, 6H), 5.23 (s, 2H).

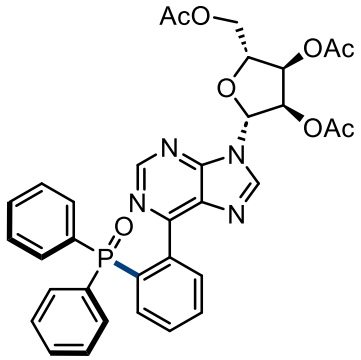
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.3 (d, *J* = 3.2 Hz) (C_q), 151.3 (C_q), 151.3 (CH), 144.2 (CH), 139.5 (d, *J* = 6.9 Hz) (C_q), 135.3 (d, *J* = 10.5 Hz) (CH), 135.0 (C_q), 133.5 (d, *J* = 106.8 Hz) (C_q), 131.9 (d, *J* = 139.6 Hz) (C_q), 131.7 (CH), 131.6 (CH), 131.5 (CH), 131.4 (CH), 130.7 (d, *J* = 2.8 Hz) (CH), 129.0 (CH), 128.9 (CH), 128.4 (CH), 127.9 (CH), 127.6 (d, *J* = 12.3 Hz) (CH), 47.0 (CH_2).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.40.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{24}N_4OP$ 487.1682; Found 487.1678.

IR (ATR): 3060, 1716, 1580, 1437, 1108, 906, 691, 647, 532 cm^{-1}.

(2R,3R,4R,5R)-2-(Acetoxymethyl)-5-(6-(2-(diphenylphosphoryl)phenyl)-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate (**3d**)



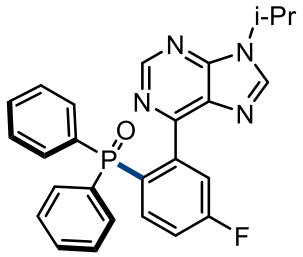
Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.25) yielded **3d** (119.7 mg, 61%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.14 (s, 1H), 7.92 – 7.83 (m, 2H), 7.73 – 7.66 (m, 2H), 7.64 – 7.56 (m, 4H), 7.36 – 7.31 (m, 2H), 7.29 – 7.22 (m, 4H), 6.17 (d, *J* = 4.7 Hz, 1H), 5.93 – 5.85 (m, 1H), 5.69 (t, *J* = 5.3 Hz, 1H), 4.51 – 4.35 (m, 3H), 2.16 – 2.11 (m, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2 (C_q), 169.4 (C_q), 169.3 (C_q), 157.2 (d, *J* = 3.2 Hz) (C_q), 151.5 (CH), 150.8 (C_q), 142.7 (CH), 139.2 (d, *J* = 6.9 Hz) (C_q), 135.3 (d, *J* = 10.3 Hz) (CH), 134.3 (C_q), 134.2 (C_q), 133.1 (C_q), 132.9 (C_q), 132.8 (C_q), 131.9 (C_q), 131.8 (C_q), 131.6 (CH), 131.6 (CH), 131.5 (CH), 131.5 (CH), 131.0 (CH), 130.9 (CH), 130.9 (CH), 129.1 (d, *J* = 11.9 Hz) (CH), 127.7 (d, *J* = 12.3 Hz) (CH), 86.5 (CH), 80.0 (CH), 73.1 (CH), 70.3 (CH), 62.9 (CH_2), 20.6 (CH_3), 20.4 (CH_3), 20.3 (CH_3).

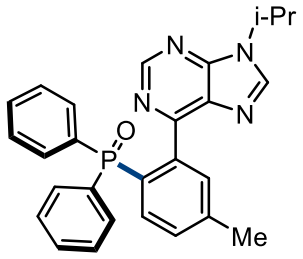
^{31}P NMR (121 MHz, $CDCl_3$) δ 29.06.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for$C_{34}H_{32}N_4O_8P$ 655.1952; Found 655.1948.
IR (ATR): 1745, 1582, 1212, 901, 720, 541 m^{-1}.

(4-Fluoro-2-(9-isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3e**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.22) yielded **3e** (112.2 mg, 82%) as a colorless sticky oil.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.07 (s, 1H), 7.70 – 7.58 (m, 5H), 7.51 – 7.43 (m, 1H), 7.38 – 7.24 (m, 6H), 7.21 – 7.12 (m, 1H), 4.90 – 4.78 (m, 1H), 1.61 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.8 (C_q), 163.9 (d, J_{C-F} = 251.6 Hz) (C_q), 156.5 (t, *J* = 3.1 Hz) (C_q), 151.0 (CH), 150.7 (C_q), 142.4 (C_q), 142.2 (CH), 133.9 (CH), 133.7 (d, *J* = 1.8 Hz) (CH), 132.2 (d, *J* = 27.9 Hz) (C_q), 131.1 (d, *J* = 3.3 Hz) (CH), 131.0 (d, *J* = 1.8 Hz) (CH), 127.7 (d, *J* = 12.8 Hz) (CH), 119.9 (dd, *J* = 97.2, 17.6 Hz) (C_q), 117.0 (dd, *J* = 24.6, 5.1 Hz) (CH), 47.2 (CH), 22.3 (CH_3).
^{31}P NMR (121 MHz, $CDCl_3$) δ 23.85.
^{19}F NMR (282 MHz, $CDCl_3$) δ -94.79.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{23}FN_4OP$ 457.1588; Found 457.1590.
IR (ATR): 2978, 2227, 1561, 1438, 1195, 1117, 906, 716 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)-4-methylphenyl)diphenylphosphine oxide (**3f**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.3) yielded **3f** (85.5 mg, 63%) as a colorless sticky oil.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.02 (s, 1H), 7.79 – 7.57 (m, 6H), 7.36 (d, *J* = 7.9 Hz, 1H), 7.30 – 7.18 (m, 6H), 4.90 – 4.74 (m, 1H), 2.46 (s, 3H), 1.59 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.8 (d, *J* = 3.3 Hz) (C_q), 150.9 (CH), 150.9 (C_q), 142.1 (d, *J* = 2.6 Hz) (C_q), 141.9 (CH), 139.6 (d, *J* = 7.3 Hz) (C_q), 135.3 (d, *J* = 10.6 Hz) (CH), 133.8 (d, *J* = 106.4 Hz) (C_q), 132.1 (d, *J* = 9.9 Hz) (CH), 131.6 (d, *J* = 9.5 Hz) (CH), 131.6 (C_q), 130.6 (d, *J* = 2.6 Hz) (CH), 129.7 (d,

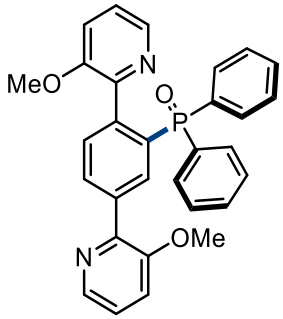
J = 12.1 Hz) (CH), 129.0 (d, *J* = 103.4 Hz) (C_q), 127.5 (d, *J* = 12.1 Hz) (CH), 47.1 (CH), 22.4 (CH_3), 21.4 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.76.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{27}H_{26}N_4OP$ 453.1839; Found 453.1847.

IR (ATR): 3055, 2977, 2225, 1574, 1436, 1192, 907, 704 cm^{-1}.

(2,5-Bis(3-methoxypyridin-2-yl)phenyl)diphenylphosphine oxide (**3g**)



Prepared according to standard procedure A using $[Ru(OAc)_2(p\text{-cymene})]$ (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.10) yielded **3g** (91.8 mg, 62%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 – 8.09 (m, 3H), 7.95 (dd, *J* = 4.7, 1.1 Hz, 1H), 7.60 – 7.52 (m, 4H), 7.47 (dd, *J* = 8.0, 4.2 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.27 – 7.20 (m, 4H), 7.13 – 7.07 (m, 2H), 6.99 – 6.93 (m, 1H), 6.75 (dd, *J* = 8.4, 1.1 Hz, 1H), 3.53 (s, 3H), 3.27 (s, 3H).

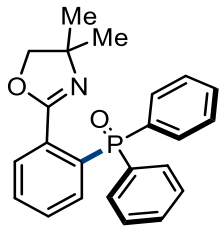
^{13}C NMR (75 MHz, $CDCl_3$) δ 153.6 (C_q), 153.2 (C_q), 148.6 (d, *J* = 3.5 Hz) (C_q), 146.2 (C_q), 142.2 (d, *J* = 8.0 Hz) (C_q), 141.3 (CH), 139.9 (CH), 136.7 (d, *J* = 12.7 Hz) (C_q), 135.0 (d, *J* = 12.7 Hz) (CH), 134.1 (d, *J* = 104.6 Hz) (C_q), 132.2 (d, *J* = 2.6 Hz) (CH), 131.9 (d, *J* = 9.8 Hz) (CH), 131.3 (d, *J* = 10.5 Hz) (CH), 130.8 (d, *J* = 2.8 Hz) (CH), 130.2 (d, *J* = 101.9 Hz) (C_q), 127.8 (d, *J* = 12.1 Hz) (CH), 123.4 (CH), 123.2 (CH), 118.5 (CH), 116.4 (CH), 55.1 (CH_3), 54.2 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.23.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{26}N_2O_3P$ 493.1676; Found 493.1689.

IR (ATR): 3055, 2834, 1580, 1425, 1179, 1015, 705, 540 cm^{-1}.

(2-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenyl)diphenylphosphine oxide (**3h**)



Prepared according to standard procedure A using $[Ru(OAc)_2(p\text{-cymene})]$ (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.23) yielded **3h** (39.4 mg, 35%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 7.5, 4.0 Hz, 1H), 7.72 – 7.64 (m, 4H), 7.58 – 7.51 (m, 1H), 7.49 – 7.40 (m, 8H), 3.55 (s, 2H), 1.09 (s, 6H).

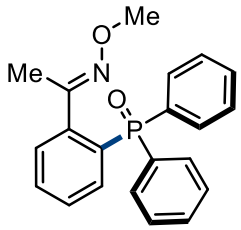
^{13}C NMR (75 MHz, $CDCl_3$) δ 162.4 (d, J = 3.2 Hz) (C_q), 134.8 (d, J = 10.9 Hz) (CH), 133.5 (d, J = 106.8 Hz) (C_q), 132.7 (d, J = 6.2 Hz) (C_q), 131.8 (d, J = 2.4 Hz) (CH), 131.7 (d, J = 99.2 Hz) (C_q), 131.5 (d, J = 9.7 Hz) (CH), 131.3 (d, J = 2.9 Hz) (CH), 131.2 (CH), 130.1 (d, J = 12.0 Hz) (CH), 128.3 (d, J = 12.3 Hz) (CH), 79.1 (CH_2), 67.3 (C_q), 27.8 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.50.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}NO_2P$ 376.1461; Found 376.1472.

IR (ATR): 2964, 1659, 1437, 1177, 963, 693, 543cm^{-1}.

(E)-(2-(1-(Methoxyimino)ethyl)phenyl)diphenylphosphine oxide (3**i**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.33) yielded **3i** (52.1 mg, 50%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 – 7.57 (m, 4H), 7.48 – 7.34 (m, 8H), 7.32 – 7.24 (m, 2H), 3.40 (s, 3H), 1.85 (s, 3H).

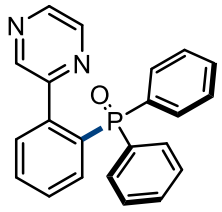
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.5 (d, J = 3.5 Hz) (C_q), 142.5 (d, J = 7.4 Hz) (C_q), 134.3 (CH), 133.5 (d, J = 95.1 Hz) (C_q), 132.1 (d, J = 9.8 Hz) (CH), 131.9 (d, J = 2.7 Hz) (CH), 131.5 (d, J = 102.5 Hz) (C_q), 131.4 (d, J = 2.7 Hz) (CH), 129.5 (d, J = 9.5 Hz) (CH), 128.2 (d, J = 12.3 Hz) (CH), 127.8 (d, J = 12.3 Hz) (CH), 61.2 (CH_3), 16.6 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 30.23.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{21}NO_2P$ 350.1304; Found 350.1314.

IR (ATR): 1436, 1312, 1181, 1037, 875, 692, 529 cm^{-1}.

Diphenyl(2-(pyrazin-2-yl)phenyl)phosphine oxide (**3j**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.38) yielded **3j** (29 mg, 27%) as a colorless solid. M.p.: 160-161 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.88 – 8.82 (m, 1H), 8.28 (d, J = 2.4 Hz, 1H), 8.23 – 8.19 (m, 1H), 7.68 – 7.56 (m, 6H), 7.50 – 7.34 (m, 8H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 153.8 (d, J = 4.0 Hz) (C_q), 145.8 (CH), 143.1 (CH), 142.9 (CH), 142.3 (d, J = 7.5 Hz) (C_q), 134.3 (d, J = 11.5 Hz) (CH), 132.9 (d, J = 105.2 Hz) (C_q), 132.1 (d, J = 100.2 Hz) (C_q),

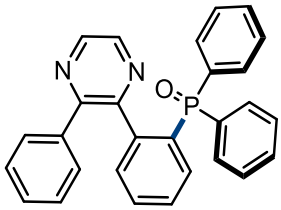
132.0 (d, J = 2.5 Hz) (CH), 131.7 (d, J = 9.6 Hz) (CH), 131.5 (d, J = 2.8 Hz) (CH), 128.5 (CH), 128.4 (CH), 128.3 (d, J = 12.2 Hz) (CH).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.76.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}N_2OP$ 357.1151; Found 357.1146.

IR (ATR): 3053, 1437, 1196, 1104, 1019, 715, 540 cm^{-1}.

Diphenyl(2-(3-phenylpyrazin-2-yl)phenyl)phosphine oxide (**3k**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(p-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.22) yielded **3k** (44.1 mg, 34%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 2.4 Hz, 1H), 8.20 (d, J = 2.4 Hz, 1H), 7.53 – 7.41 (m, 10H), 7.40 – 7.33 (m, 5H), 7.25 – 7.16 (m, 4H).

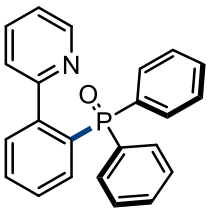
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0 (d, J = 3.4 Hz) (C_q), 152.7 (C_q), 144.1 (d, J = 6.6 Hz) (C_q), 142.6 (CH), 140.8 (CH), 138.1 (C_q), 134.2 (d, J = 11.4 Hz) (CH), 133.6 (d, J = 105.1 Hz) (C_q), 131.8 (d, J = 9.8 Hz) (CH), 131.7 (CH), 131.4 (d, J = 2.7 Hz) (CH), 131.2 (d, J = 2.5 Hz) (CH), 130.4 (d, J = 92.9 Hz) (C_q), 129.9 (CH), 128.3 (CH), 128.2 (d, J = 12.2 Hz) (CH), 127.8 (CH), 127.6 (d, J = 12.2 Hz) (CH).

^{31}P NMR (162 MHz, $CDCl_3$) δ 29.83.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{22}N_2OP$ 433.1464; Found 433.1460.

IR (ATR): 3055, 1389, 1118, 1018, 856, 694, 542 cm^{-1}.

Diphenyl(2-(pyridin-2-yl)phenyl)phosphine oxide (**3l**)



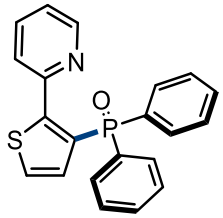
Prepared according to standard procedure A using [Ru(OAc)$_2$(p-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.40) yielded **3l** (54.2 mg, 51%) as a colorless solid. M.p.: 176-177 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 – 8.15 (m, 1H), 7.73 (d, J = 7.9 Hz, 1H), 7.56 – 7.49 (m, 6H), 7.41 – 7.35 (m, 2H), 7.33 – 7.27 (m, 3H), 7.26 – 7.19 (m, 4H), 6.88 – 6.83 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 157.5 (d, J = 4.1 Hz) (C_q), 148.6 (CH), 145.7 (d, J = 7.9 Hz) (C_q), 135.3 (CH), 134.3 (d, J = 11.8 Hz) (CH), 133.1 (d, J = 105.2 Hz) (C_q), 131.9 (d, J = 2.6 Hz) (CH), 131.5 (d, J = 9.5 Hz) (CH), 131.3 (CH), 131.1 (d, J = 2.8 Hz) (CH), 131.1 (d, J = 101.3 Hz) (C_q), 128.0 (d, J = 12.2 Hz) (CH), 127.6 (d, J = 12.3 Hz) (CH), 125.6 (CH), 121.9 (CH).

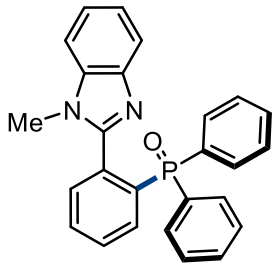
^{31}P NMR (121 MHz, $CDCl_3$) δ 29.12.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}NOP$ 356.1199; Found 356.1204.
IR (ATR): 3057, 2142, 1584, 1437, 1181, 1104, 694, 540 cm^{-1}.

Diphenyl(2-(pyridin-2-yl)thiophen-3-yl)phosphine oxide (**3m**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.25) yielded **3m** (96.4 mg, 89%) as a colorless sticky oil.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 – 8.36 (m, 1H), 8.26 – 8.21 (m, 1H), 7.71 – 7.63 (m, 4H), 7.43 – 7.30 (m, 8H), 7.01 – 6.94 (m, 1H), 6.72 (td, *J* = 5.2, 1.1 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 154.0 (d, *J* = 11.0 Hz) (C_q), 150.9 (d, *J* = 2.1 Hz) (C_q), 148.8 (CH), 136.2 (CH), 134.0 (d, *J* = 16.6 Hz) (CH), 133.0 (d, *J* = 107.4 Hz) (C_q), 131.6 (d, *J* = 2.9 Hz) (CH), 131.5 (d, *J* = 9.9 Hz) (CH), 129.4 (d, *J* = 103.0 Hz) (C_q), 128.3 (d, *J* = 12.4 Hz) (CH), 126.5 (d, *J* = 16.4 Hz) (CH), 124.2 (CH), 122.6 (CH).
^{31}P NMR (121 MHz, $CDCl_3$) δ 22.02.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}NOPS$ 362.0763; Found 362.0770.
IR (ATR): 3050, 1582, 1436, 1162, 996, 696, 537 cm^{-1}.

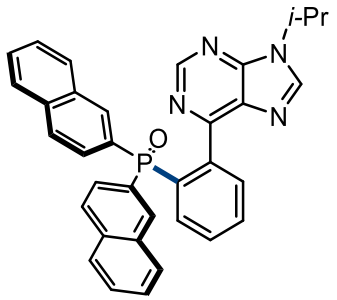
(2-(1-methyl-1H-benzo[d]imidazol-2-yl)phenyl)diphenylphosphine oxide (**3n**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.34) yielded **3n** (50.3 mg, 41%) as a colorless sticky oil.
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 – 7.89 (m, 1H), 7.64 – 7.56 (m, 2H), 7.54 – 7.46 (m, 4H), 7.43 – 7.38 (m, 2H), 7.23 – 7.07 (m, 8H), 7.01 – 6.96 (m, 1H), 3.25 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 151.2 (d, *J* = 4.1 Hz) (C_q), 141.9 (C_q), 134.8 (C_q), 134.3 (d, *J* = 9.5 Hz) (CH), 134.0 (d, *J* = 100.0 Hz) (C_q), 133.5 (d, *J* = 8.2 Hz) (C_q), 131.8 (CH), 131.7 (d, *J* = 10.1 Hz) (CH), 131.5 (CH), 131.4 (d, *J* = 106.0 Hz) (C_q), 131.3 (d, *J* = 3.0 Hz) (CH), 129.9 (d, *J* = 11.2 Hz) (CH), 127.8 (d, *J* = 12.5 Hz) (CH), 122.7 (CH), 122.1 (CH), 119.6 (CH), 109.4 (CH), 30.9 (CH_3).
^{31}P NMR (121 MHz, $CDCl_3$) δ 28.70.

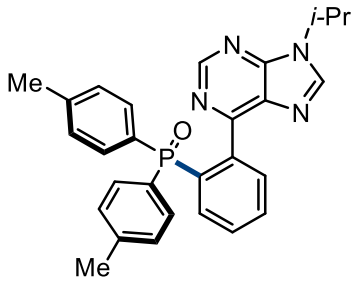
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{22}N_2OP$ 409.1464; Found 409.1460.
IR (ATR): 3057, 1716, 1422, 1118, 906, 689, 535, 449 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di(naphthalen-2-yl)phosphine oxide (**3o**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.18) yielded **3o** (116.0 mg, 72%) as a colorless sticky oil.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.28 (d, *J* = 13.9 Hz, 2H), 7.97 – 7.89 (m, 2H), 7.84 (s, 1H), 7.76 – 7.63 (m, 9H), 7.57 – 7.51 (m, 1H), 7.49 – 7.38 (m, 4H), 4.44 (h, *J* = 6.7 Hz, 1H), 1.32 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.3 (d, *J* = 3.2 Hz) (C_q), 150.9 (CH), 150.7 (C_q), 141.9 (CH), 139.8 (d, *J* = 7.2 Hz) (C_q), 135.5 (d, *J* = 10.6 Hz) (CH), 134.0 (d, *J* = 2.3 Hz) (C_q), 133.2 (d, *J* = 9.2 Hz) (CH), 132.3 (d, *J* = 101.4 Hz) (C_q), 132.0 (C_q), 131.9 (C_q), 131.7 (CH), 131.5 (CH), 130.9 (d, *J* = 106.6 Hz) (C_q), 129.0 (d, *J* = 12.0 Hz) (CH), 128.7 (CH), 127.5 (d, *J* = 17.2 Hz) (CH), 127.3 (d, *J* = 12.1 Hz) (CH), 126.7 (d, *J* = 10.5 Hz) (CH), 126.3 (CH), 47.0 (CH), 22.0 (CH_3).
^{31}P NMR (121 MHz, $CDCl_3$) δ 28.59.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{34}H_{28}N_4OP$ 539.1995; Found 539.1989.
IR (ATR): 3054, 1576, 1391, 1188, 1085, 931, 814, 645, 477 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di-p-tolylphosphine oxide (**3p**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.15) yielded **3p** (102.1 mg, 73%) as a colorless sticky oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.03 (s, 1H), 7.88 (dd, *J* = 7.3, 3.9 Hz, 1H), 7.77 (dd, *J* = 13.5, 7.7 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.51 – 7.45 (m, 5H), 7.06 – 7.01 (m, 4H), 4.85 – 4.75 (m, 1H), 2.26 (s, 6H), 1.58 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7 (d, *J* = 3.2 Hz) (C_q), 151.0 (CH), 151.0 (C_q), 141.9 (CH), 141.0 (d,

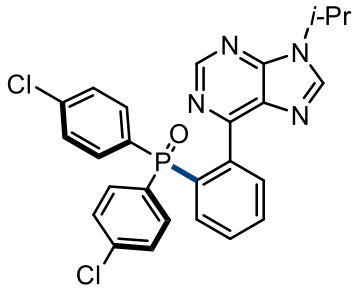
J = 2.8 Hz) (C_q), 139.7 (d, *J* = 6.9 Hz) (C_q), 135.2 (d, *J* = 10.6 Hz) (CH), 132.7 (d, *J* = 101.0 Hz) (C_q), 131.7 (C_q), 131.6 (d, *J* = 4.8 Hz) (CH), 131.5 (d, *J* = 3.7 Hz) (CH), 131.3 (d, *J* = 2.5 Hz) (CH), 130.6 (d, *J* = 108.9 Hz) (C_q), 128.8 (d, *J* = 12.0 Hz) (CH), 128.4 (d, *J* = 12.7 Hz) (CH), 47.1 (CH), 22.3 (CH_3), 21.4 (CH_3), 21.4 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 29.37.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{28}N_4OP$ 467.1995; Found 467.2006.

IR (ATR): 2978, 1580, 1331, 1100, 931, 733, 536 cm^{-1}.

Bis(4-chlorophenyl)(2-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**3q**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.38) yielded **3q** (77.4 mg, 51%) as a colorless solid. M.p.: 198-199 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.99 (s, 1H), 7.91 – 7.78 (m, 2H), 7.68 – 7.62 (m, 1H), 7.55 – 7.44 (m, 5H), 7.17 – 7.11 (m, 4H), 4.86 – 4.69 (m, 1H), 1.56 (d, *J* = 6.8 Hz, 6H).

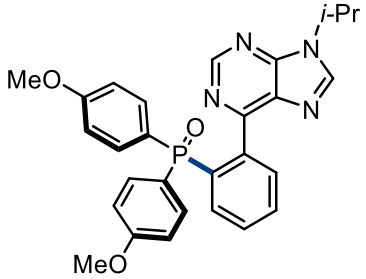
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1 (d, *J* = 3.3 Hz) (C_q), 151.1 (C_q), 150.8 (CH), 142.2 (CH), 139.5 (d, *J* = 7.4 Hz) (C_q), 137.5 (d, *J* = 3.4 Hz) (C_q), 135.3 (d, *J* = 10.3 Hz) (CH), 133.0 (d, *J* = 10.8 Hz) (CH), 132.0 (d, *J* = 2.6 Hz) (CH), 132.0 (d, *J* = 108.3 Hz) (C_q), 131.8 (d, *J* = 9.4 Hz) (CH), 131.5 (C_q), 131.4 (d, *J* = 103.2 Hz) (C_q), 129.2 (d, *J* = 12.2 Hz) (CH), 128.0 (d, *J* = 13.0 Hz) (CH), 47.4 (CH), 22.3 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 27.88.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{22}Cl_2N_4OP$ 507.0903; Found 507.0920.

IR (ATR): 2978, 1582, 1390, 1193, 1086, 1013, 751, 559 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-methoxyphenyl)phosphine oxide (**3r**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.13) yielded **3r** (129.9 mg, 87%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.97 (s, 1H), 7.83 (dd, *J* = 13.3, 7.6 Hz, 1H), 7.72 – 7.67 (m,

1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.40 (m, 5H), 6.65 (dd, *J* = 8.7, 2.0 Hz, 4H), 4.78 – 4.69 (m, 1H), 3.66 (s, 6H), 1.52 (d, *J* = 6.8 Hz, 6H).

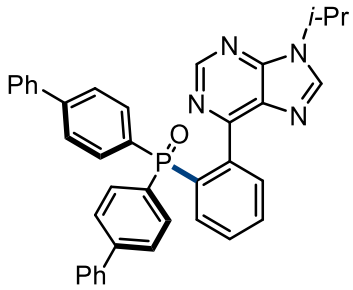
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.9 (C_q), 161.3 (d, *J* = 2.9 Hz) (C_q), 156.8 (d, *J* = 3.4 Hz) (C_q), 150.8 (CH), 150.7 (C_q), 141.9 (CH), 139.3 (d, *J* = 7.5 Hz) (C_q), 134.9 (d, *J* = 10.1 Hz) (CH), 133.3 (d, *J* = 11.3 Hz) (CH), 131.8 (d, *J* = 45.0 Hz) (C_q), 131.2 (d, *J* = 2.1 Hz) (CH), 131.0 (CH), 128.7 (d, *J* = 11.8 Hz) (CH), 124.5 (d, *J* = 113.1 Hz) (C_q), 113.0 (d, *J* = 13.4 Hz) (CH), 54.9 (CH_3), 47.1 (CH), 22.1 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.04.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{28}N_4O_3P$ 499.1894; Found 499.1900.

IR (ATR): 2978, 1596, 1248, 1101, 1024, 931, 734, 532 cm^{-1}.

Di([1,1'-biphenyl]-4-yl)(2-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**3s**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.15) yielded **3s** (88.6 mg, 50%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.04 – 7.96 (m, 2H), 7.92 – 7.88 (m, 1H), 7.78 – 7.70 (m, 5H), 7.62 – 7.52 (m, 5H), 7.49 – 7.44 (m, 5H), 7.42 – 7.34 (m, 5H), 4.69 – 4.56 (m, 1H), 1.33 (d, *J* = 6.7 Hz, 6H).

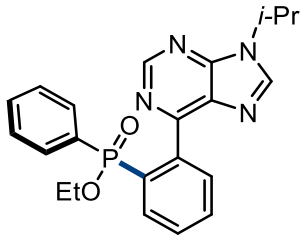
^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2 (C_q), 156.6 (d, *J* = 3.3 Hz) (C_q), 151.0 (CH), 151.0 (C_q), 143.4 (d, *J* = 2.7 Hz) (C_q), 141.9 (CH), 139.7 (C_q), 139.6 (d, *J* = 7.4 Hz) (C_q), 135.4 (d, *J* = 10.3 Hz) (CH), 132.4 (d, *J* = 101.9 Hz) (C_q), 132.2 (d, *J* = 10.2 Hz) (CH), 132.1 (d, *J* = 107.8 Hz) (C_q), 131.6 (CH), 131.6 (CH), 129.1 (d, *J* = 12.0 Hz) (CH), 128.8 (CH), 127.9 (CH), 127.0 (CH), 126.2 (d, *J* = 12.7 Hz) (CH), 47.1 (CH), 22.0 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.01.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{38}H_{32}N_4OP$ 591.2308; Found 591.2320.

IR (ATR): 2978, 1597, 1391, 1177, 1102, 1007, 733, 529 cm^{-1}.

Ethyl (2-(9-isopropyl-9H-purin-6-yl)phenyl)(phenyl)phosphinate (**3t**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol

scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.20) yielded **3t** (37.6 mg, 31%) as a colorless solid. M.p.: 153-154 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.22 – 8.13 (m, 1H), 7.94 (s, 1H), 7.77 – 7.72 (m, 1H), 7.61 – 7.52 (m, 4H), 7.26 – 7.17 (m, 3H), 4.91 – 4.79 (m, 1H), 3.96 – 3.83 (m, 2H), 1.58 (d, *J* = 6.8 Hz, 6H), 1.10 (t, *J* = 7.0 Hz, 3H).

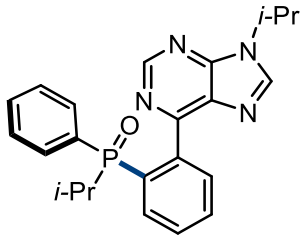
^{13}C NMR (75 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.6 Hz) (C_q), 151.2 (C_q), 151.0 (CH), 142.1 (CH), 141.3 (C_q), 139.6 (d, *J* = 9.1 Hz) (C_q), 134.3 (d, *J* = 8.0 Hz) (CH), 133.1 (d, *J* = 140.9 Hz) (C_q), 132.0 (CH), 131.7 (d, *J* = 2.6 Hz) (CH), 131.2 (d, *J* = 10.5 Hz) (CH), 131.0 (d, *J* = 2.9 Hz) (CH), 131.0 (d, *J* = 133.7 Hz) (C_q), 129.0 (d, *J* = 12.0 Hz) (CH), 127.7 (d, *J* = 13.6 Hz) (CH), 60.7 (d, *J* = 5.7 Hz) (CH_2), 47.3 (CH), 22.5 (CH_3), 22.5 (CH_3), 16.1 (d, *J* = 6.9 Hz) (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.94.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{24}N_4O_2P$ 407.1631; Found 407.1634.

IR (ATR): 2977, 1581, 1330, 1214, 1024, 930, 735, 648, 558 cm^{-1}.

Isopropyl(2-(9-isopropyl-9H-purin-6-yl)phenyl)(phenyl)phosphine oxide (**3u**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.16) yielded **3u** (72.2 mg, 60%) as a colorless sticky oil.

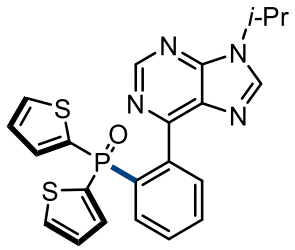
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.45 – 8.34 (m, 1H), 7.84 (s, 1H), 7.64 – 7.54 (m, 3H), 7.22 – 7.14 (m, 2H), 6.93 – 6.85 (m, 3H), 4.84 – 4.70 (m, 1H), 3.17 – 3.03 (m, 1H), 1.56 (dd, *J* = 6.8, 4.4 Hz, 6H), 1.31 – 1.15 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2 (d, *J* = 3.2 Hz) (C_q), 150.8 (C_q), 150.6 (CH), 142.0 (CH), 138.3 (d, *J* = 7.8 Hz) (C_q), 134.3 (d, *J* = 6.9 Hz) (CH), 132.9 (d, *J* = 95.7 Hz) (C_q), 132.3 (d, *J* = 90.5 Hz) (C_q), 131.7 (C_q), 131.0 (d, *J* = 9.1 Hz) (CH), 130.9 (d, *J* = 2.4 Hz) (CH), 130.2 (d, *J* = 8.9 Hz) (CH), 129.7 (d, *J* = 2.6 Hz) (CH), 128.8 (d, *J* = 10.4 Hz) (CH), 127.1 (d, *J* = 11.3 Hz) (CH), 47.2 (CH), 26.8 (d, *J* = 73.3 Hz) (CH), 22.4 (CH_3), 22.2 (CH_3), 16.0 (d, *J* = 3.4 Hz) (CH_3), 15.9 (d, *J* = 2.6 Hz) (CH_3). ^{31}P NMR (162 MHz, $CDCl_3$) δ 39.61.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{26}N_4OP$ 405.1839; Found 405.1841.

IR (ATR): 2975, 1582, 1393, 1215, 1176, 1026, 734, 537 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di(thiophen-2-yl)phosphine oxide (**3v**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.26) yielded **3v** (28.3 mg, 21%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.09 – 8.01 (m, 3H), 7.74 – 7.67 (m, 1H), 7.61 – 7.47 (m, 5H), 7.00 – 6.96 (m, 2H), 4.96 – 4.82 (m, 1H), 1.63 (d, *J* = 6.8 Hz, 6H).

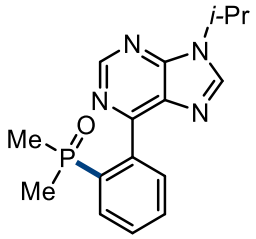
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1 (d, *J* = 3.4 Hz) (C_q), 151.2 (C_q), 151.1 (CH), 142.2 (CH), 139.4 (d, *J* = 7.3 Hz) (C_q), 136.2 (d, *J* = 10.8 Hz) (CH), 135.8 (d, *J* = 123.5 Hz) (C_q), 134.8 (d, *J* = 10.9 Hz) (CH), 133.1 (d, *J* = 113.4 Hz) (C_q), 133.1 (d, *J* = 5.5 Hz) (CH), 132.0 (d, *J* = 2.7 Hz) (CH), 131.8 (d, *J* = 10.0 Hz) (CH), 131.7 (C_q), 129.2 (d, *J* = 12.9 Hz) (CH), 127.5 (d, *J* = 14.9 Hz) (CH), 47.2 (CH), 22.5 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 14.49.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{20}N_4OPS_2$ 451.0811; Found 451.0817.

IR (ATR): 2977, 1576, 1331, 1190, 1004, 931, 715, 527 cm^{-1}.

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)dimethylphosphine oxide (**3w**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.04) yielded **3w** (55.6 mg, 59%) as a colorless solid. M.p.: 210-211 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.34 – 8.23 (m, 1H), 8.16 (s, 1H), 8.05 – 7.97 (m, 1H), 7.69 – 7.59 (m, 2H), 5.06 – 4.90 (m, 1H), 1.73 – 1.64 (m, 12H).

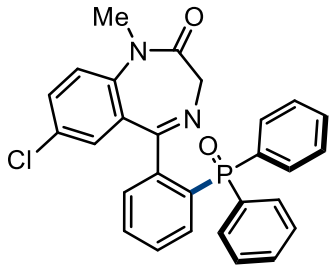
^{13}C NMR (75 MHz, $CDCl_3$) δ 157.3 (d, *J* = 2.6 Hz) (C_q), 151.8 (C_q), 150.9 (CH), 142.8 (CH), 137.4 (d, *J* = 7.2 Hz) (C_q), 134.5 (d, *J* = 91.6 Hz) (C_q), 133.5 (d, *J* = 7.9 Hz) (CH), 132.3 (C_q), 132.1 (d, *J* = 9.0 Hz) (CH), 131.2 (d, *J* = 2.6 Hz) (CH), 129.6 (d, *J* = 10.9 Hz) (CH), 47.5 (CH), 22.5 (CH_3), 19.5 (d, *J* = 73.1 Hz) (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 36.29.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{20}N_4OP$ 315.1369; Found 315.1371.

IR (ATR): 2977, 1582, 1331, 1172, 932, 734, 649, 445 cm^{-1}.

7-Chloro-5-(2-(diphenylphosphoryl)phenyl)-1-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (**3x**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.18) yielded **3x** (130.6 mg, 90%) as a colorless solid. M.p.: 238-239 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 – 7.48 (m, 1H), 7.42 – 7.25 (m, 12H), 7.24 – 7.17 (m, 1H), 7.12 – 7.03 (m, 2H), 6.69 (d, *J* = 2.1 Hz, 1H), 4.46 (d, *J* = 10.9 Hz, 1H), 3.49 (d, *J* = 11.2 Hz, 1H), 3.38 (s, 3H).

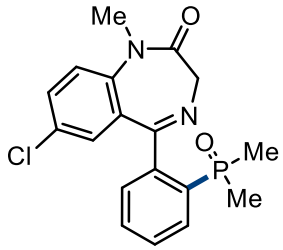
^{13}C NMR (75 MHz, $CDCl_3$) δ 169.7 (d, *J* = 3.6 Hz) (C_q), 168.3 (C_q), 143.7 (d, *J* = 6.4 Hz) (C_q), 142.3 (C_q), 134.1 (d, *J* = 11.6 Hz) (CH), 132.0 (d, *J* = 100.1 Hz) (C_q), 131.6 (CH), 131.6 (CH), 131.5 (CH), 130.9 (CH), 129.5 (d, *J* = 168.7 Hz) (C_q), 129.4 (CH), 128.6 (d, *J* = 12.2 Hz) (CH), 128.2 (d, *J* = 12.3 Hz) (CH), 122.4 (CH), 56.3 (CH_2), 35.4 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 30.64.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{23}ClN_2O_2P$ 485.1180; Found 485.1190.

IR (ATR): 3057, 1666, 1485, 1402, 1116, 918, 717, 526 cm^{-1}.

7-Chloro-5-(2-(dimethylphosphoryl)phenyl)-1-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (**3y**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.11) yielded **3y** (96.6 mg, 89%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 11.9, 7.5 Hz, 1H), 7.51 – 7.37 (m, 3H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.16 – 7.09 (m, 1H), 7.03 (d, *J* = 2.4 Hz, 1H), 4.74 (d, *J* = 10.3 Hz, 1H), 3.77 (d, *J* = 10.2 Hz, 1H), 3.37 (s, 3H), 1.69 (dd, *J* = 48.9, 12.9 Hz, 6H).

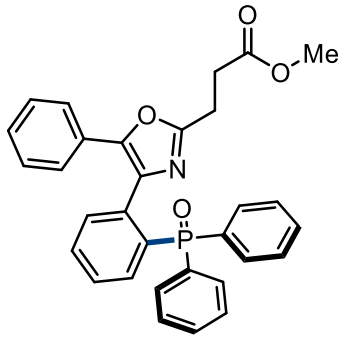
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0 (C_q), 168.6 (C_q), 142.2 (C_q), 142.1 (C_q), 134.8 (d, *J* = 93.9 Hz) (C_q), 131.7 (CH), 131.5 (d, *J* = 3.5 Hz) (CH), 131.2 (d, *J* = 8.7 Hz) (CH), 131.0 (d, *J* = 1.8 Hz) (CH), 130.0 (d, *J* = 117.6 Hz) (C_q), 129.6 (CH), 129.4 (CH), 129.3 (C_q), 122.5 (CH), 56.5 (CH_2), 35.1 (CH_3), 19.8 (d, *J* = 29.6 Hz) (CH_3), 18.8 (d, *J* = 28.1 Hz) (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 36.45.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}ClN_2O_2P$ 361.0867; Found 361.0870.

IR (ATR): 2915, 1665, 1470, 1300, 1168, 931, 722, 433 cm^{-1}.

Methyl 3-(4-(2-(diphenylphosphoryl)phenyl)-5-phenyloxazol-2-yl)propanoate (**3z**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.24) yielded **3z** (71.5 mg, 47%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 – 7.96 (m, 1H), 7.58 – 7.46 (m, 6H), 7.33 – 7.25 (m, 3H), 7.20 – 7.08 (m, 7H), 7.06 – 6.99 (m, 2H), 3.61 (s, 3H), 2.82 (t, *J* = 7.6 Hz, 2H), 2.58 (t, *J* = 7.6 Hz, 2H).

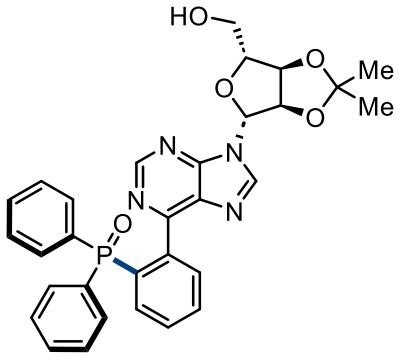
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4 (C_q), 159.9 (C_q), 146.1 (C_q), 136.3 (d, *J* = 8.3 Hz) (C_q), 134.9 (d, *J* = 9.4 Hz) (CH), 133.3 (C_q), 133.0 (d, *J* = 100.4 Hz) (C_q), 132.7 (d, *J* = 103.7 Hz) (C_q), 132.2 (CH), 132.0 (d, *J* = 9.6 Hz) (CH), 131.8 (d, *J* = 10.1 Hz) (CH), 131.3 (d, *J* = 2.7 Hz) (CH), 128.8 (d, *J* = 11.6 Hz) (CH), 128.2 (CH), 127.8 (C_q), 127.7 (CH), 127.6 (CH), 125.0 (CH), 51.8 (CH_3), 30.1 (CH_2), 22.9 (CH_2).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.61.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{31}H_{27}NO_4P$ 508.1672; Found 508.1677.

IR (ATR): 3052, 1737, 1437, 1331, 1179, 1118, 692, 545 cm^{-1}.

(2-(9-((3aR,4R,6R,6aR)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3aa**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.16) yielded **3aa** (73.3 mg, 43%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.02 (s, 1H), 7.84 – 7.71 (m, 2H), 7.66 – 7.59 (m, 1H), 7.57 – 7.45 (m, 5H), 7.32 – 7.24 (m, 2H), 7.22 – 7.14 (m, 4H), 5.84 (d, *J* = 4.5 Hz, 1H), 5.49 (s, 1H), 5.12 – 4.99 (m, 2H), 4.47 – 4.40 (m, 1H), 3.83 (dd, *J* = 12.6, 1.5 Hz, 1H), 3.68 (d, *J* = 11.0 Hz, 1H), 1.58 (s, 3H), 1.32 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 157.9 (d, *J* = 3.2 Hz) (C_q), 150.7 (CH), 150.1 (C_q), 144.1 (CH), 139.2 (d, *J* = 6.9 Hz) (C_q), 135.3 (d, *J* = 10.4 Hz) (CH), 134.2 (d, *J* = 4.6 Hz) (C_q), 132.5 (d, *J* = 100.7 Hz) (C_q),

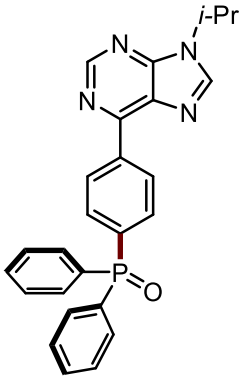
132.3 (d, J = 97.3 Hz) (C_q), 131.7 (CH), 131.6 (CH), 131.1 (d, J = 2.7 Hz) (CH), 129.3 (d, J = 12.0 Hz) (CH), 127.9 (d, J = 2.1 Hz) (CH), 127.7 (d, J = 2.2 Hz) (CH), 114.1 (C_q), 93.7 (CH), 86.2 (CH), 82.9 (CH), 81.5 (CH), 63.2 (CH_2), 27.5 (CH_3), 25.2 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.19.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{31}H_{30}N_4O_5P$ 569.1948; Found 569.1966.

IR (ATR): 2989, 1579, 1384, 1171, 1070, 849, 719, 535 cm^{-1}.

(4-(9-Isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4a**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.44) yielded **4a** (107.7 mg, 82%) as a colorless solid. M.p.: 185-186 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (s, 1H), 8.79 (dd, J = 8.3, 2.5 Hz, 2H), 8.10 (s, 1H), 7.78 (dd, J = 11.6, 8.3 Hz, 2H), 7.65 – 7.54 (m, 4H), 7.42 – 7.36 (m, 2H), 7.34 – 7.28 (m, 4H), 4.85 – 4.74 (m, 1H), 1.49 (d, J = 6.8 Hz, 6H).

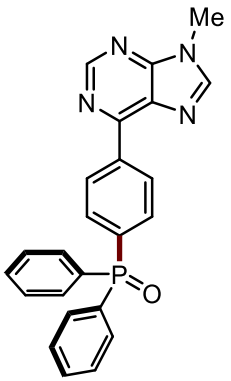
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5 (C_q), 151.9 (C_q), 151.5 (CH), 142.4 (CH), 138.8 (d, J = 2.9 Hz) (C_q), 134.3 (d, J = 102.6 Hz) (C_q), 131.9 (d, J = 104.3 Hz) (C_q), 131.8 (d, J = 10.0 Hz) (CH), 131.6 (d, J = 4.5 Hz) (CH), 131.6 (d, J = 2.6 Hz) (CH), 131.3 (C_q), 129.1 (d, J = 12.0 Hz) (CH), 128.1 (d, J = 12.1 Hz) (CH), 47.0 (CH), 22.0 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 28.57.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{24}N_4OP$ 439.1682; Found 439.1687.

IR (ATR): 3058, 2978, 1576, 1326, 1184, 1117, 805, 537 cm^{-1}.

(4-(9-Methyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4b**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.40) yielded **4b** (52.9 mg, 43%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.85 (dd, *J* = 8.4, 2.6 Hz, 2H), 8.12 (s, 1H), 7.90 – 7.83 (m, 2H), 7.74 – 7.66 (m, 4H), 7.56 – 7.52 (m, 2H), 7.49 – 7.44 (m, 4H), 3.94 (s, 3H).

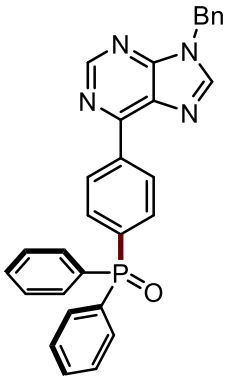
^{13}C NMR (75 MHz, $CDCl_3$) δ 153.4 (d, *J* = 0.9 Hz) (C_q), 153.0 (C_q), 152.4 (CH), 145.4 (CH), 139.0 (d, *J* = 2.9 Hz) (C_q), 134.7 (d, *J* = 102.8 Hz) (C_q), 132.4 (d, *J* = 10.1 Hz) (CH), 132.2 (CH), 132.1 (d, *J* = 104.6 Hz) (C_q), 132.1 (d, *J* = 2.9 Hz) (CH), 131.2 (C_q), 129.6 (d, *J* = 12.1 Hz) (CH), 128.5 (d, *J* = 12.2 Hz) (CH), 29.9 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.17.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{20}N_4OP$ 411.1369; Found 411.1368.

IR (ATR): 3059, 1578, 1437, 1180, 1121, 927, 733, 537 cm^{-1}.

(4-(9-Benzyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4c**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.38) yielded **4c** (76.0 mg, 52%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (s, 1H), 8.86 (dd, *J* = 8.2, 2.6 Hz, 2H), 8.10 (s, 1H), 7.86 (dd, *J* = 11.6, 8.2 Hz, 2H), 7.73 – 7.67 (m, 4H), 7.57 – 7.52 (m, 2H), 7.50 – 7.44 (m, 4H), 7.38 – 7.30 (m, 5H), 5.47 (s, 2H).

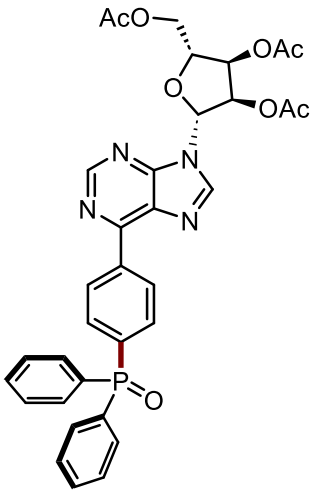
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.5 (C_q), 152.70 (C_q), 152.6 (CH), 144.6 (CH), 138.9 (d, *J* = 2.9 Hz) (C_q), 134.9 (d, *J* = 102.7 Hz) (C_q), 135.0 (Cq), 132.3 (d, *J* = 10.0 Hz) (CH), 132.2 (d, *J* = 104.4 Hz) (C_q), 132.1 (CH), 132.0 (d, *J* = 3.9 Hz) (CH), 131.2 (C_q), 129.6 (d, *J* = 12.0 Hz) (CH), 129.1 (CH), 128.6 (d, *J* = 4.4 Hz) (CH), 128.4 (CH), 127.8 (CH), 47.3 (CH_2).

^{31}P NMR (162 MHz, $CDCl_3$) δ 28.91.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{24}N_4OP$ 487.1682; Found 487.1695.

IR (ATR): 3061, 1577, 1325, 1119, 908, 722, 645, 536 cm^{-1}.

(2R,3R,4R,5R)-2-(Acetoxymethyl)-5-(6-(4-(diphenylphosphoryl)phenyl)-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate (**4d**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.40) yielded **4d** (45.3 mg, 23%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.84 (dd, *J* = 8.6, 2.6 Hz, 2H), 8.29 (s, 1H), 7.91 – 7.84 (m, 2H), 7.75 – 7.67 (m, 4H), 7.59 – 7.53 (m, 2H), 7.51 – 7.45 (m, 4H), 6.29 (d, *J* = 5.2 Hz, 1H), 6.00 (t, *J* = 5.4 Hz, 1H), 5.73 – 5.66 (m, 1H), 4.51 – 4.37 (m, 3H), 2.18 – 2.07 (m, 9H).

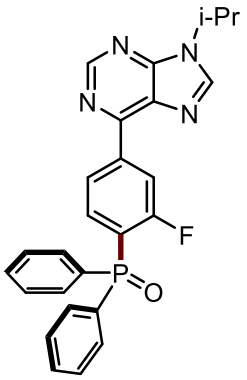
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.3 (C_q), 169.6 (C_q), 169.4 (C_q), 154.1 (C_q), 152.7 (CH), 152.2 (C_q), 143.1 (CH), 138.6 (d, *J* = 2.9 Hz) (C_q), 135.2 (d, *J* = 102.4 Hz) (C_q), 132.4 (d, *J* = 10.0 Hz) (CH), 132.2 (d, *J* = 104.5 Hz) (C_q), 132.1 (d, *J* = 10.0 Hz) (CH), 132.0 (CH), 132.1 (C_q), 129.6 (d, *J* = 12.0 Hz), (CH) 128.6 (d, *J* = 12.2 Hz) (CH), 86.5 (CH), 80.4 (CH), 73.1 (CH), 70.6 (CH), 63.0 (CH_2), 20.8 (CH_3), 20.5 (CH_3), 20.4 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.83.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{34}H_{32}N_4O_8P$ 655.1952; Found 655.1965.

IR (ATR): 2925, 1746, 1580, 1366, 1214, 1046, 739, 537 cm^{-1}.

(2-Fluoro-4-(9-isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4e**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.40) yielded **4e** (93.1 mg, 68%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.83 – 8.72 (m, 1H), 8.64 – 8.52 (m, 1H), 8.22 (s, 1H), 8.15 – 8.03 (m, 1H), 7.85 – 7.73 (m, 4H), 7.61 – 7.45 (m, 6H), 5.07 – 4.90 (m, 1H), 1.68 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.9 (d, $J_{C\text{-}F}$ = 249.8 Hz) (C_q), 152.5 (C_q), 151.9 (CH), 151.8 (d, *J* = 2.5

Hz) (C_q), 142.8 (CH), 142.4 (dd, *J* = 8.4, 2.3 Hz) (C_q), 135.1 – 134.5 (m) (CH), 132.2 (d, *J* = 2.8 Hz) (CH), 131.9 (d, *J* = 108.2 Hz) (C_q), 131.7 (dd, *J* = 10.6, 1.8 Hz) (CH), 128.5 (d, *J* = 12.8 Hz) (CH), 125.6 (dd, *J* = 10.6, 3.3 Hz) (CH), 122.1 (dd, *J* = 19.1 Hz, 99.0 Hz) (C_q), 116.9 (dd, *J* = 25.1, 5.7 Hz) (CH), 47.5 (CH), 22.5 (CH_3).

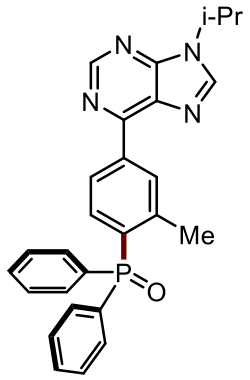
^{31}P NMR (121 MHz, $CDCl_3$) δ 24.44.

^{19}F NMR (282 MHz, $CDCl_3$) δ -98.88.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{23}FN_4OP$ 457.1588; Found 457.1600.

IR (ATR): 3057, 2978, 1574, 1436, 1104, 897, 690, 521 cm^{-1}.

(4-(9-Isopropyl-9H-purin-6-yl)-2-methylphenyl)diphenylphosphine oxide (**4f**)



Prepared according to standard procedure A using [Ru(OAc)$_2$(*p*-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.43) yielded **4f** (50.2 mg, 37%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.67 – 8.51 (m, 2H), 8.20 (s, 1H), 7.76 – 7.66 (m, 4H), 7.61 – 7.54 (m, 2H), 7.53 – 7.45 (m, 4H), 7.24 (dd, *J* = 13.8, 8.1 Hz, 1H), 5.08 – 4.91 (m, 1H), 2.61 (s, 3H), 1.68 (d, *J* = 6.8 Hz, 6H).

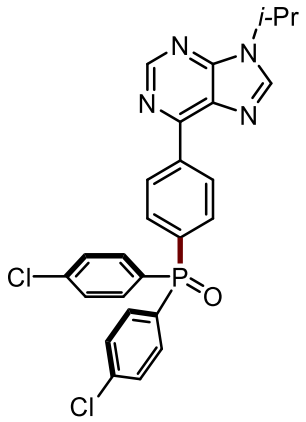
^{13}C NMR (75 MHz, $CDCl_3$) δ 152.9 (d, *J* = 94.3 Hz) (C_q), 152.0 (CH), 143.7 (d, *J* = 8.1 Hz) (C_q), 142.4 (CH), 139.1 (d, *J* = 2.6 Hz) (C_q), 133.8 (d, *J* = 13.6 Hz) (CH), 132.4 (d, *J* = 103.8 Hz) (C_q), 132.4 (C_q), 132.2 (d, *J* = 10.3 Hz) (CH), 132.0 (CH), 131.9 (d, *J* = 2.6 Hz) (CH), 131.8 (C_q), 128.6 (d, *J* = 12.1 Hz) (CH), 126.6 (d, *J* = 12.8 Hz) (CH), 47.4 (CH), 22.5(CH_3), 21.8 (d, *J* = 4.4 Hz) (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 31.59.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{27}H_{26}N_4OP$ 453.1839; Found 453.1828.

IR (ATR): 2977, 2226, 1573, 1325, 1116, 807, 693, 547 cm^{-1}.

Bis(4-chlorophenyl)(4-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**4g**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.44) yielded **4g** (94.2 mg, 62%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.85 (dd, *J* = 8.5, 2.7 Hz, 2H), 8.18 (s, 1H), 7.83 – 7.75 (m, 2H), 7.63 – 7.55 (m, 4H), 7.45 – 7.40 (m, 4H), 4.96 (h, *J* = 6.8 Hz, 1H), 1.64 (d, *J* = 6.8 Hz, 6H).

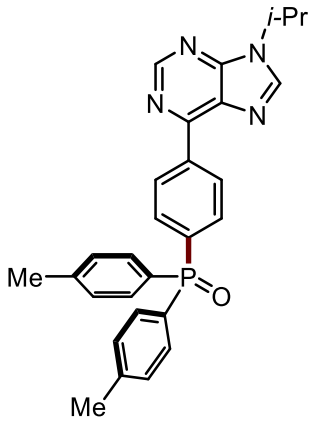
^{13}C NMR (75 MHz, $CDCl_3$) δ 152.9 (d, *J* = 1.0 Hz) (C_q), 152.3 (C_q), 152.0 (CH), 142.6 (CH), 139.5 (d, *J* = 2.9 Hz) (C_q), 138.9 (d, *J* = 3.4 Hz) (C_q), 133.5 (d, *J* = 104.7 Hz) (C_q), 133.3 (d, *J* = 10.9 Hz) (CH), 132.1 (d, *J* = 10.2 Hz) (CH), 131.7 (C_q), 130.3 (d, *J* = 106.0 Hz) (C_q), 129.7 (d, *J* = 12.2 Hz) (CH), 129.0 (d, *J* = 12.8 Hz) (CH), 47.4 (CH), 22.4 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 27.54.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{22}Cl_2N_4OP$ 507.0903; Found 507.0913.

IR (ATR): 2977, 1576, 1388, 1177, 1084, 1013, 930, 729, 562 cm^{-1}.

(4-(9-Isopropyl-9H-purin-6-yl)phenyl)di-p-tolylphosphine oxide (**4h**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.42) yielded **4h** (62.8 mg, 45%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.89 – 8.85 (m, 2H), 8.23 (s, 1H), 7.93 – 7.87 (m, 2H), 7.65 – 7.59 (m, 4H), 7.32 – 7.29 (m, 4H), 5.10 – 4.96 (m, 1H), 2.44 (s, 6H), 1.72 (d, J = 6.7 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 153.5 (C_q), 152.3 (C_q), 152.1 (CH), 142.5 (CH), 142.4 (C_q), 138.9 (d, *J* = 3.0 Hz) (C_q), 135.3 (d, *J* = 102.7 Hz) (C_q), 132.3 (d, *J* = 10.1 Hz) (CH), 132.1 (d, *J* = 10.1 Hz) (CH),

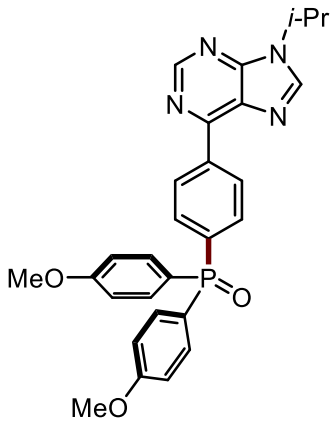
131.8 (C_q), 129.5 (d, J = 12.0 Hz) (CH), 129.2 (d, J = 12.5 Hz) (CH), δ 129.2 (d, J = 106.8 Hz) (C_q), 47.4 (CH), 22.5 (CH_3), 21.6 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 29.16.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{28}N_4OP$ 467.1995; Found 467.2016.

IR (ATR): 2904, 1577, 1327, 1183, 1116, 930, 731, 542 cm^{-1}.

(4-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-methoxyphenyl)phosphine oxide (**4i**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.33) yielded **4i** (96.6 mg, 65%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.99 (d, J = 1.2 Hz, 1H), 8.81 (dd, J = 8.2, 2.5 Hz, 2H), 8.17 (s, 1H), 7.90 – 7.81 (m, 2H), 7.62 – 7.53 (m, 4H), 6.95 – 6.91 (m, 4H), 5.02 – 4.87 (m, 1H), 3.80 (d, J = 1.3 Hz, 6H), 1.63 (d, J = 6.8 Hz, 6H).

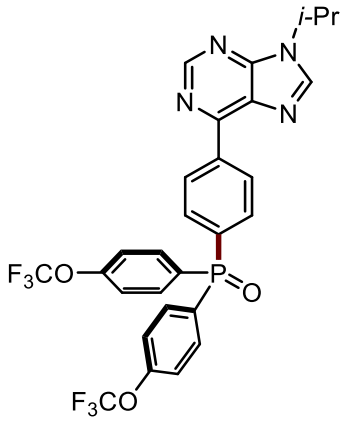
^{13}C NMR (75 MHz, $CDCl_3$) δ 162.4 (d, J = 2.8 Hz) (C_q), 153.4 (C_q), 152.2 (C_q), 152.0 (CH), 142.5 (CH), 138.8 (d, J = 2.9 Hz) (C_q), 135.5 (d, J = 103.5 Hz) (C_q), 133.9 (d, J = 11.3 Hz) (CH), 132.2 (d, J = 10.1 Hz) (CH), 131.7 (C_q), 129.4 (d, J = 12.0 Hz) (CH), 123.6 (d, J = 111.2 Hz) (C_q), 114.0 (d, J = 13.2 Hz), 55.2 (CH), 47.3 (CH_3), 22.4 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.82.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{28}N_4O_3P$ 499.1894; Found 499.1895.

IR (ATR): 2977, 1569, 1250, 1118, 1026, 929, 731, 535 cm^{-1}.

(4-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-(trifluoromethoxy)phenyl)phosphine oxide (**4j**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.47) yielded **4j** (111.0 mg, 61%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.88 (dd, *J* = 8.0, 1.7 Hz, 2H), 8.19 (s, 1H), 7.87 – 7.70 (m, 6H), 7.32 (d, *J* = 8.1 Hz, 4H), 4.98 (p, *J* = 6.8 Hz, 1H), 1.66 (d, *J* = 6.8 Hz, 6H).

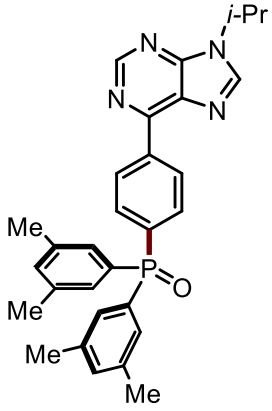
^{13}C NMR (75 MHz, $CDCl_3$) δ 153.0 (C_q), 152.4 (C_q), 152.2 (C_q), 152.1 (CH), 142.6 (CH), 139.7 (d, *J* = 2.4 Hz) (C_q), 134.1 (d, *J* = 11.0 Hz) (CH), 132.3 (d, *J* = 72.8 Hz) (C_q), 132.2 (d, *J* = 10.1 Hz) (CH), 130.5 (d, *J* = 105.8 Hz) (C_q), 129.8 (d, *J* = 12.1 Hz) (CH), 120.6 (d, *J* = 12.7 Hz) (CH), 120.2 (q, *J* = 259.0 Hz) (C_q), 47.5 (CH), 22.5 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 26.78.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{22}F_6N_4O_3P$ 607.1328; Found 607.1335.

IR (ATR): 2980, 1579, 1501, 1252, 1164, 1117, 748, 563 cm^{-1}.

Bis(3,5-dimethylphenyl)(4-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**4k**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.51) yielded **4k** (75.4 mg, 51%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.83 (dd, *J* = 8.4, 2.5 Hz, 2H), 8.18 (s, 1H), 7.86 (dd, *J* = 11.5, 8.4 Hz, 2H), 7.30 (d, *J* = 12.3 Hz, 4H), 7.15 (s, 2H), 4.97 (p, *J* = 6.8 Hz, 1H), 2.30 (s, 12H), 1.66 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 153.5 (C_q), 152.3 (C_q), 152.0 (CH), 142.4 (C_q), 138.8 (d, *J* = 2.8 Hz) (C_q), 138.1 (d, *J* = 12.8 Hz) (C_q), 135.3 (d, *J* = 101.7 Hz) (C_q), 133.7 (d, *J* = 2.8 Hz) (CH), 132.4 (d, *J* = 10.0

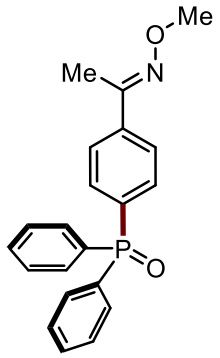
Hz) (CH), 132.1 (d, J = 103.5 Hz) (C_q), 131.7 (C_q), 129.6 (d, J = 9.9 Hz) (CH), 129.4 (d, J = 12.0 Hz) (CH), 47.4 (CH), 22.5 (CH_3), 21.2 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 29.43.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{32}N_4OP$ 495.2308; Found 495.2314.

IR (ATR): 2977, 1575, 1326, 1182, 849, 730, 569, 530 cm^{-1}.

(E)-(4-(1-(Methoxyimino)ethyl)phenyl)diphenylphosphine oxide (**4l**)



Prepared according to standard procedure A using [$Ru(OAc)_2$(p-cymene)] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.30) yielded **4l** (31.8 mg, 30%) as a colorless sticky oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.76 (m, 2H), 7.74 – 7.67 (m, 6H), 7.61 – 7.57 (m, 2H), 7.53 – 7.48 (m, 4H), 4.05 (s, 3H), 2.26 (s, 3H).

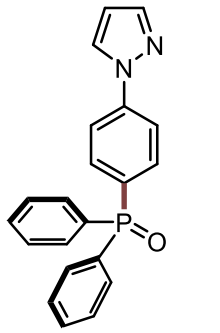
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7 (C_q), 140.0 (d, J = 2.9 Hz) (C_q), 132.9 (d, J = 103.9 Hz) (C_q), 132.3 (d, J = 104.6 Hz) (C_q), 132.2 (d, J = 9.8 Hz) (CH), 132.1 (CH), 132.0 (CH), 128.5 (d, J = 12.0 Hz) (CH), 126.0 (d, J = 12.4 Hz) (CH), 62.2 (CH_3), 12.5 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 28.87.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{21}NO_2P$ 350.1304; Found 350.1310.

IR (ATR): 2935, 1436, 1181, 1118, 1046, 897, 709, 554 cm^{-1}.

(4-(1H-pyrazol-1-yl)phenyl)diphenylphosphine oxide (**4m**)

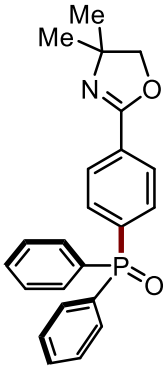


Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.53) yielded **4m** (33.0 mg, 32%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, J = 2.5 Hz, 1H), 7.84 – 7.64 (m, 9H), 7.58 – 7.52 (m, 2H), 7.50

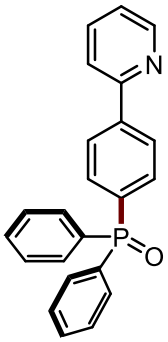
– 7.44 (m, 4H), 6.49 (dd, J = 2.5, 1.9 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 142.6 (d, J = 3.1 Hz) (C_q), 141.9 (CH), 133.6 (d, J = 10.7 Hz) (CH), 132.3 (d, J = 104.8 Hz) (C_q), 132.1 (d, J = 3.7 Hz) (CH), 132.0 (CH), 130.1 (d, J = 106.0 Hz) (C_q), 128.6 (d, J = 12.2 Hz) (CH), 126.8 (CH), 118.6 (d, J = 12.6 Hz) (CH), 108.4 (CH).
^{31}P NMR (121 MHz, $CDCl_3$) δ 28.52.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{18}N_2OP$ 345.1151; Found 345.1156.
IR (ATR): 3059, 1600, 1392, 1177, 1111, 933, 726, 548 cm^{-1}.

(4-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenyl)diphenylphosphine oxide (**4n**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.49) yielded **4n** (25.3 mg, 22%) as a colorless sticky oil.
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.74 – 7.69 (m, 2H), 7.68 – 7.63 (m, 4H), 7.57 – 7.53 (m, 2H), 7.48 – 7.44 (m, 4H), 4.12 (s, 2H), 1.38 (s, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 161.2 (C_q), 135.5 (d, J = 102.3 Hz) (C_q), 132.1 (d, J = 104.6 Hz) (C_q), 132.1 (CH),132.0 (CH), 132.1 (CH), 131.4 (d, J = 2.8 Hz) (C_q), 128.6 (d, J = 12.3 Hz) (CH), 128.1 (d, J = 12.2 Hz) (CH), 79.3 (CH_2), 67.9 (C_q), 28.3 (CH_3).
^{31}P NMR (121 MHz, $CDCl_3$) δ 28.57.
HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}NO_2P$ 376.1461; Found 376.1469.
IR (ATR): 2965, 1649, 1437, 1197, 1118, 1063, 721, 547 cm^{-1}.

Diphenyl(4-(pyridin-2-yl)phenyl)phosphine oxide (**4o**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale,

purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.56) yielded **4o** (47.8 mg, 45%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.6 Hz, 1H), 8.08 (dd, *J* = 8.4, 2.5 Hz, 2H), 7.82 – 7.67 (m, 8H), 7.58 – 7.53 (m, 2H), 7.50 – 7.44 (m, 4H), 7.31 – 7.26 (m, 1H).

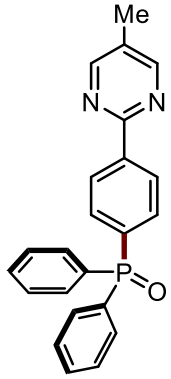
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2 (C_q), 149.9 (CH), 142.8 (d, *J* = 2.8 Hz) (C_q), 136.9 (CH), 132.8 (d, *J* = 104.2 Hz) (C_q), 132.6 (d, *J* = 10.1 Hz) (CH), 132.4 (d, *J* = 104.3 Hz) (C_q), 132.1 (d, *J* = 10.0 Hz) (CH), 132.0 (d, *J* = 2.7 Hz) (CH), 128.5 (d, *J* = 12.2 Hz) (CH), 126.9 (d, *J* = 12.3 Hz) (CH), 122.9 (CH), 121.0 (CH).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.98.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}NOP$ 356.1199; Found 356.1203.

IR (ATR): 3055, 1586, 1436, 1182, 1119, 779, 705, 553 cm^{-1}.

(4-(5-Methylpyrimidin-2-yl)phenyl)diphenylphosphine oxide (**4p**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.31) yielded **4p** (50.9 mg, 46%) as a colorless solid. M.p.: 217-218 °C

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 – 8.58 (m, 2H), 8.51 – 8.45 (m, 2H), 7.82 – 7.74 (m, 2H), 7.73 – 7.65 (m, 4H), 7.57 – 7.50 (m, 2H), 7.48 – 7.42 (m, 4H), 2.33 (s, 3H).

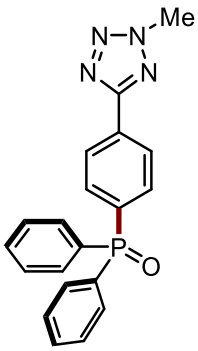
^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4 (d, *J* = 1.0 Hz) (C_q), 157.4 (CH), 140.9 (d, *J* = 2.9 Hz) (C_q), 134.2 (d, *J* = 103.4 Hz) (C_q), 132.3 (d, *J* = 10.1 Hz) (CH), 132.4 (d, *J* = 104.3 Hz) (C_q), 132.0 (d, *J* = 10.0 Hz) (CH), 131.9 (CH), 129.1 (C_q), 128.5 (d, *J* = 12.2 Hz) (CH), 127.7 (d, *J* = 12.3 Hz) (CH), 15.5 (CH_3).

^{31}P NMR (121 MHz, $CDCl_3$) δ 28.94.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}N_2OP$ 371.1308; Found 371.1311.

IR (ATR): 3058, 1542, 1429, 1195, 1118, 791, 730, 545 cm^{-1}.

(4-(2-Methyl-2H-tetrazol-5-yl)phenyl)diphenylphosphine oxide (**4q**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.51) yielded **4q** (38.9 mg, 36%) as a colorless solid. 175-176 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.20 (m, 2H), 7.83 – 7.77 (m, 2H), 7.72 – 7.66 (m, 4H), 7.59 – 7.54 (m, 2H), 7.51 – 7.45 (m, 4H), 4.41 (s, 3H).

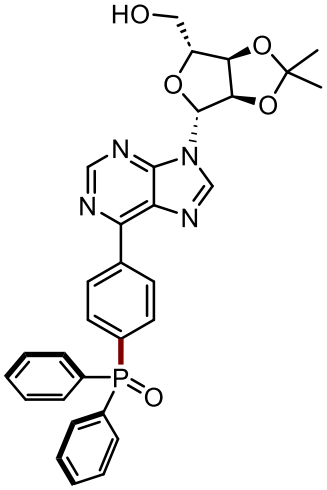
^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3 (C_q), 134.7 (d, *J* = 103.1 Hz) (C_q), 132.7 (d, *J* = 10.0 Hz) (CH), 132.1 (CH), 132.1 (d, *J* = 9.9 Hz) (CH), 131.1 (d, *J* = 99.6 Hz) (C_q), 130.6 (Cq), 128.6 (d, *J* = 12.2 Hz) (CH), 126.7 (d, *J* = 12.2 Hz) (CH), 39.6 (CH_3).

^{31}P NMR (162 MHz, $CDCl_3$) δ 28.61.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{18}N_4OP$ 361.1213; Found 361.1218.

IR (ATR): 3058, 1437, 1196, 1113, 1003, 844, 727, 562 cm^{-1}.

(4-(9-((3aR,4R,6R,6aR)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4r**)



Prepared according to standard procedure B using [$RuCl_3 \cdot 3H_2O$] (10 mol %) on a 0.3 mmol scale, purification by column chromatography on silica gel (DCM/MeOH = 20/1, R_f = 0.40) yielded **4r** (47.6 mg, 28%) as a colorless sticky oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.83 (dd, *J* = 8.4, 2.5 Hz, 2H), 8.25 (s, 1H), 7.86 (dd, *J* = 11.6, 8.4 Hz, 2H), 7.73 – 7.66 (m, 4H), 7.58 – 7.52 (m, 2H), 7.50 – 7.44 (m, 4H), 6.02 (d, *J* = 4.6 Hz, 1H), 5.63 (d, *J* = 8.3 Hz, 1H), 5.30 – 5.23 (m, 1H), 5.13 (dd, *J* = 6.0, 1.2 Hz, 1H), 4.58 – 4.53 (m, 1H), 3.98 (dd, *J* = 12.6, 1.4 Hz, 1H), 3.88 – 3.77 (m, 1H), 1.66 (s, 3H), 1.38 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 154.5 (d, *J* = 1.0 Hz) (C_q), 151.8 (CH), 151.4 (C_q), 144.4 (CH), 138.4 (d,

J = 2.9 Hz) (C_q), 135.3 (d, *J* = 102.3 Hz) (C_q), 132.9 (C_q), 132.4 (d, *J* = 10.0 Hz) (CH), 132.1 (d, *J* = 3.9 Hz) (CH), 132.1 (d, *J* = 104.5 Hz) (C_q), 132.0 (d, *J* = 3.3 Hz) (CH), 129.7 (d, *J* = 12.0 Hz) (CH), 128.6 (d, *J* = 12.2 Hz) (CH), 114.2 (C_q), 93.9 (CH), 86.3 (CH), 83.1 (CH), 81.6 (CH), 63.2 (CH_2), 27.6 (CH_3), 25.2 (CH_3).

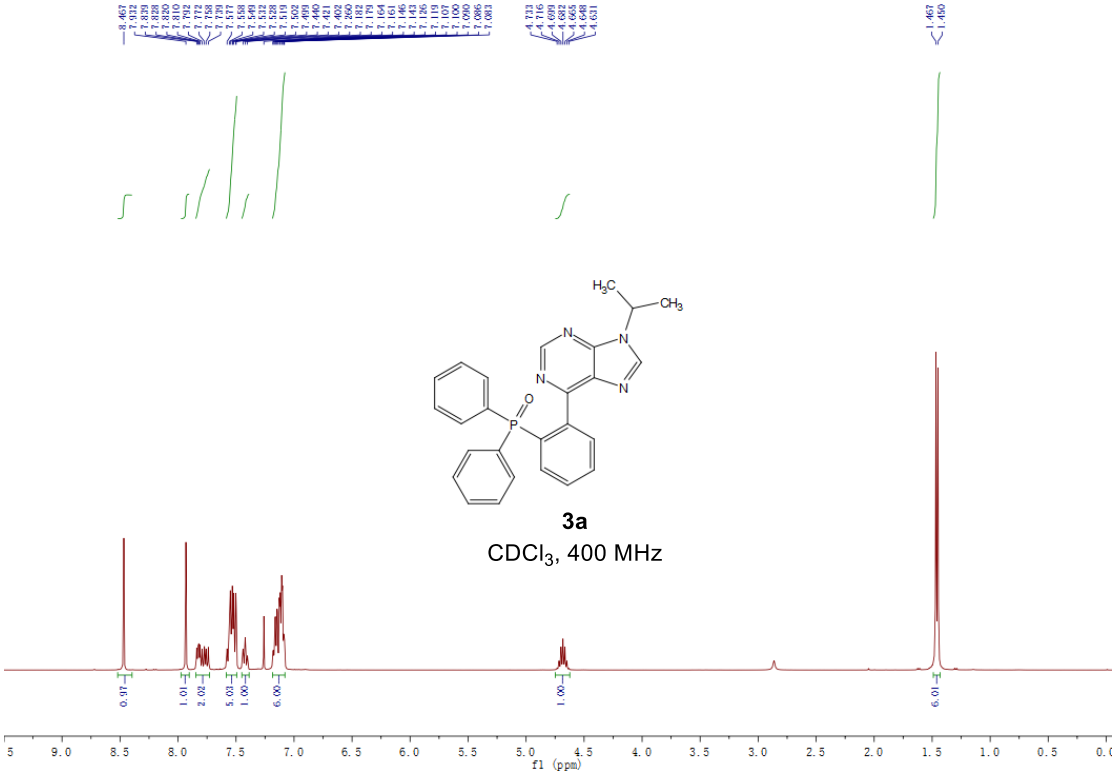
^{31}P NMR (121 MHz, $CDCl_3$) δ 28.98.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{31}H_{30}N_4O_5P$ 569.1948; Found 569.1959.

IR (ATR): 2938, 1581, 1437, 1173, 1083, 848, 718, 532 cm^{-1}.

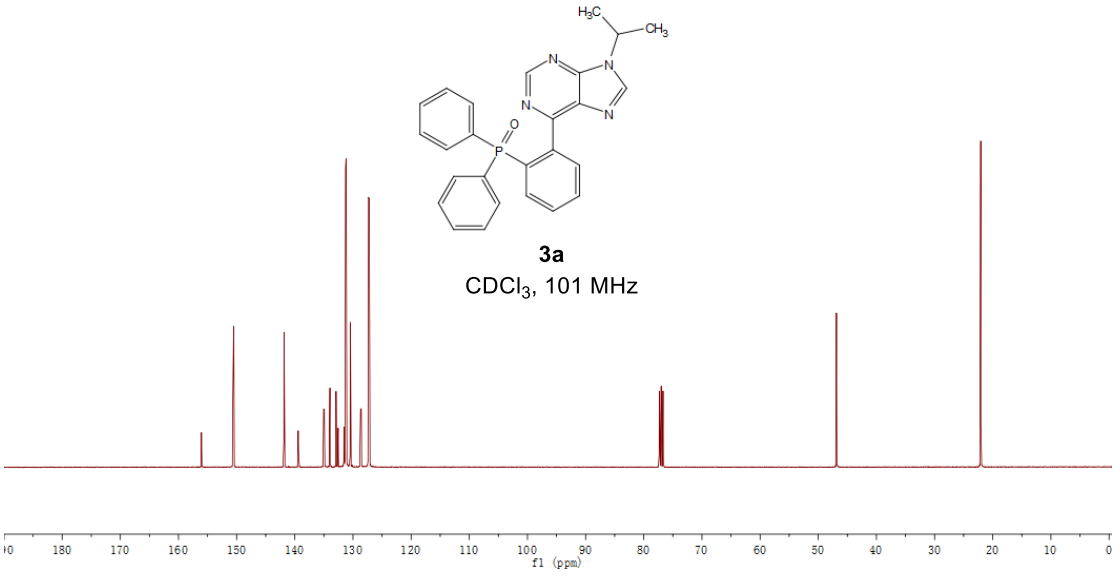
9. NMR Spectroscopic Data

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3a**)



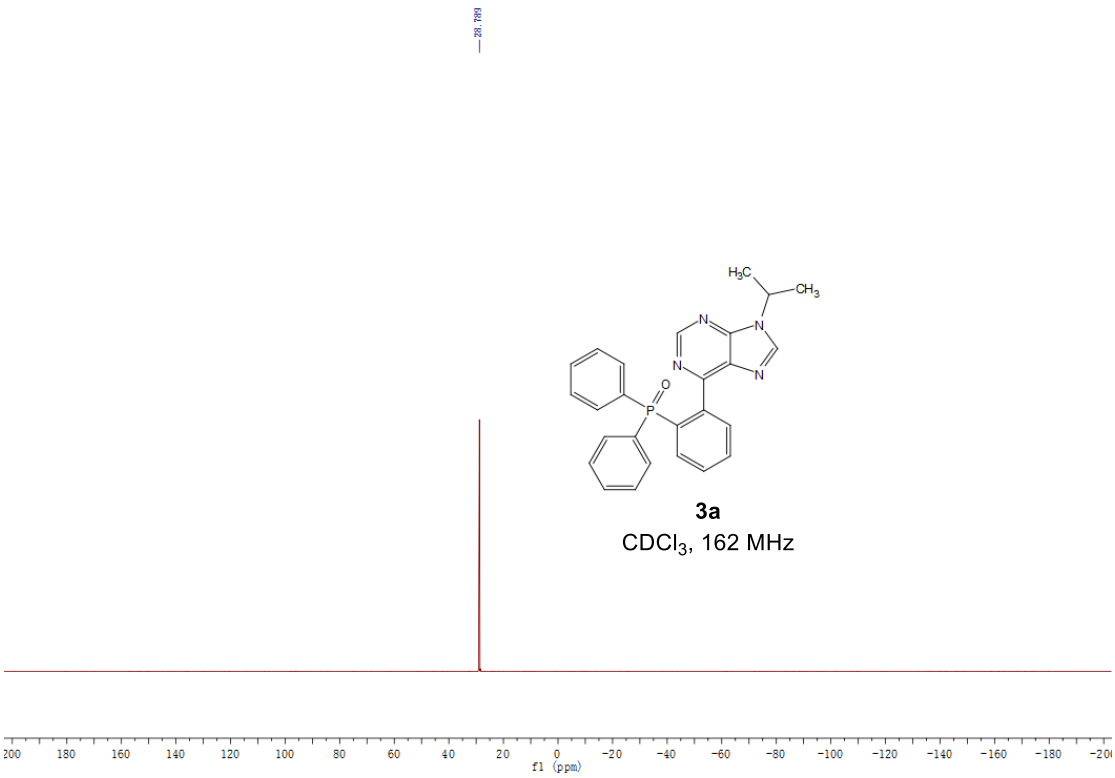
3a

$CDCl_3$, 400 MHz



3a

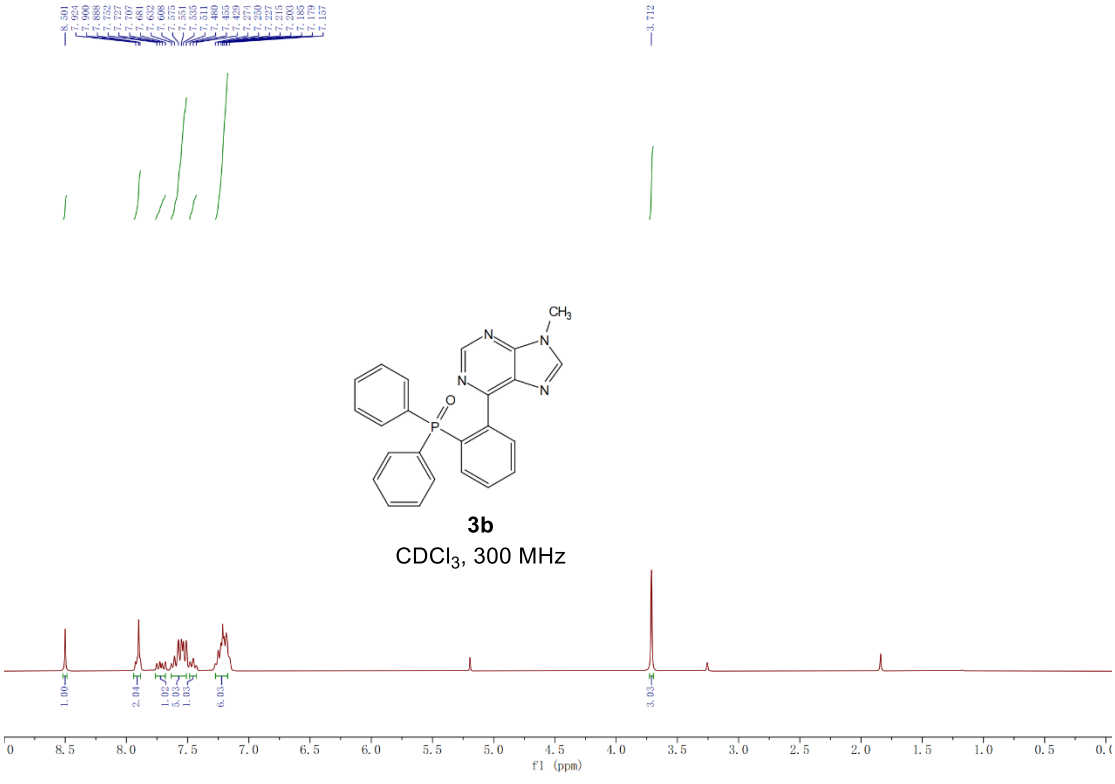
$CDCl_3$, 101 MHz



3a

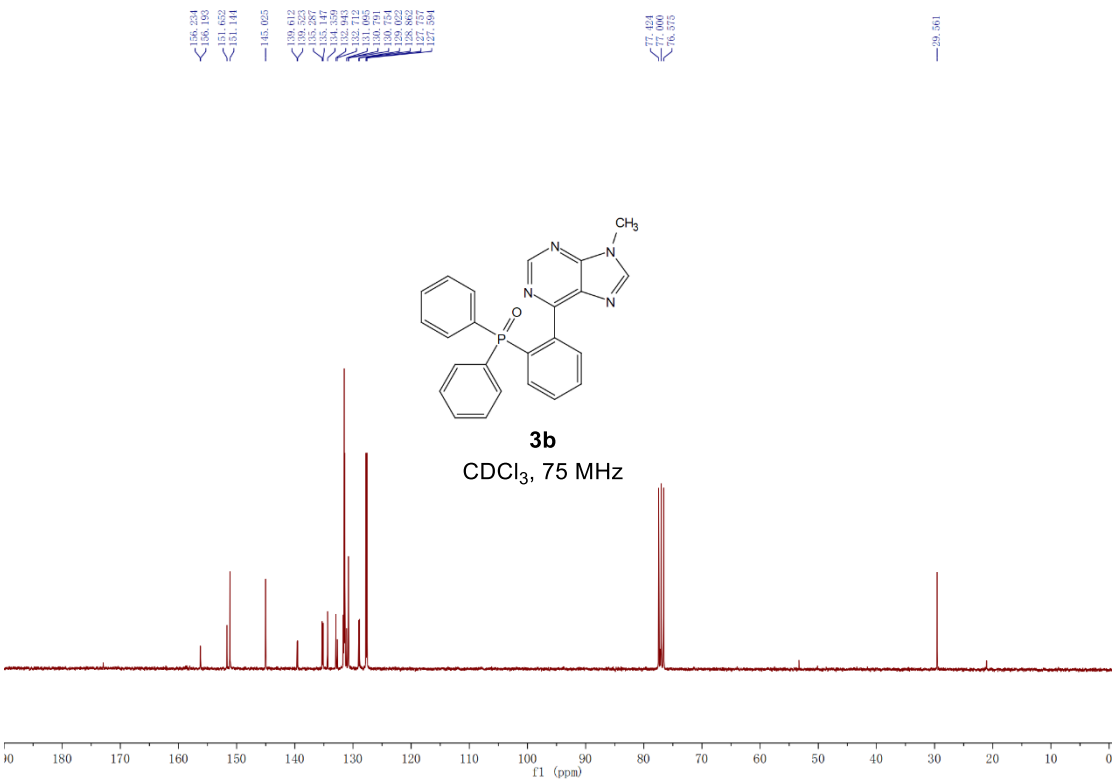
$CDCl_3$, 162 MHz

(2-(9-Methyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3b**)



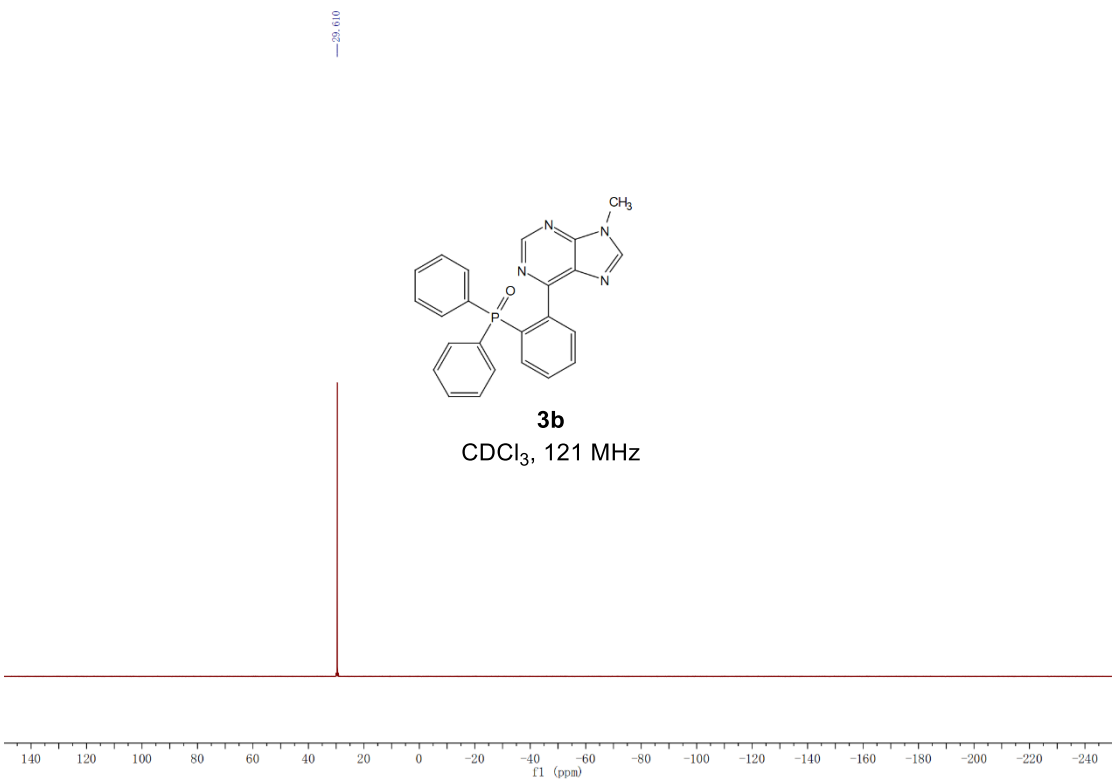
3b

$CDCl_3$, 300 MHz



3b

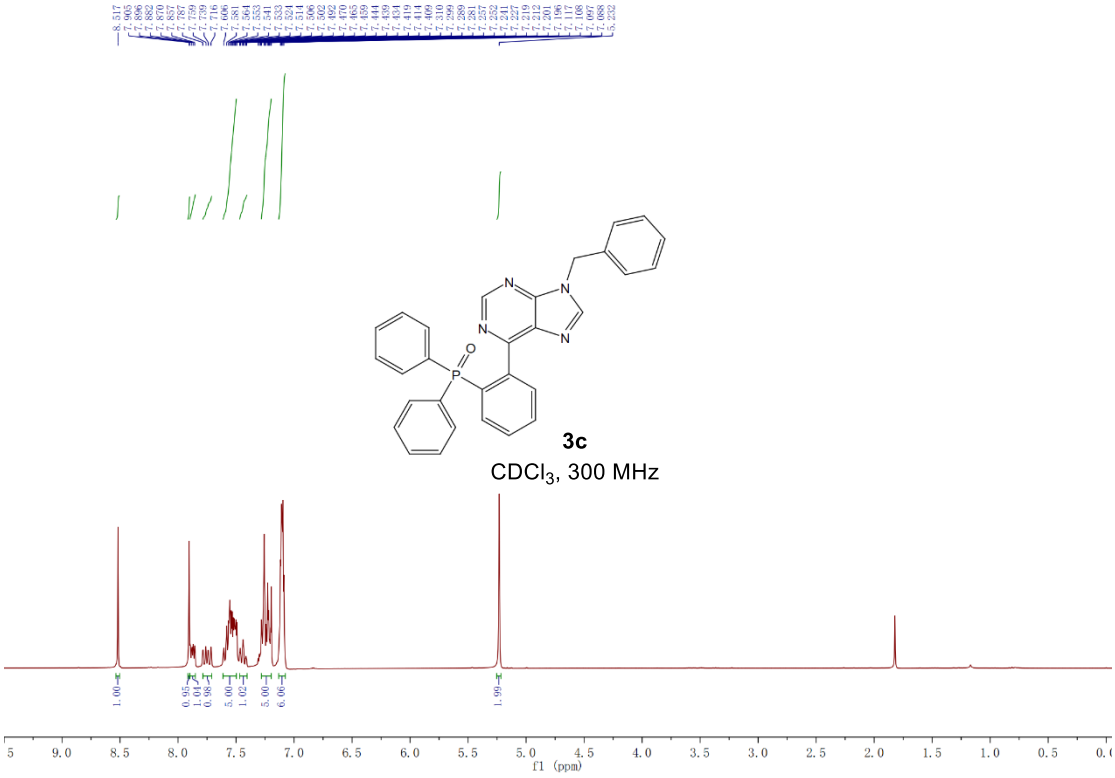
$CDCl_3$, 75 MHz

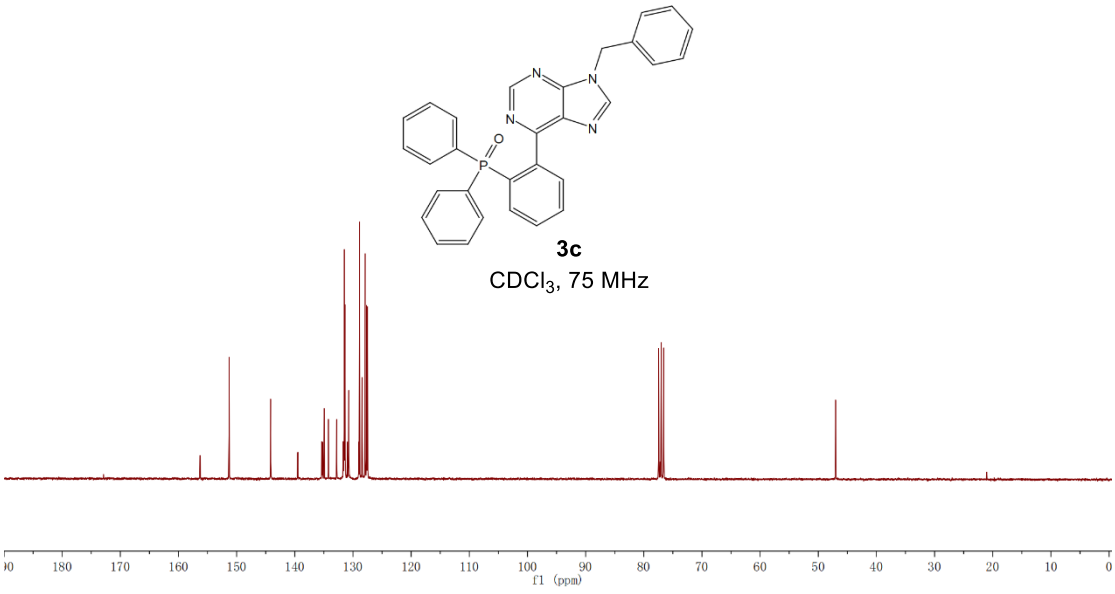


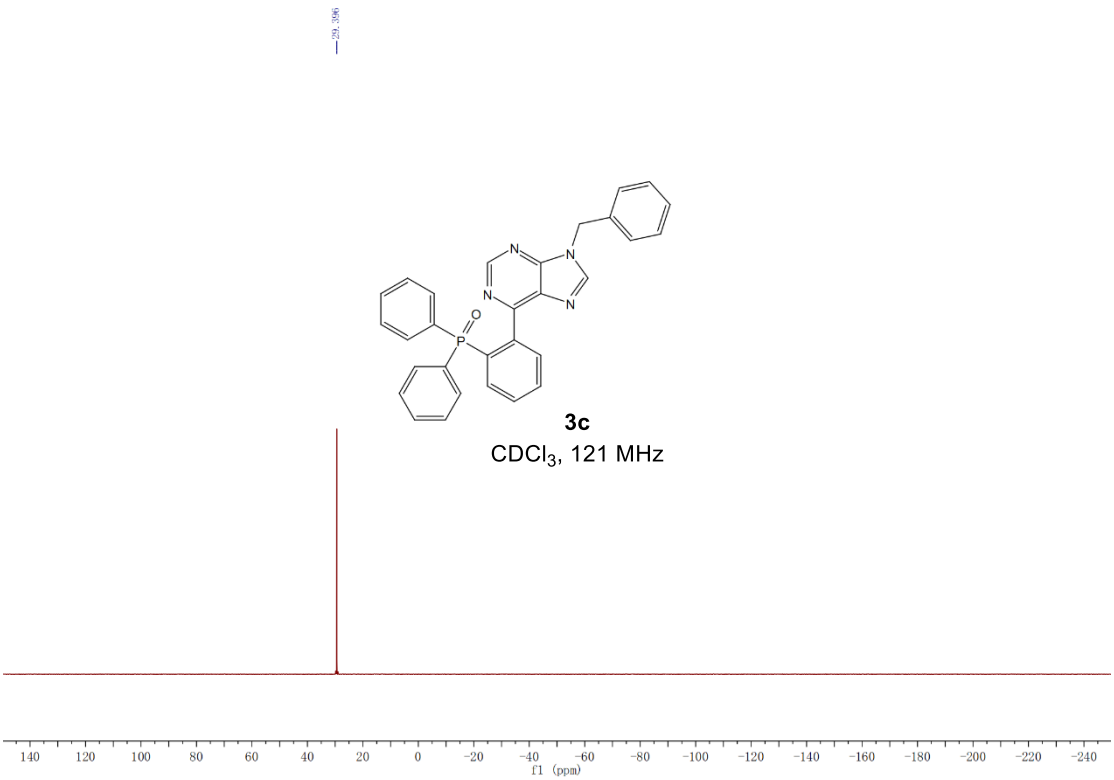
3b

$CDCl_3$, 121 MHz

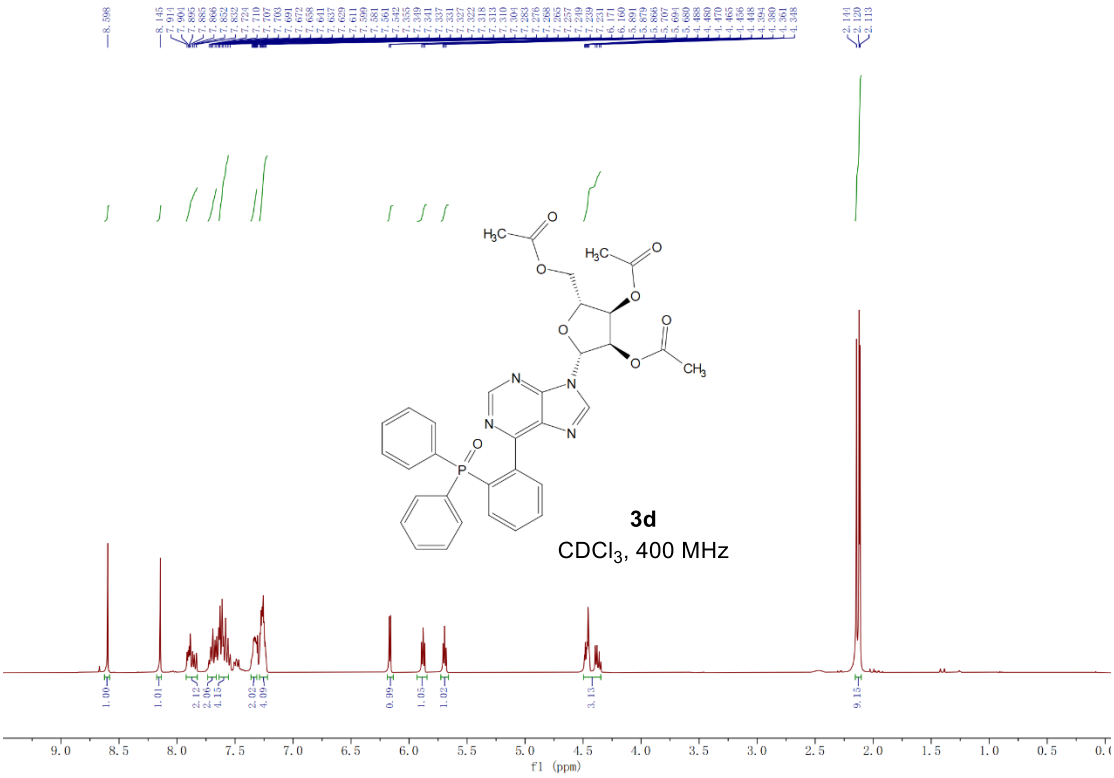
(2-(9-Benzyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3c**)

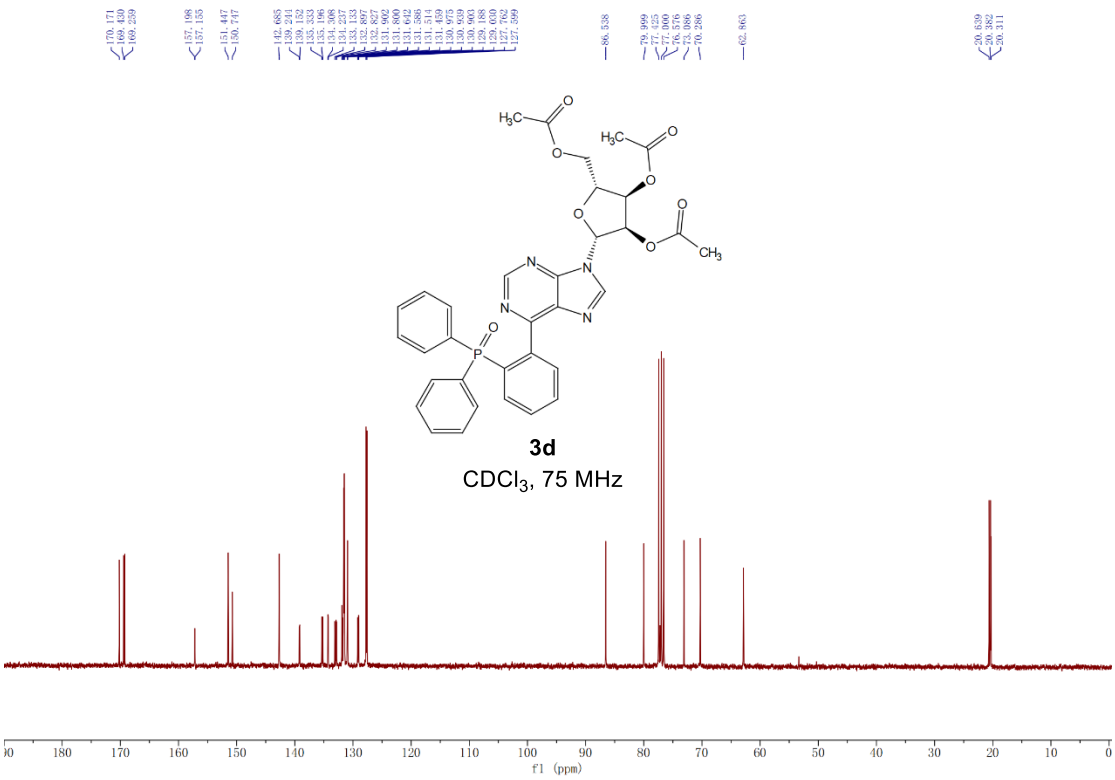


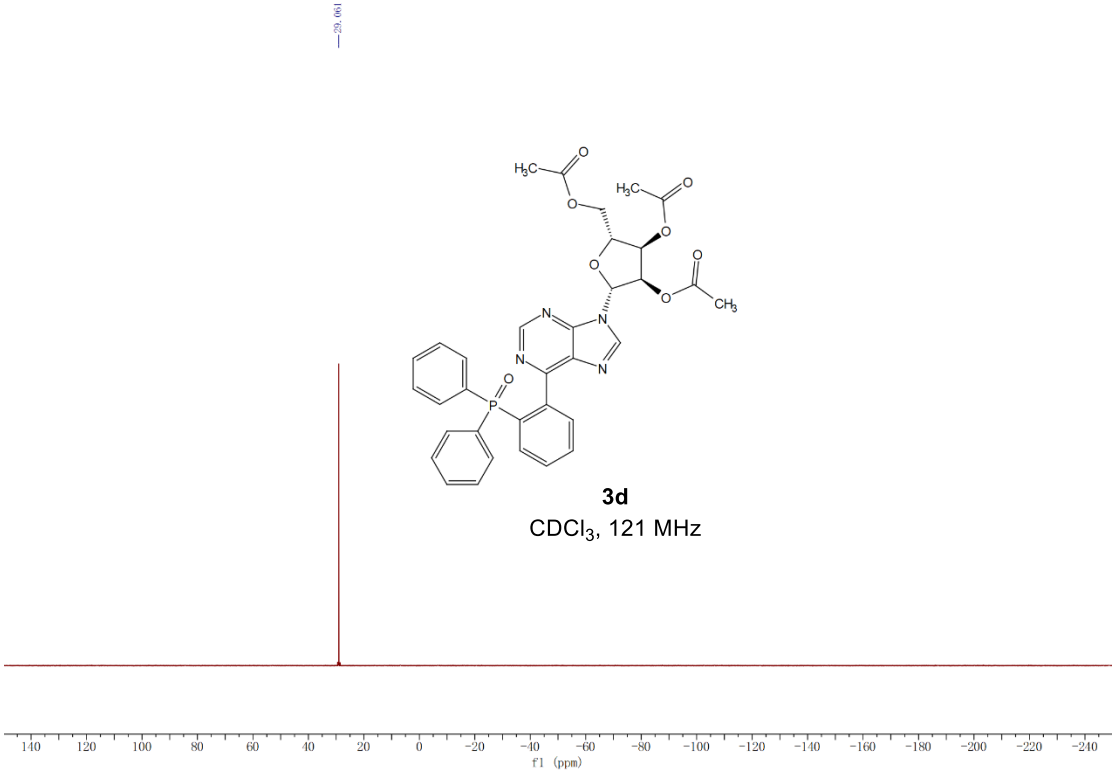




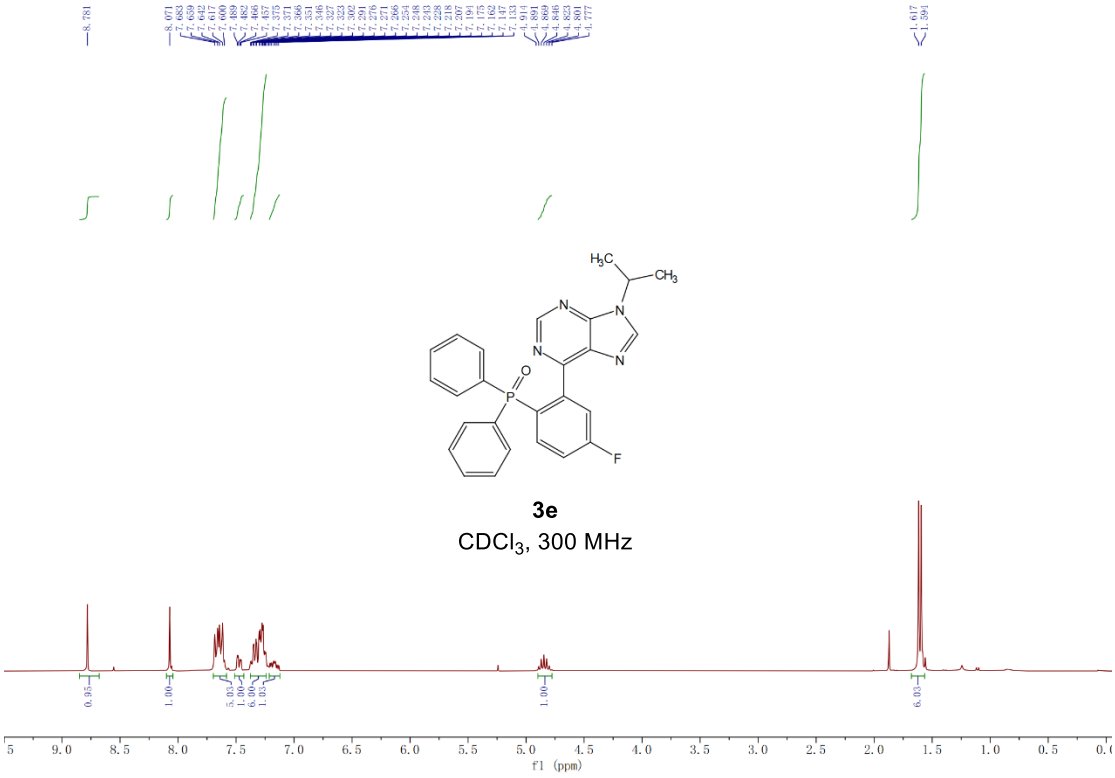
(2R,3R,4R,5R)-2-(Acetoxymethyl)-5-(6-(2-(diphenylphosphoryl)phenyl)-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate (**3d**)

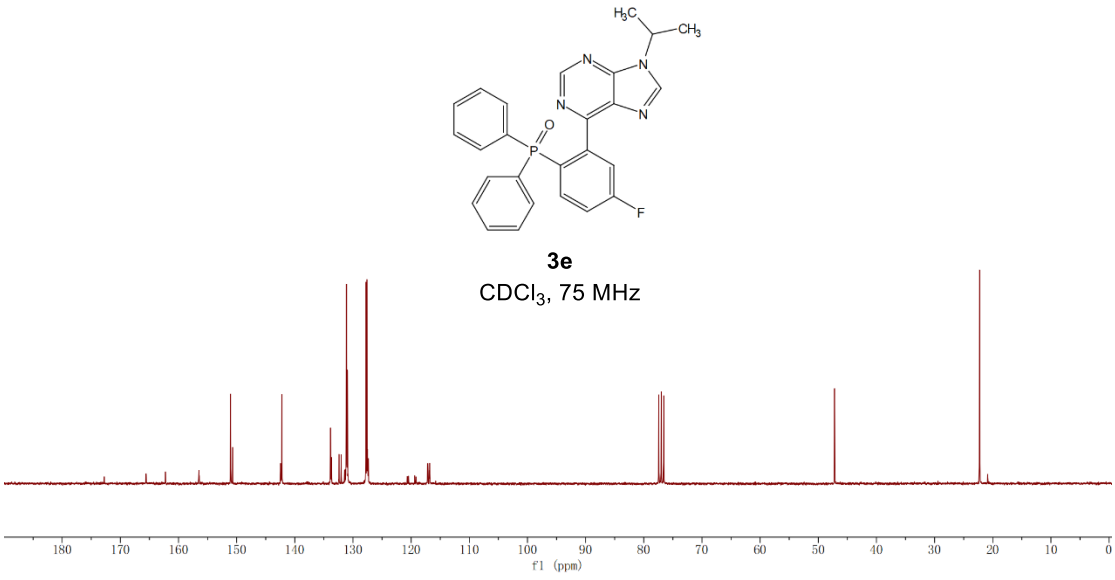


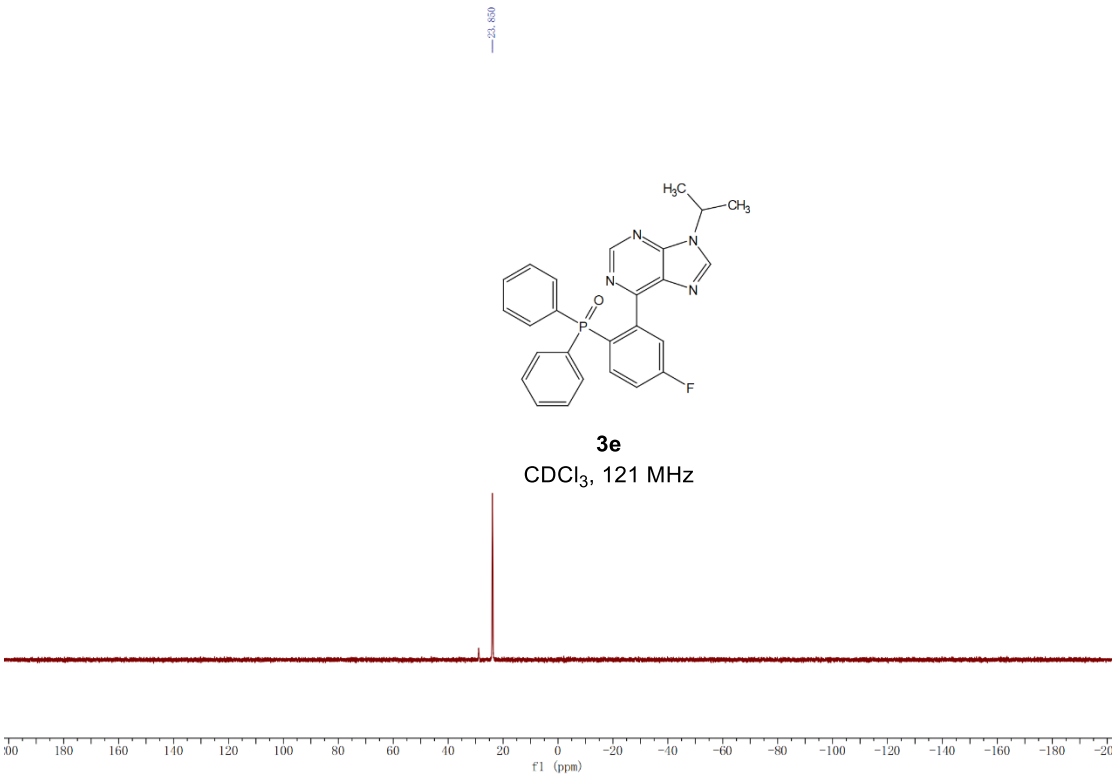

3d
CDCl3, 75 MHz
f1 (ppm)


3d
CDCl3, 121 MHz
f1 (ppm)

(4-Fluoro-2-(9-isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3e**)

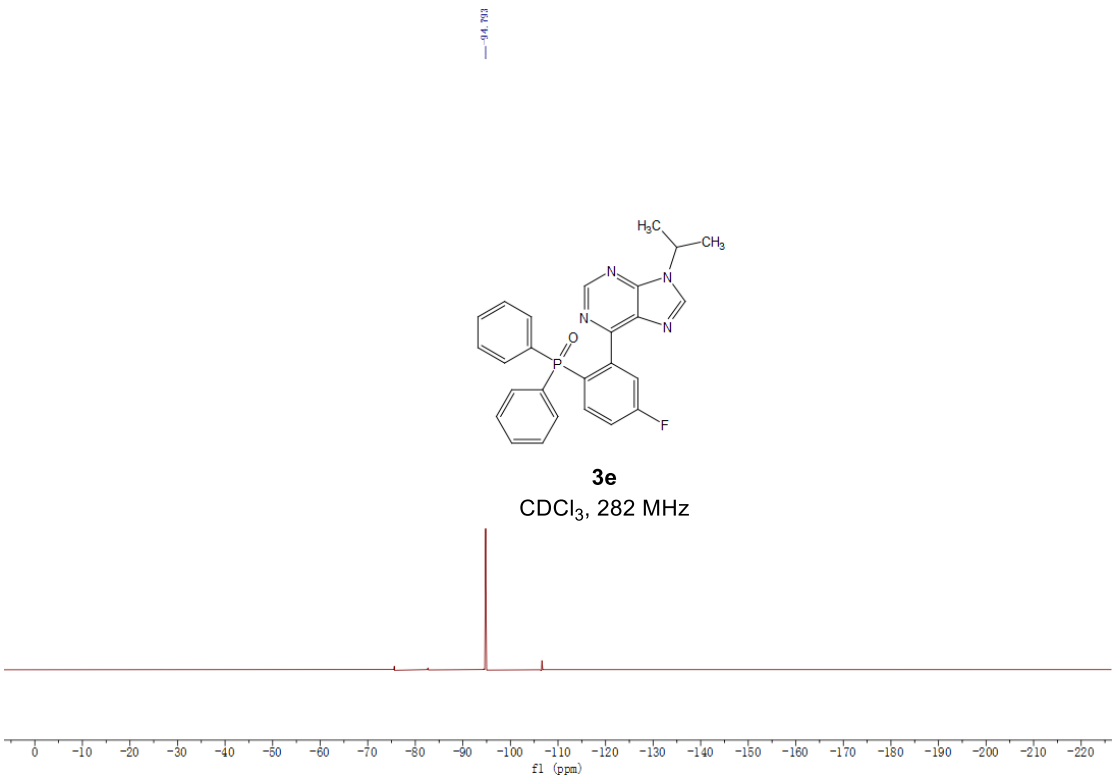






3e

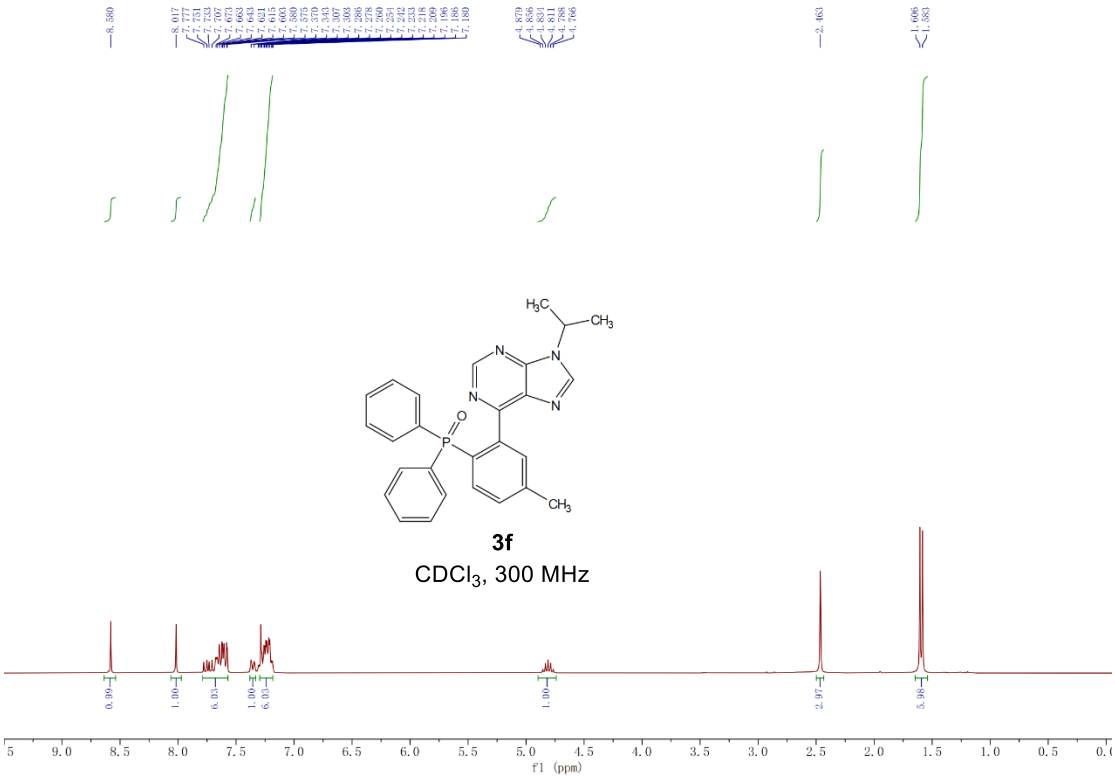
$CDCl_3$, 121 MHz

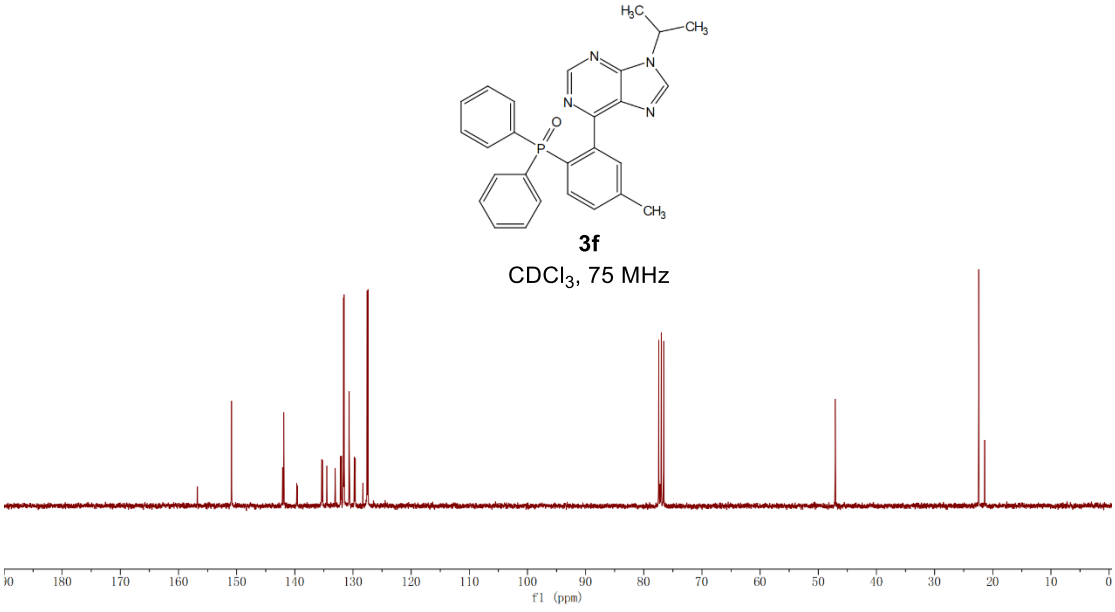


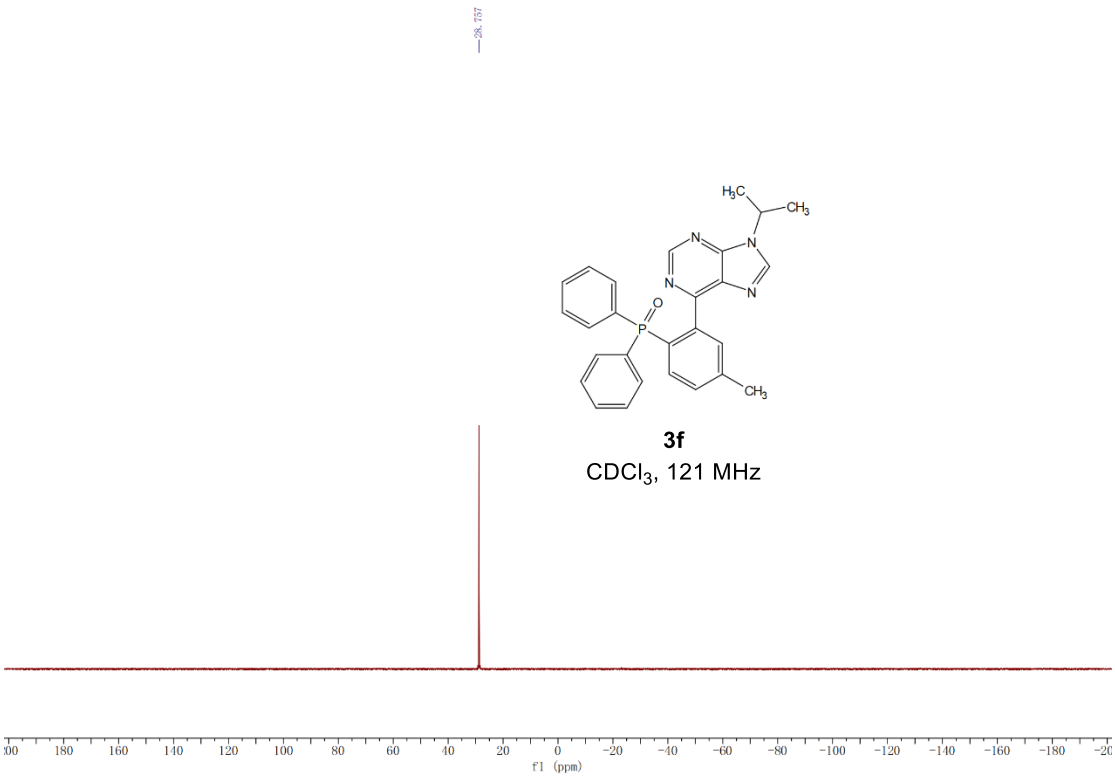
3e

$CDCl_3$, 282 MHz

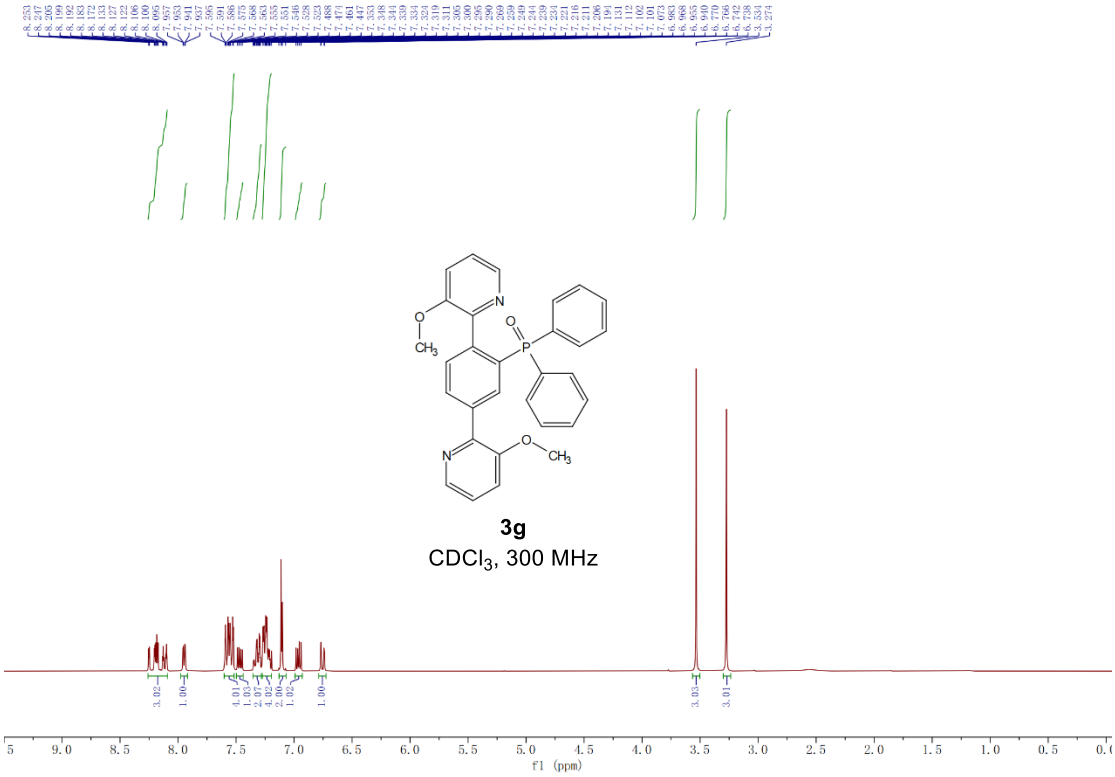
(2-(9-Isopropyl-9H-purin-6-yl)-4-methylphenyl)diphenylphosphine oxide (**3f**)

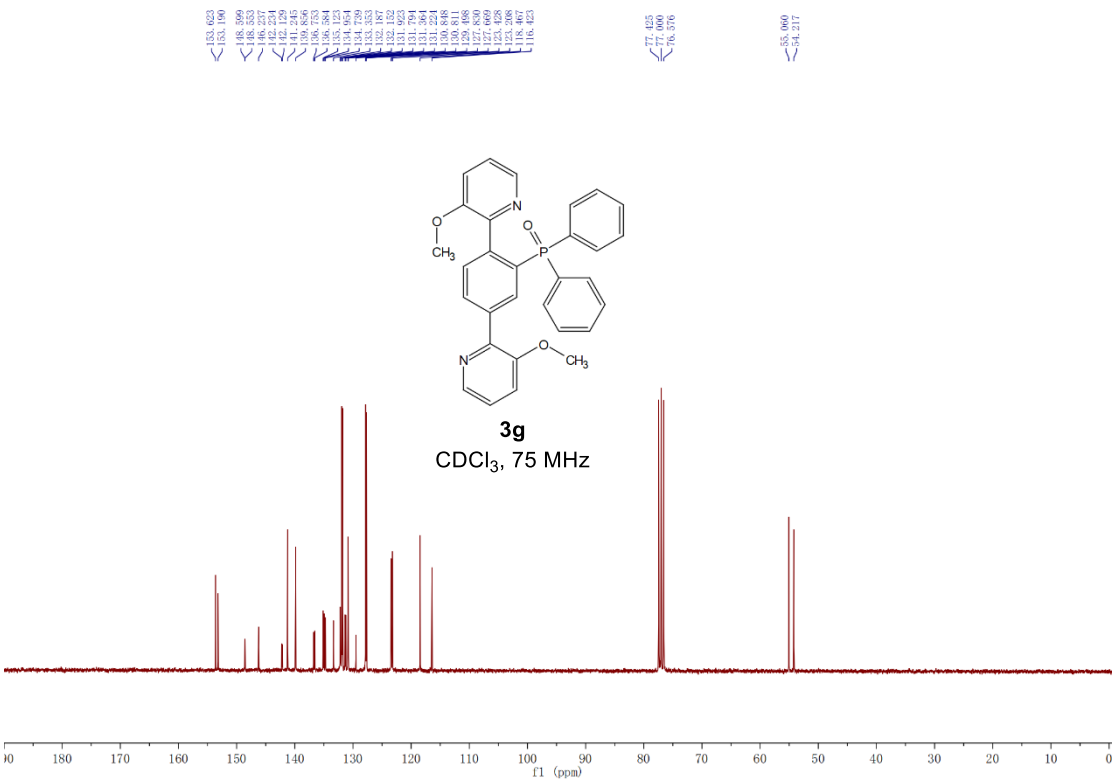


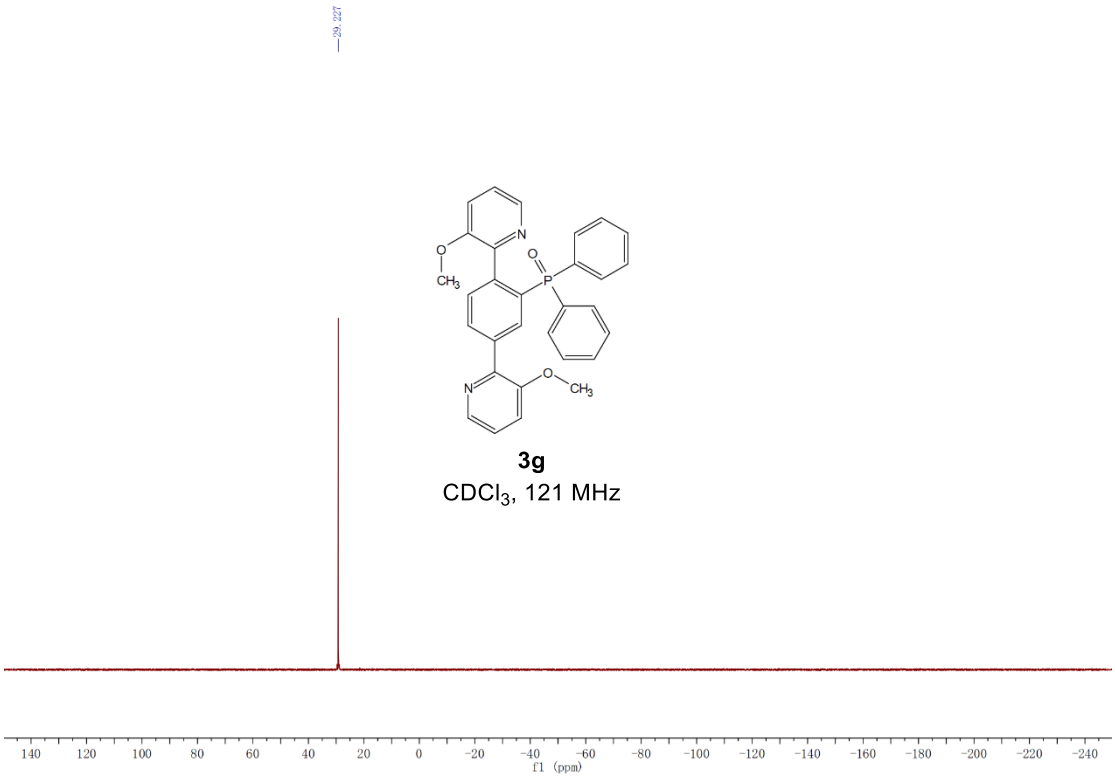




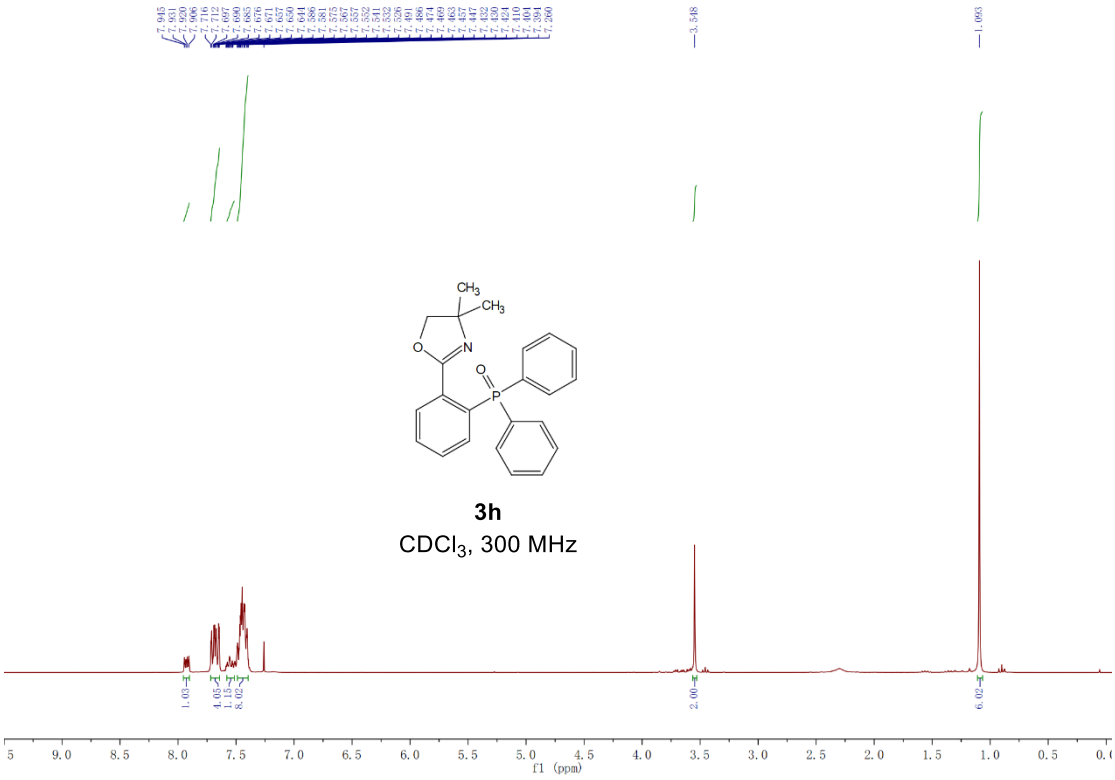
(2,5-Bis(3-methoxypyridin-2-yl)phenyl)diphenylphosphine oxide (**3g**)

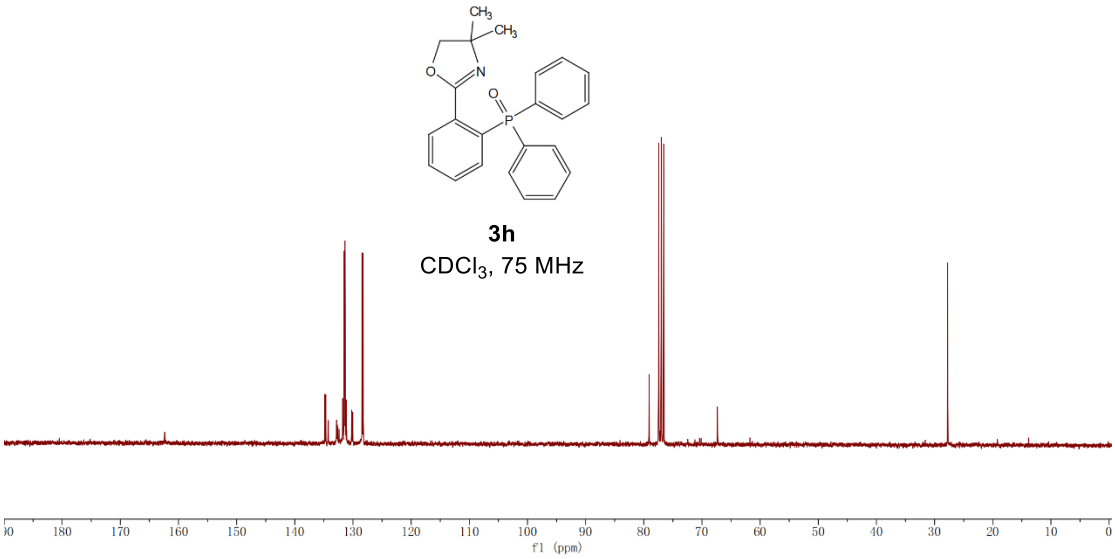


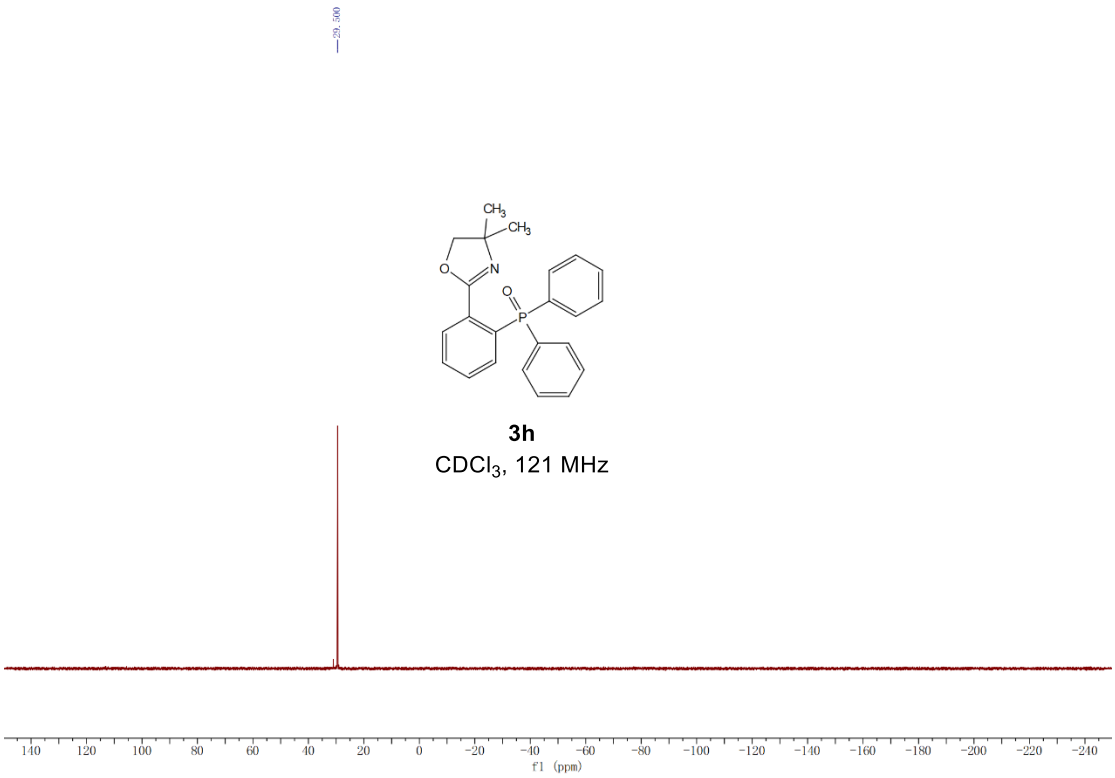

153.623
153.190
148.599
148.553
146.237
142.234
142.129
141.345
139.856
136.753
136.384
135.175
134.954
134.739
133.353
132.167
132.152
131.923
131.794
131.564
131.293
130.848
130.811
129.498
127.856
127.669
123.428
123.208
118.467
116.423
77.425
77.000
76.576
55.060
54.217
3g
CDCl3, 75 MHz
f1 (ppm)


29.227
3g
CDCl3, 121 MHz
f1 (ppm)

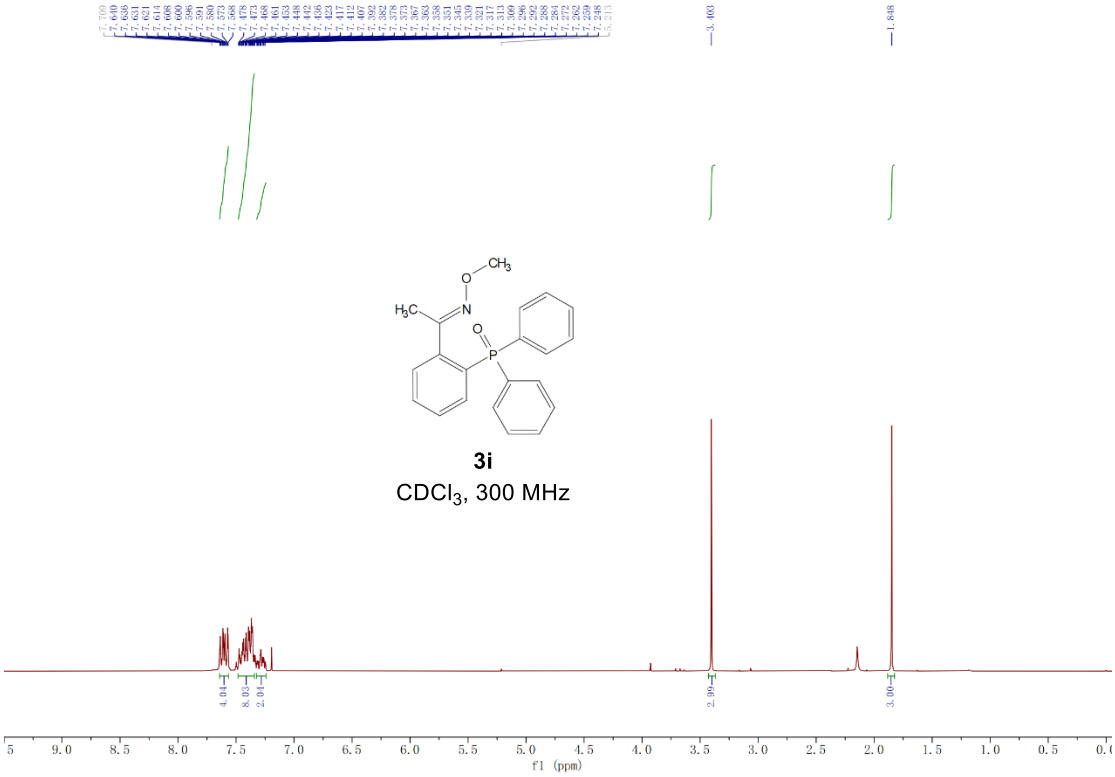
(2-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenyl)diphenylphosphine oxide (**3h**)

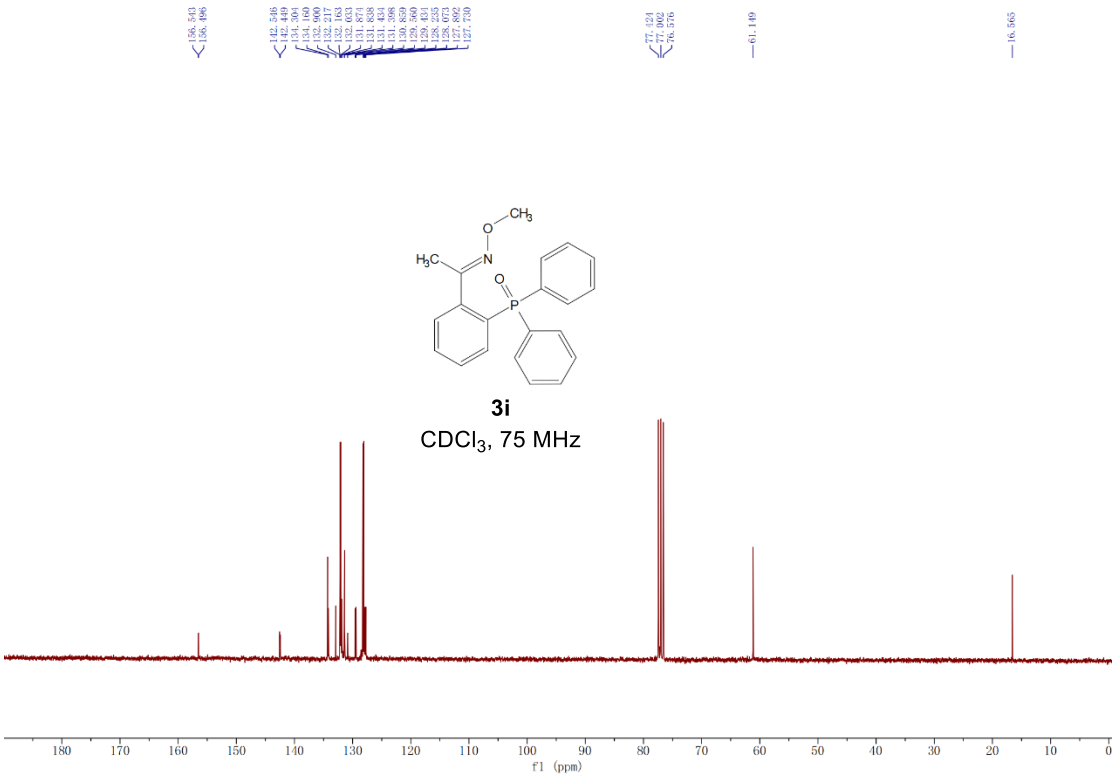






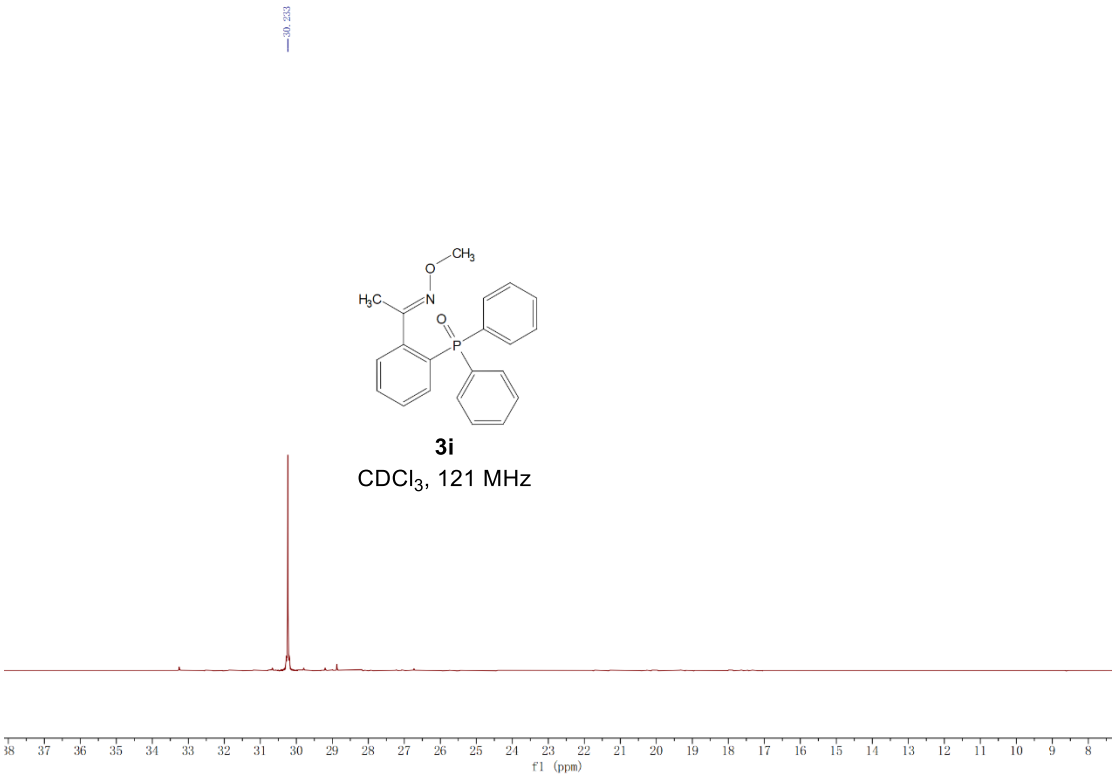
(E)-(2-(1-(Methoxyimino)ethyl)phenyl)diphenylphosphine oxide (3**i**)





3i

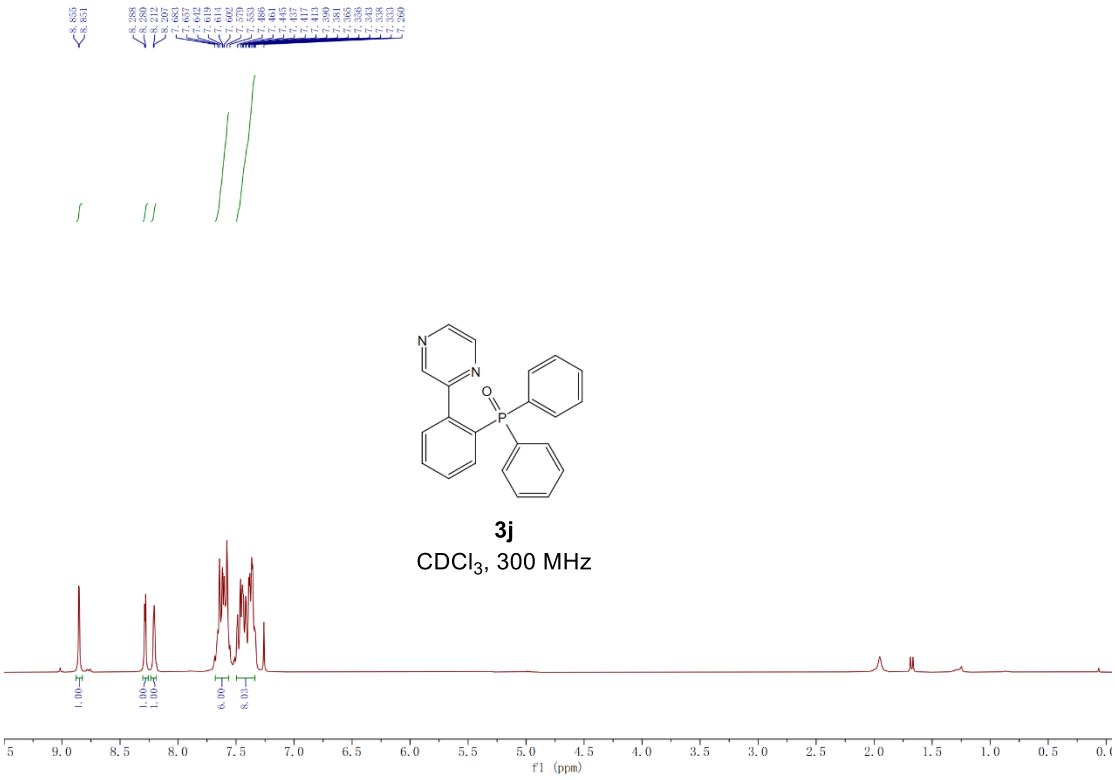
$CDCl_3$, 75 MHz

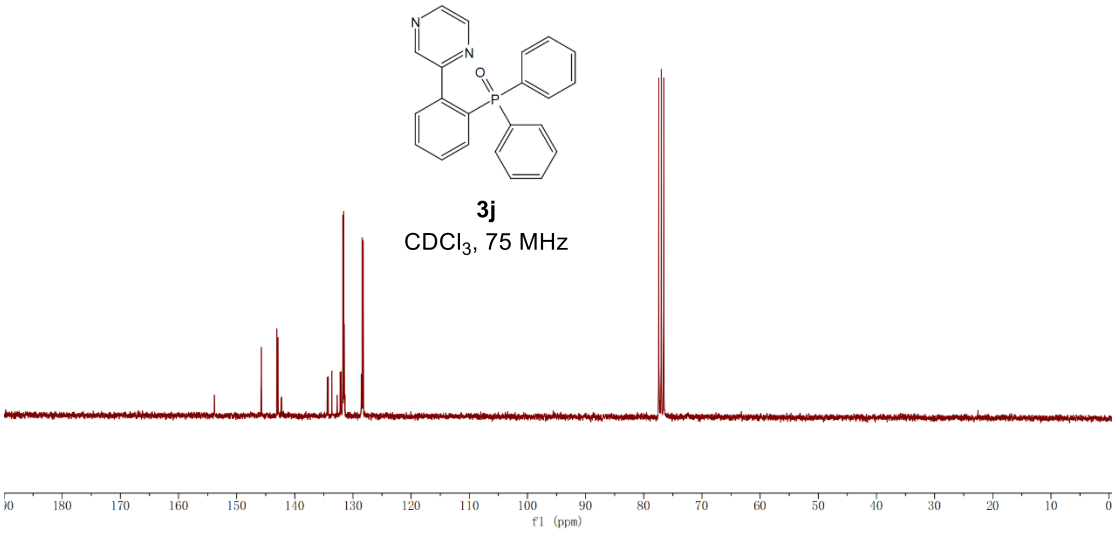


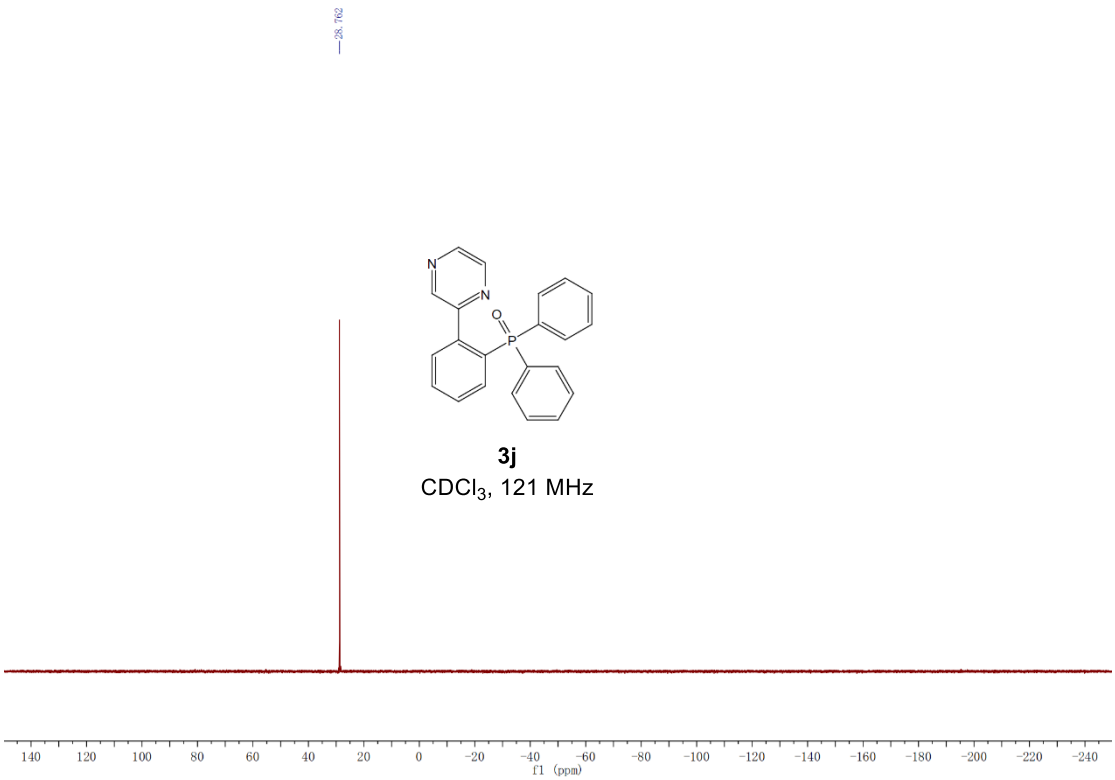
3i

$CDCl_3$, 121 MHz

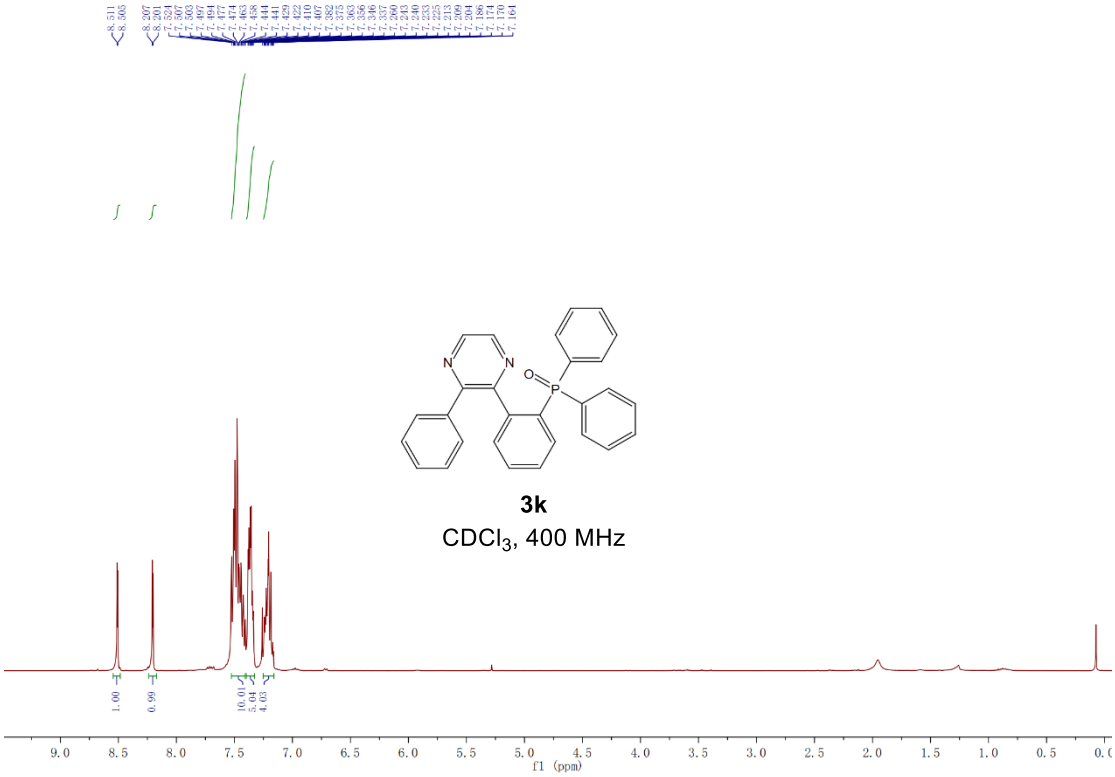
Diphenyl(2-(pyrazin-2-yl)phenyl)phosphine oxide (**3j**)

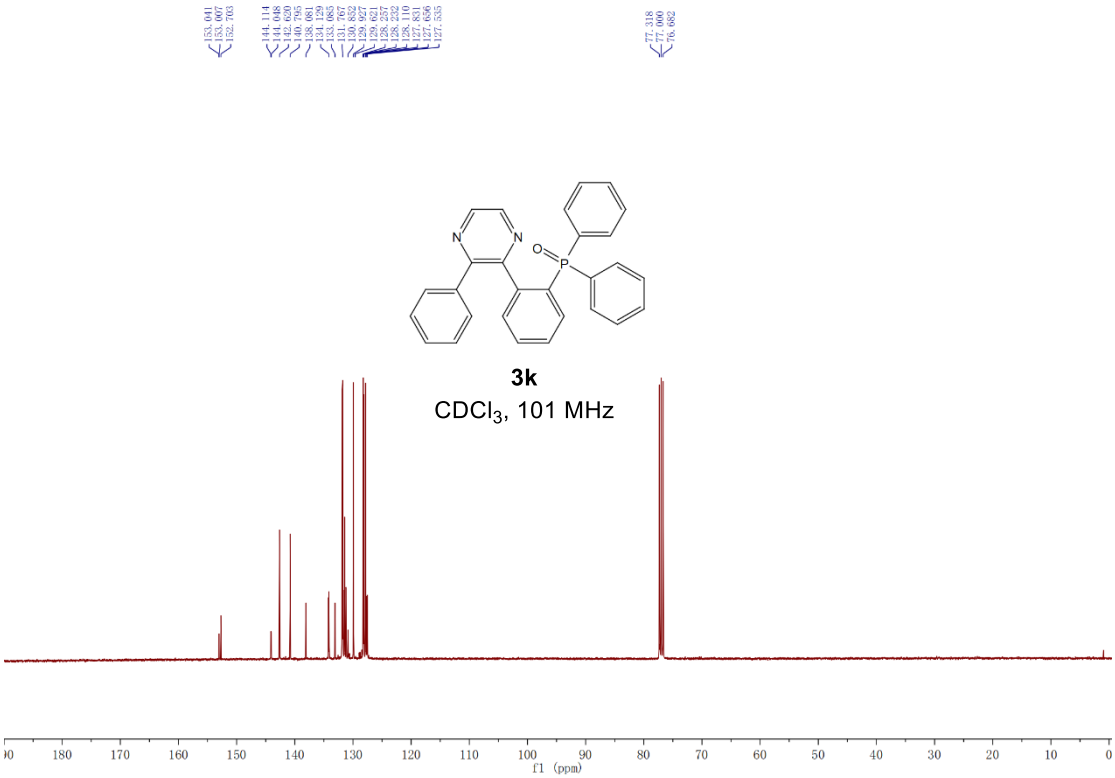


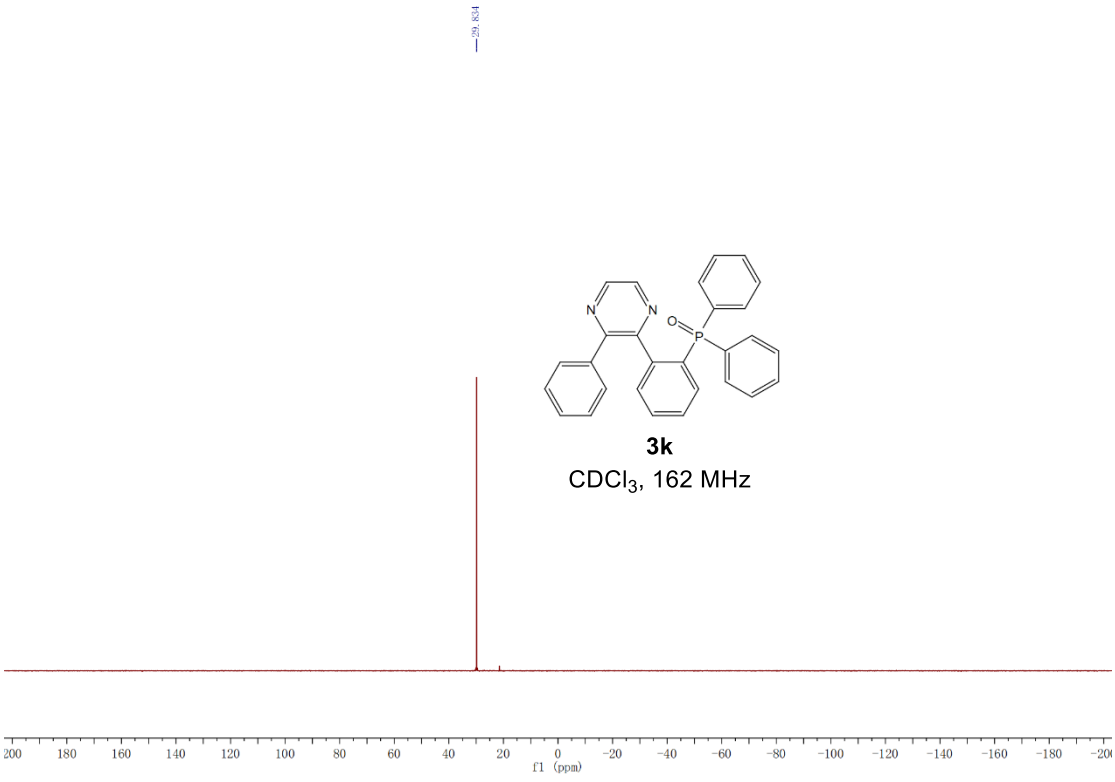




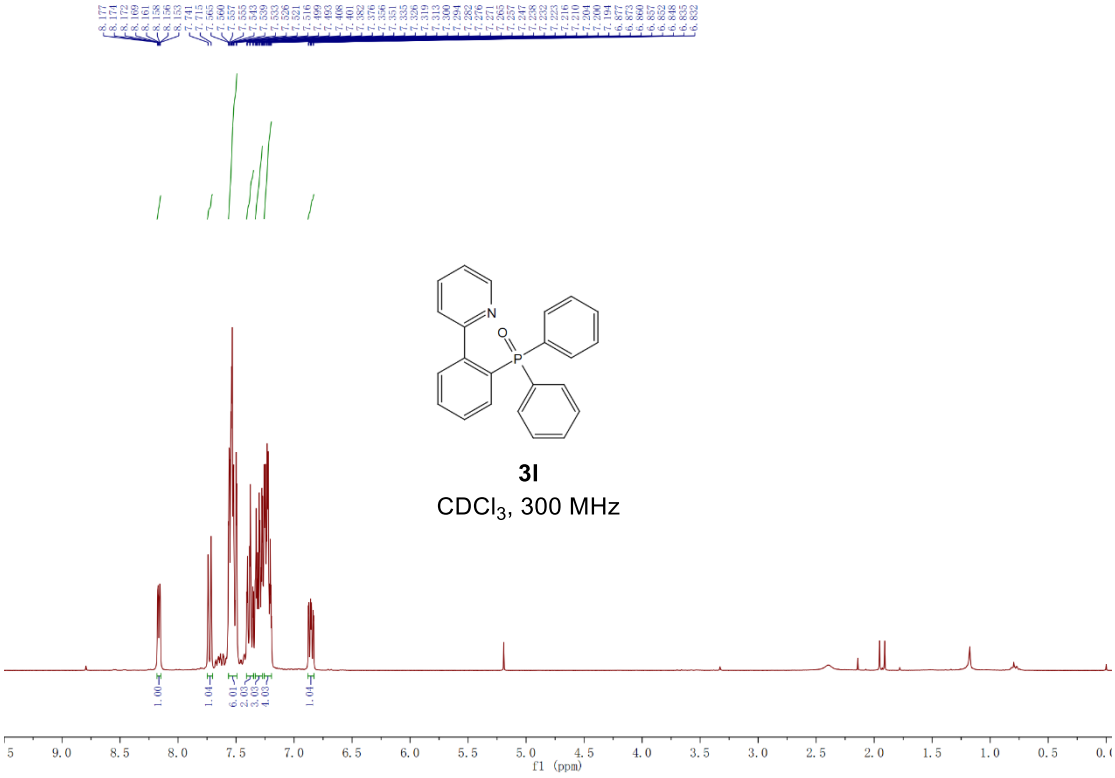
Diphenyl(2-(3-phenylpyrazin-2-yl)phenyl)phosphine oxide (**3k**)

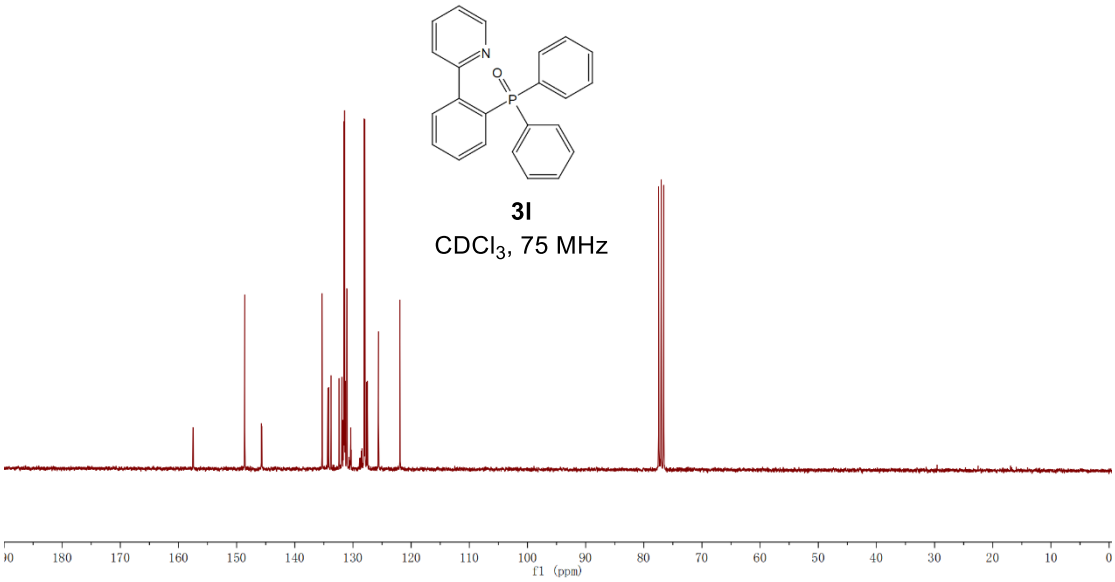


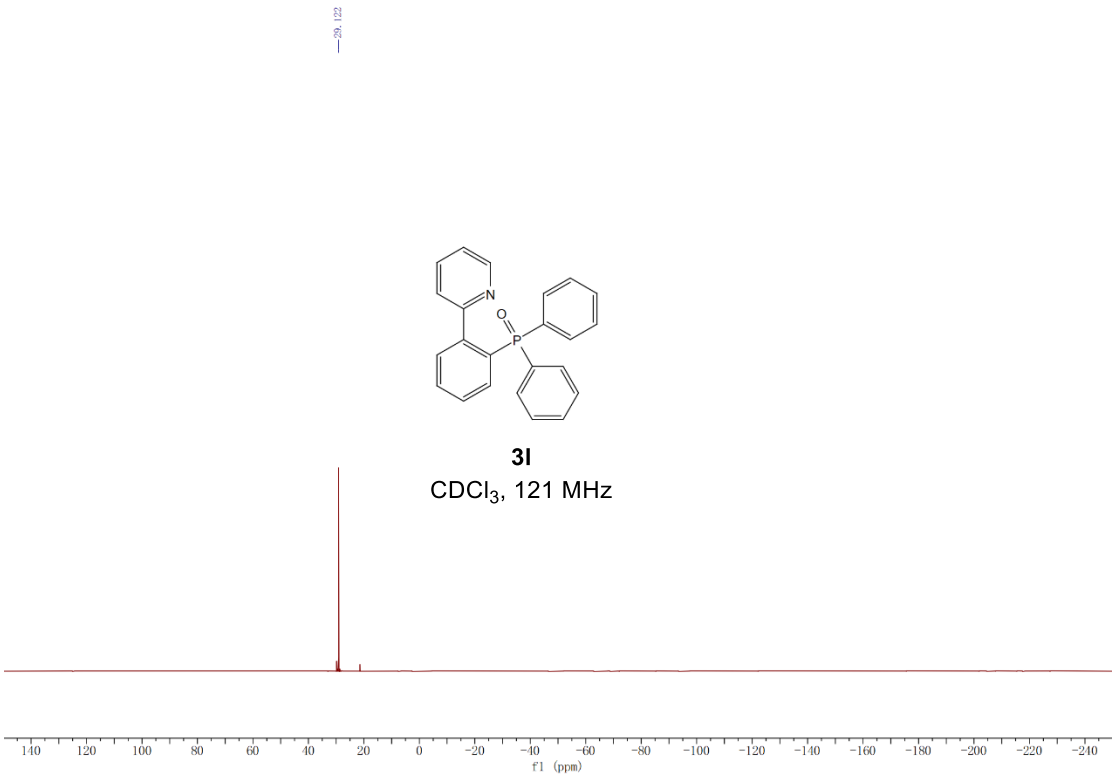

153.041
153.067
152.703
144.114
144.048
142.620
140.795
138.661
134.129
133.685
131.767
130.852
129.927
129.621
128.257
128.232
128.110
127.831
127.656
127.535
77.318
77.000
76.682
N
N
O
P
3k
CDCl3, 101 MHz
f1 (ppm)


29.834
N
N
O
P
3k
CDCl3, 162 MHz
f1 (ppm)

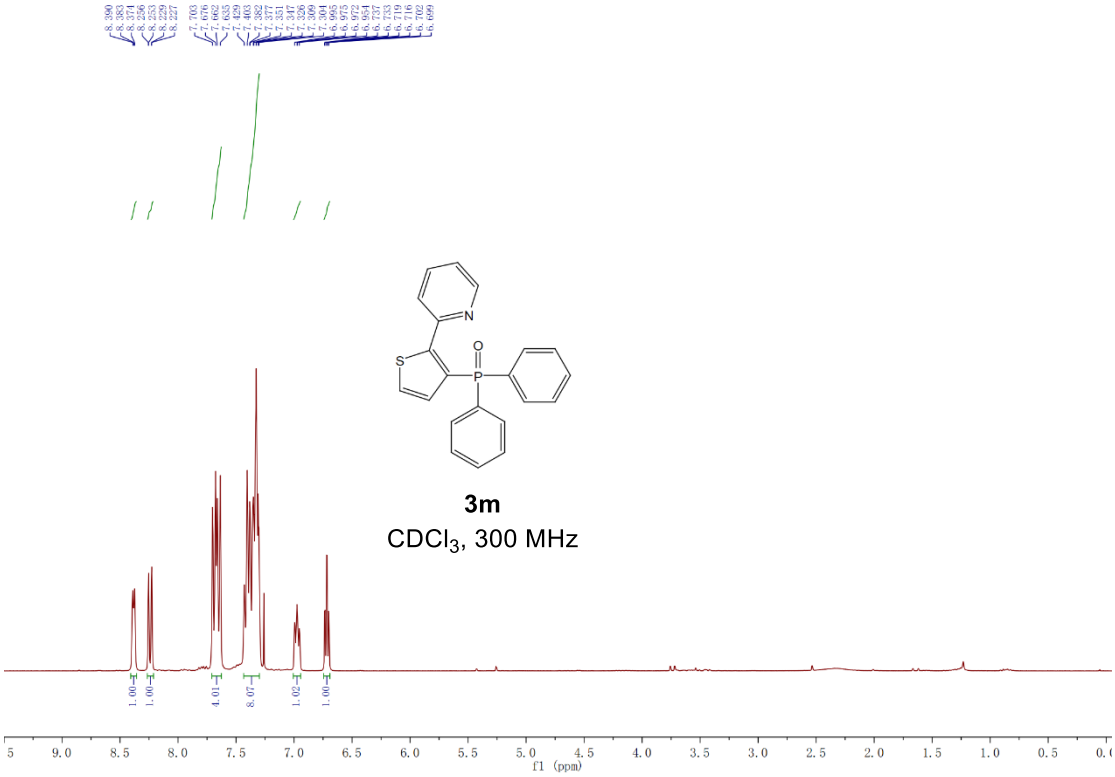
Diphenyl(2-(pyridin-2-yl)phenyl)phosphine oxide (**3l**)

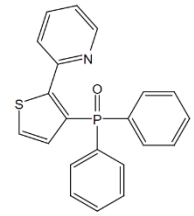






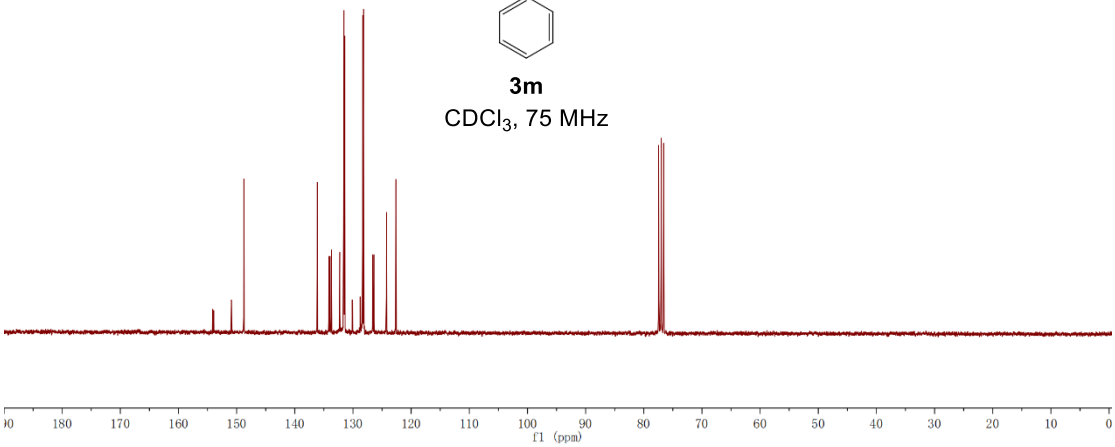
Diphenyl(2-(pyridin-2-yl)thiophen-3-yl)phosphine oxide (**3m**)

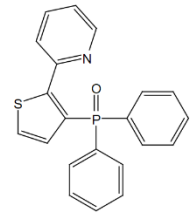




3m

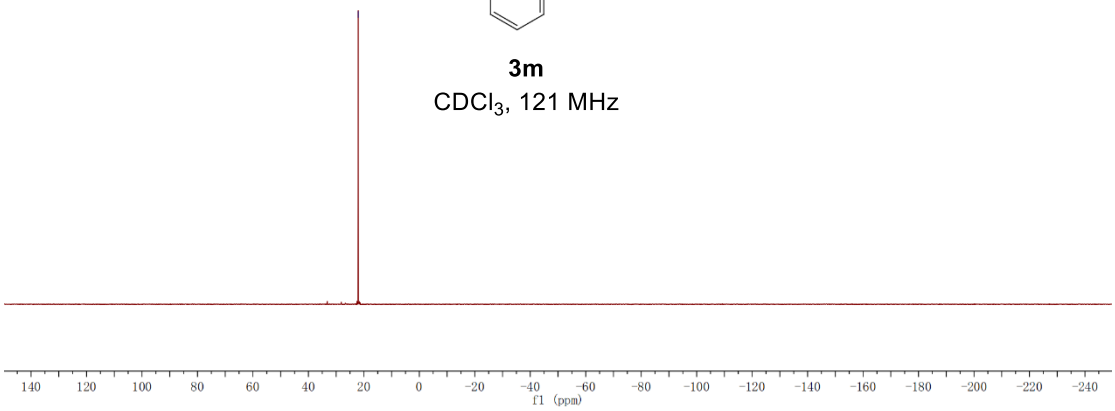
$CDCl_3$, 75 MHz



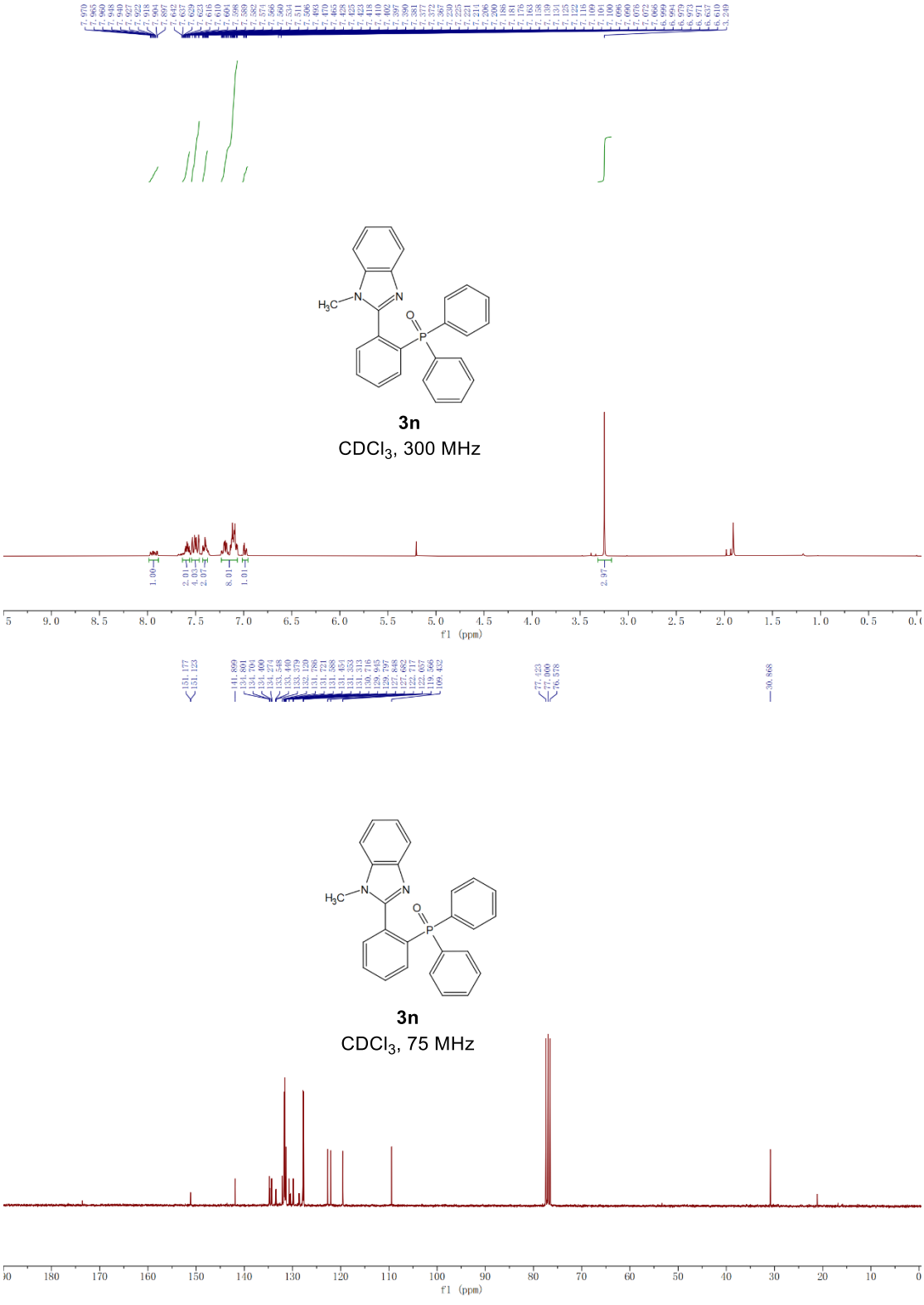


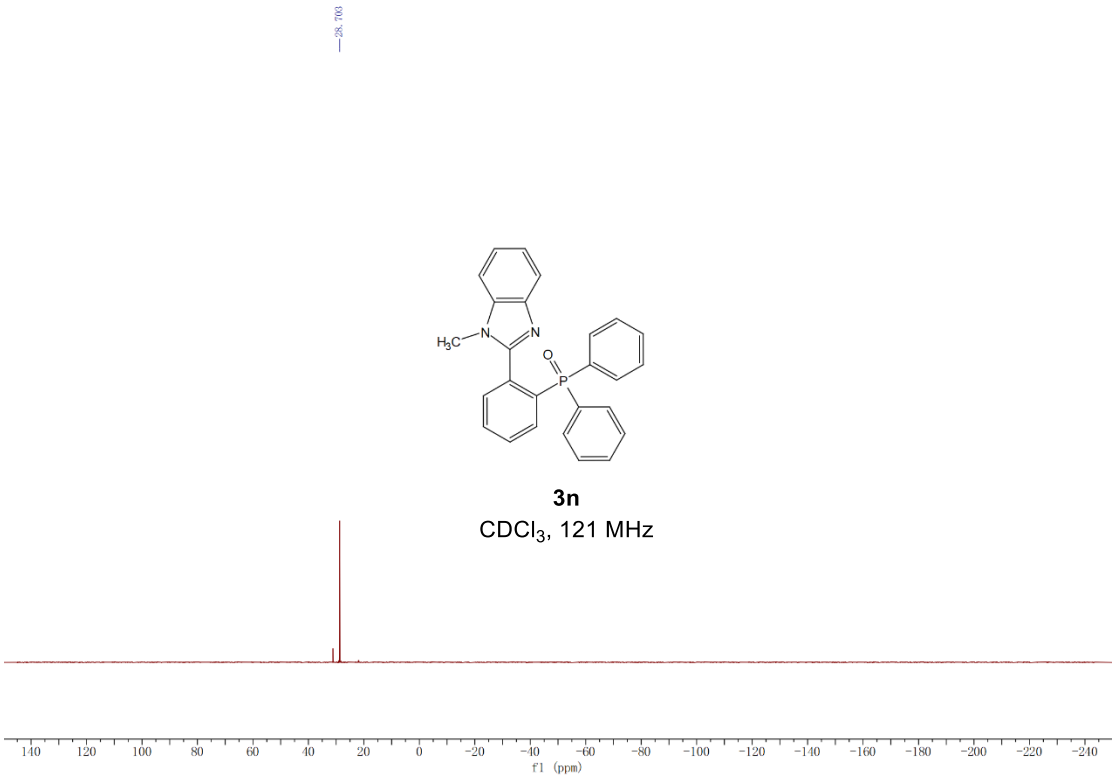
3m

$CDCl_3$, 121 MHz

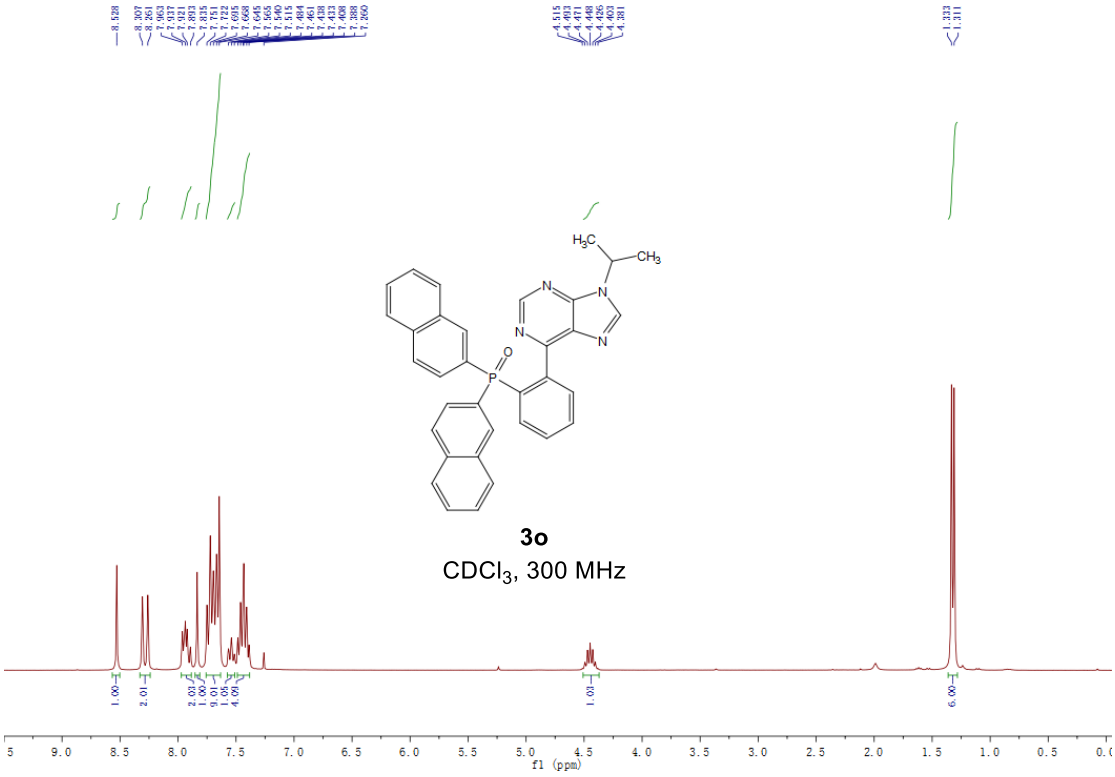


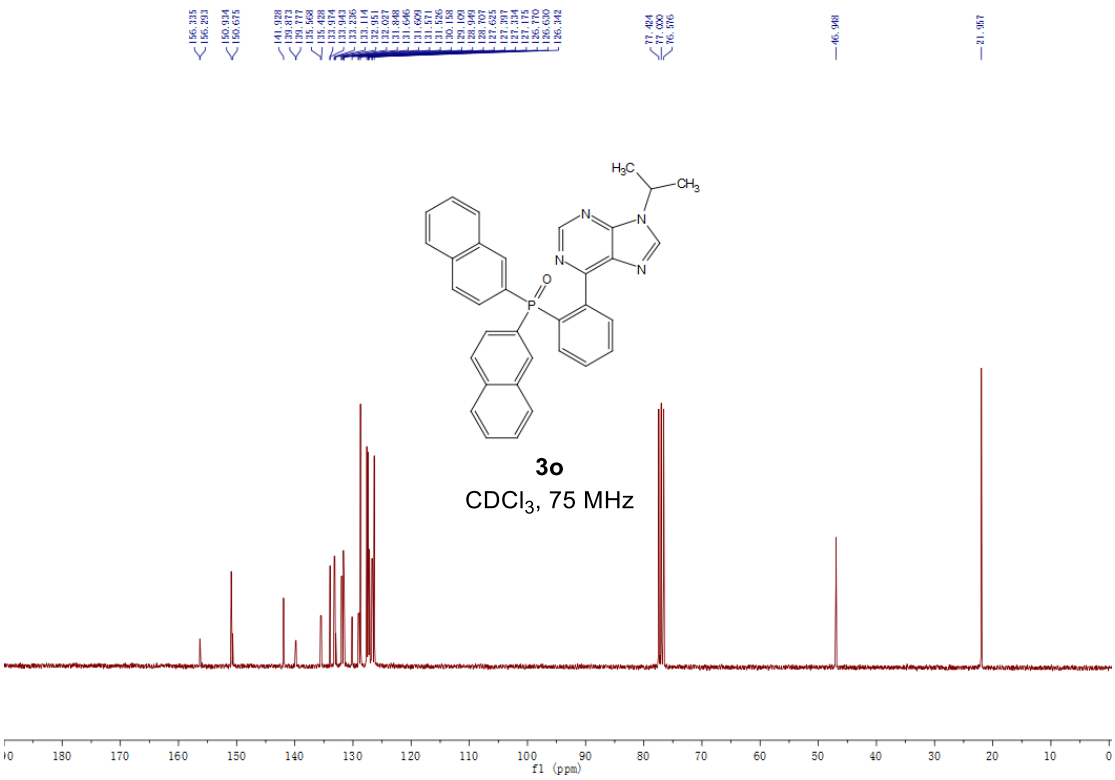
(2-(1-methyl-1H-benzo[d]imidazol-2-yl)phenyl)diphenylphosphine oxide (**3n**)





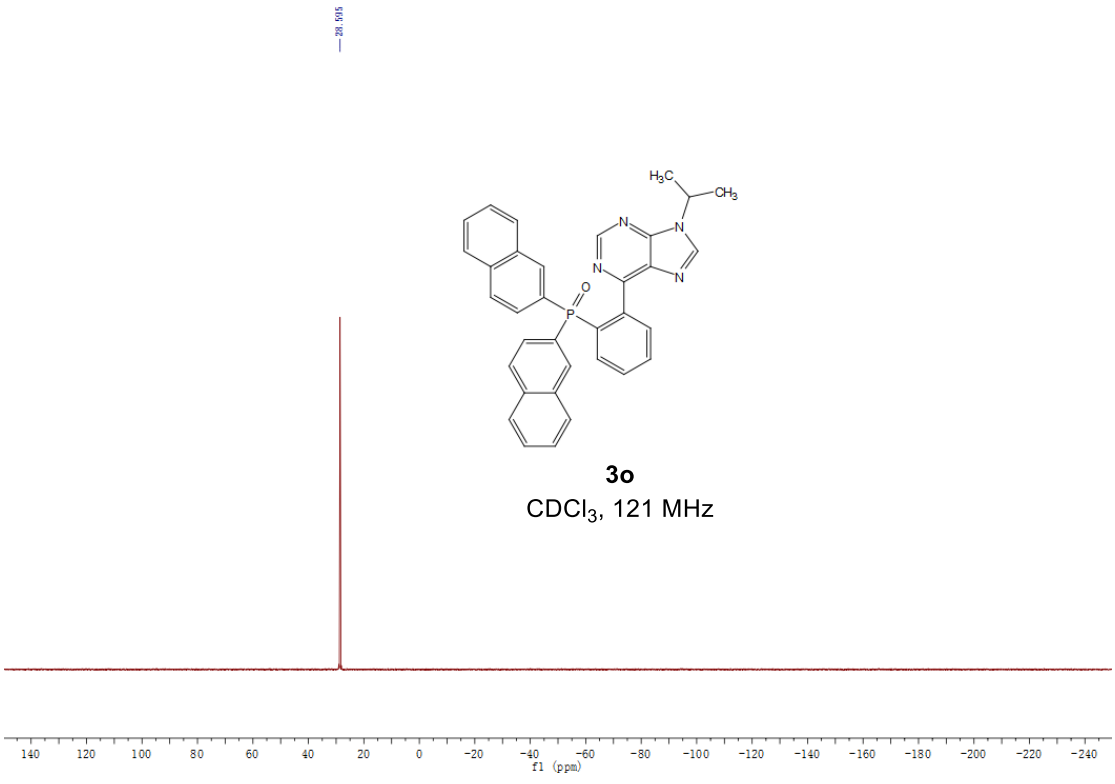
(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di(naphthalen-2-yl)phosphine oxide (**3o**)





3o

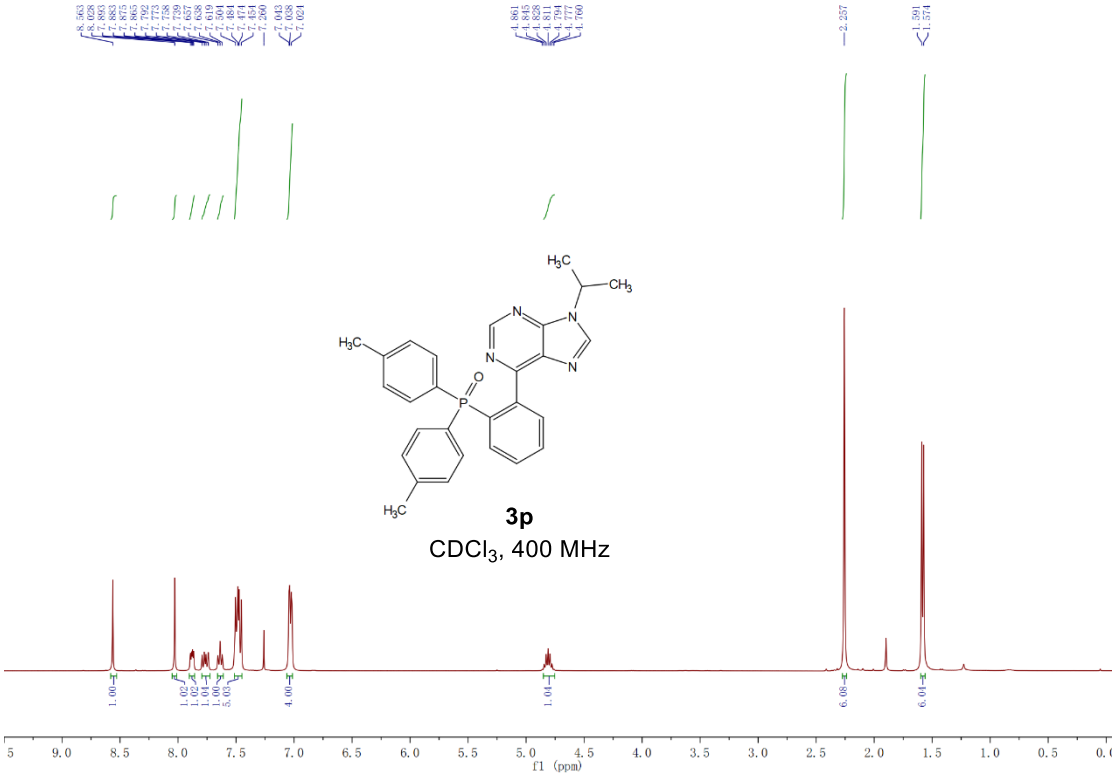
$CDCl_3$, 75 MHz

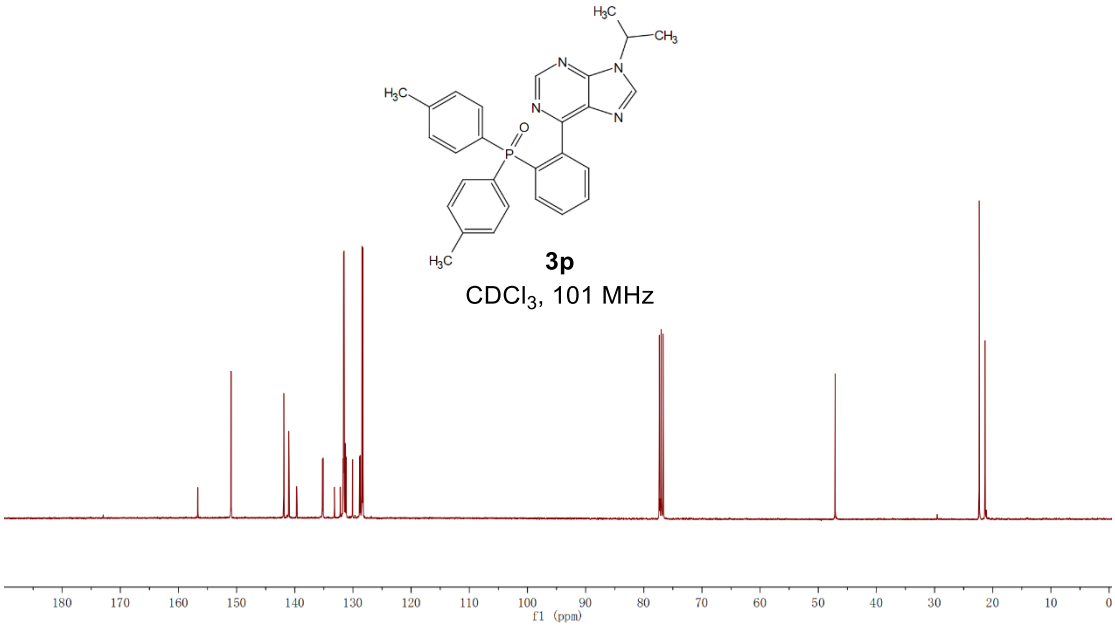


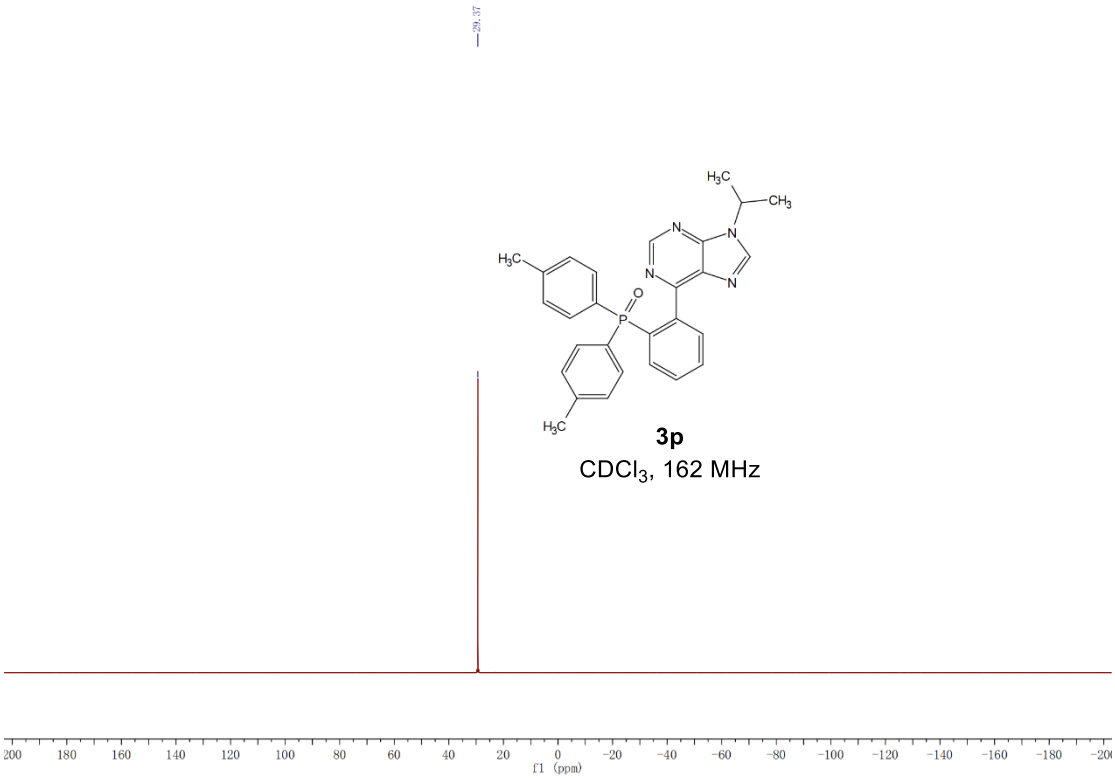
3o

$CDCl_3$, 121 MHz

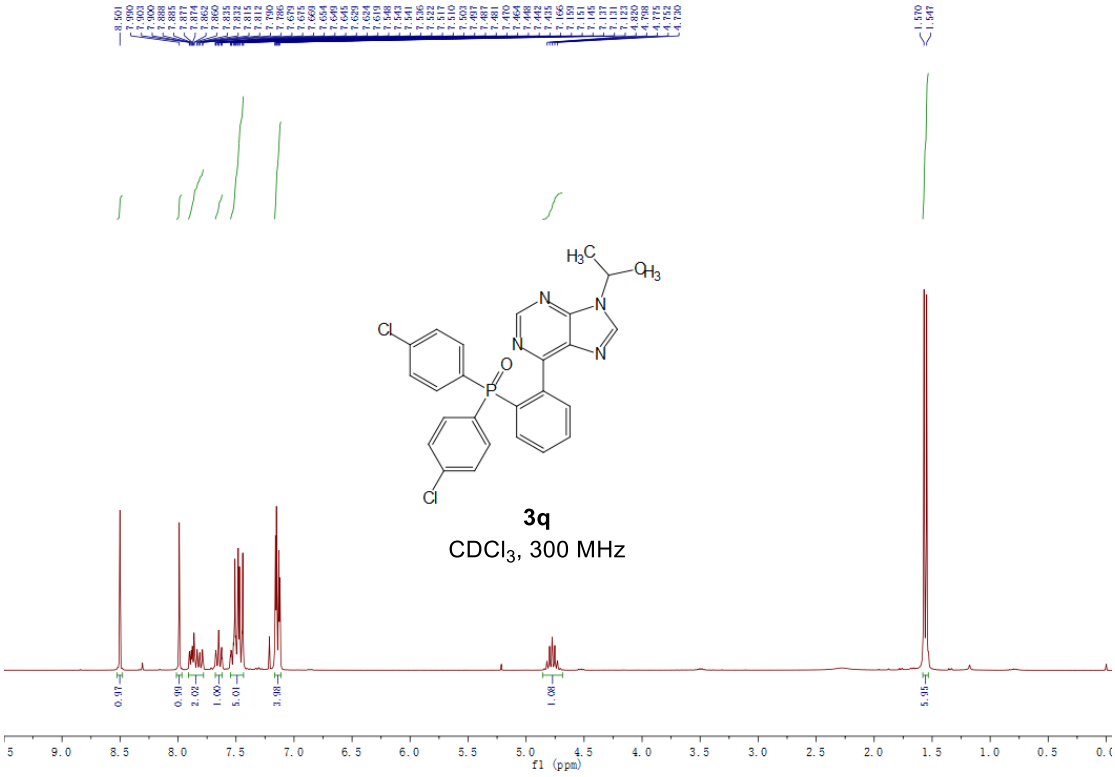
(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di-p-tolylphosphine oxide (**3p**)

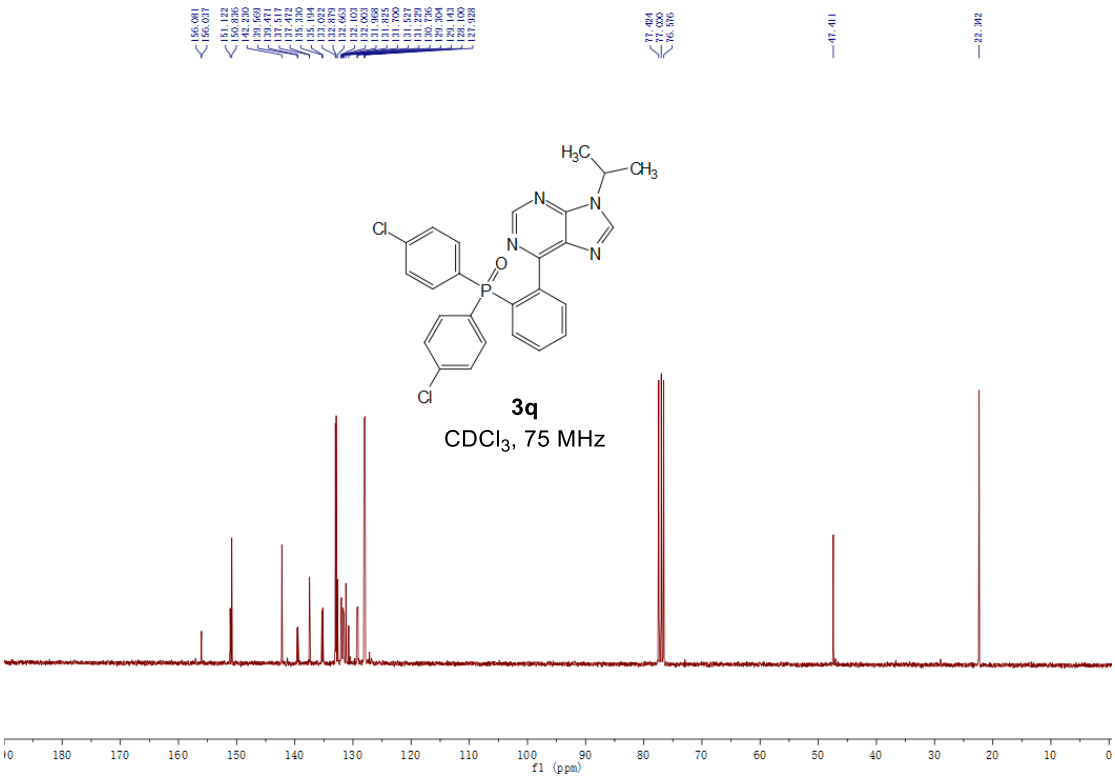


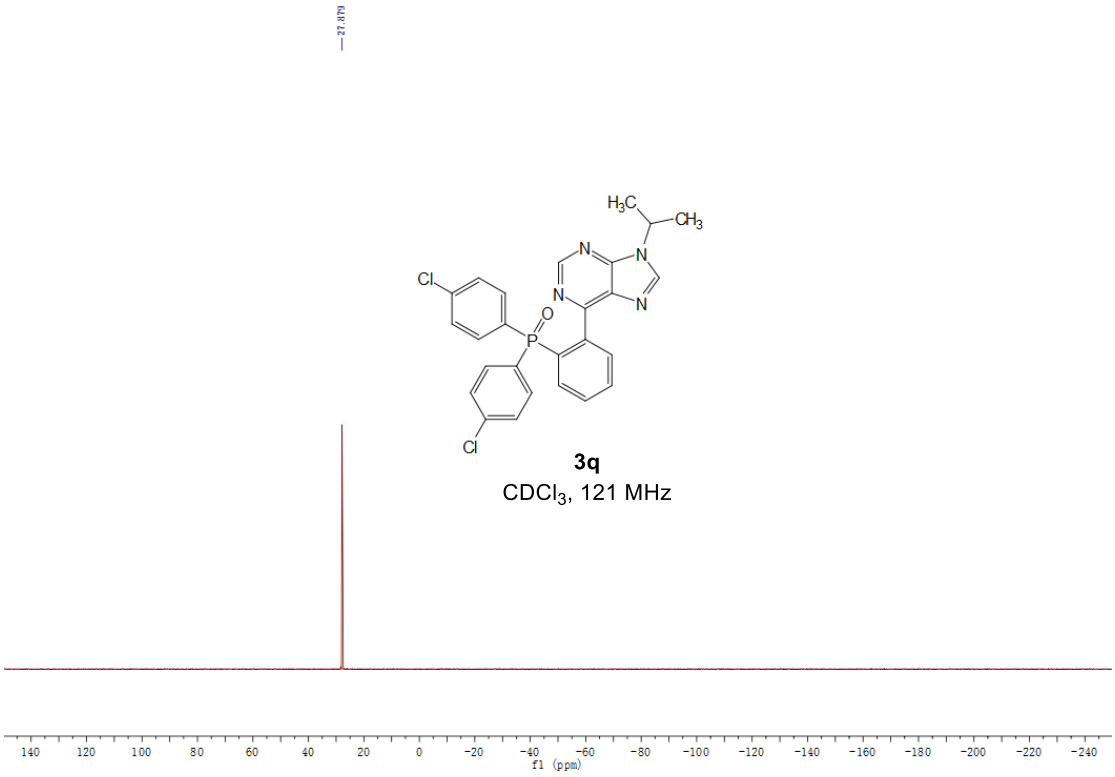




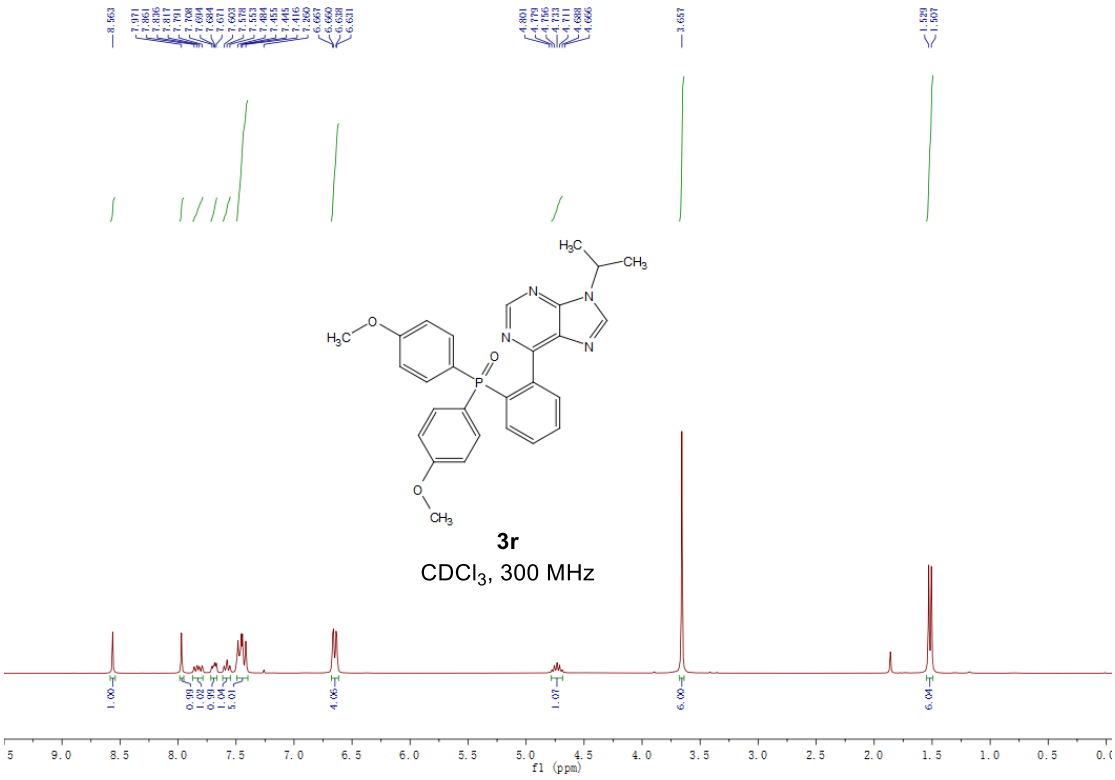
Bis(4-chlorophenyl)(2-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**3q**)

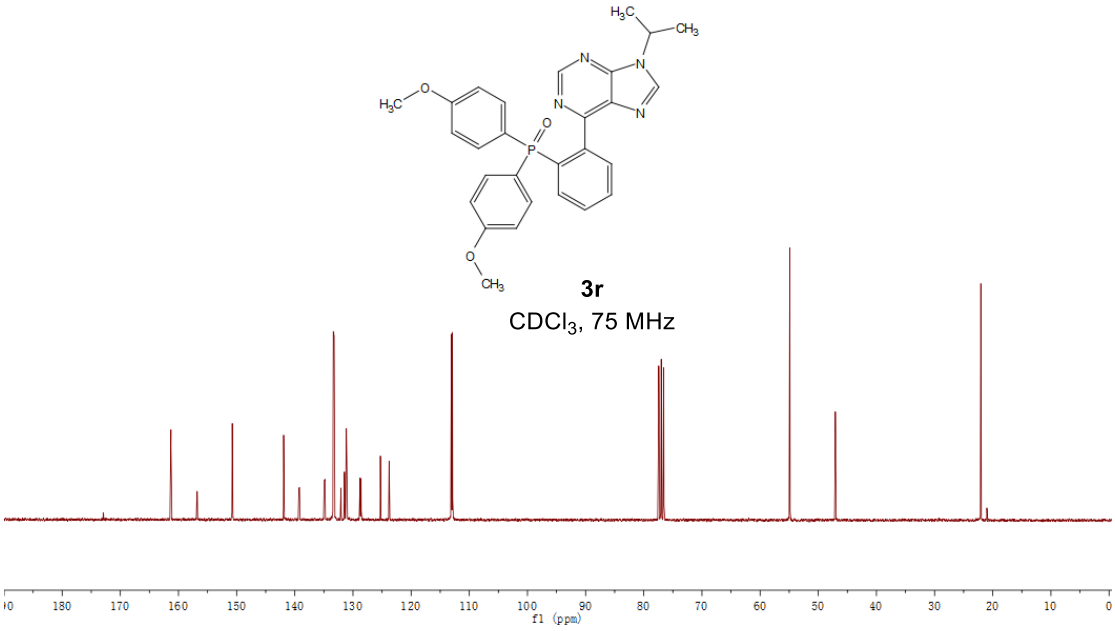


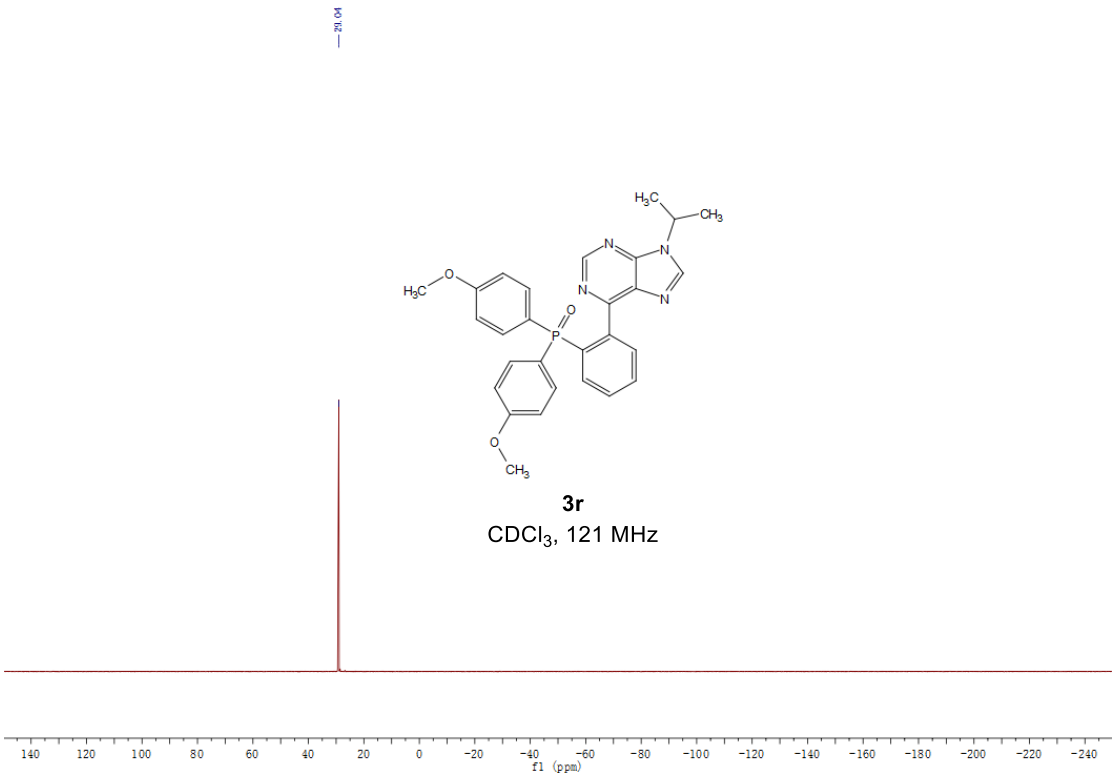

156.081
156.037
151.122
150.836
142.230
139.569
139.447
137.517
137.472
135.330
135.014
135.024
132.879
132.663
132.103
132.060
131.968
131.825
131.700
131.337
131.229
130.736
129.304
129.143
128.109
127.928
77.404
77.000
76.596
47.411
22.942
Cl
Cl
O
P
N
N
N
N
H3C
CH3
3q
CDCl3, 75 MHz
f1 (ppm)


27.879
Cl
Cl
O
P
N
N
N
N
H3C
CH3
3q
CDCl3, 121 MHz
f1 (ppm)

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-methoxyphenyl)phosphine oxide (**3r**)



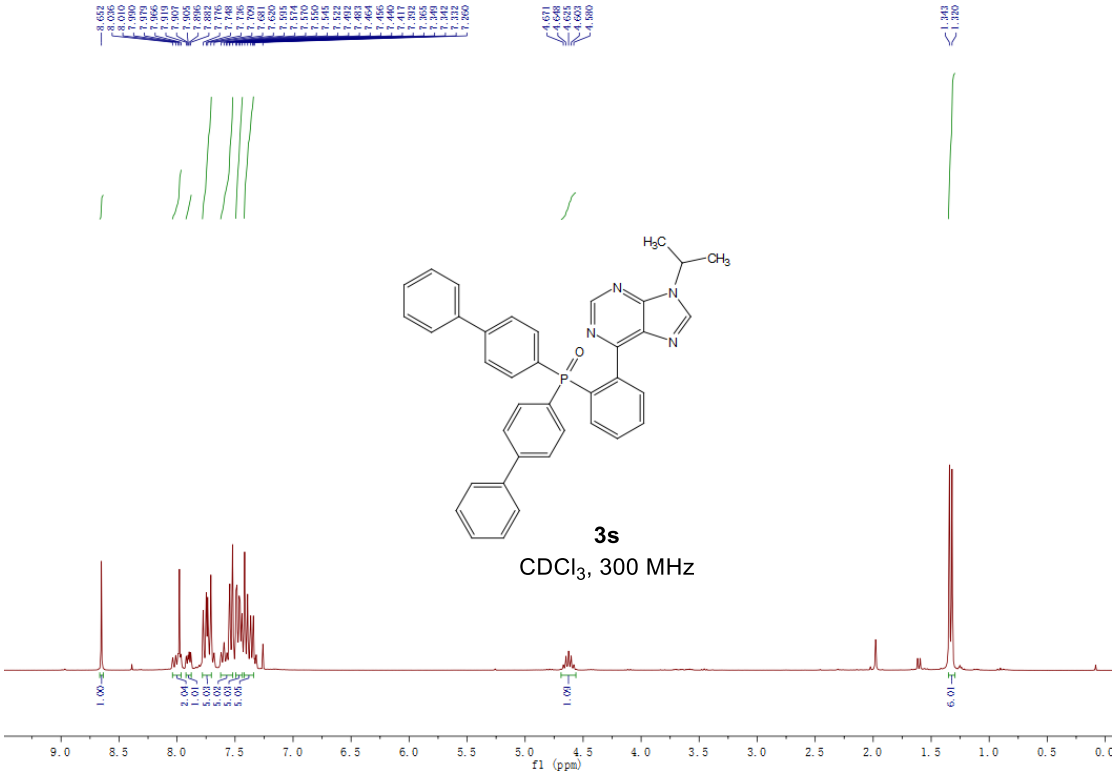




3r

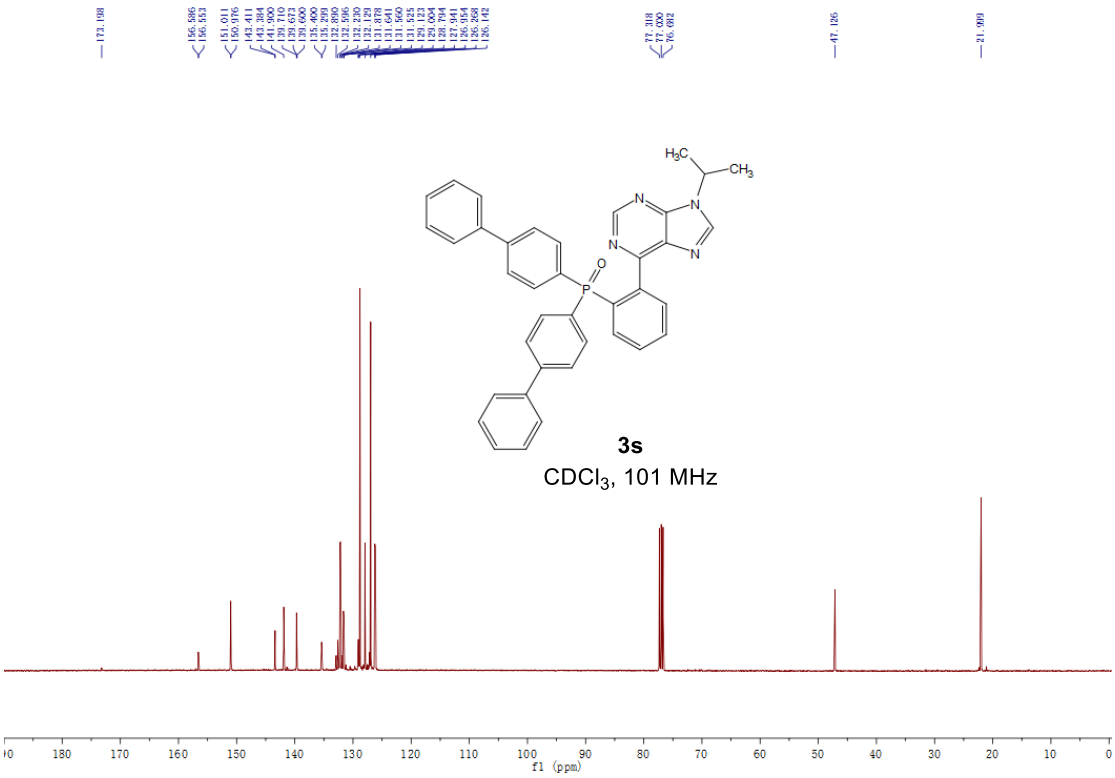
$CDCl_3$, 121 MHz

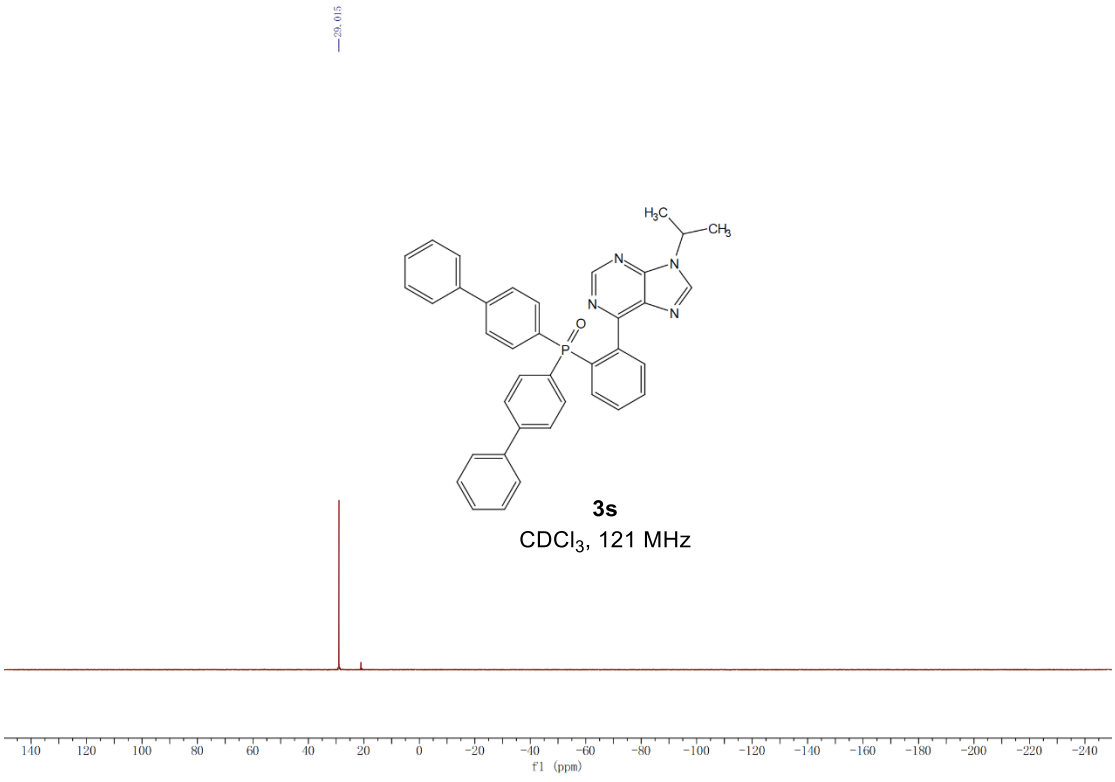
Di([1,1'-biphenyl]-4-yl)(2-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**3s**)



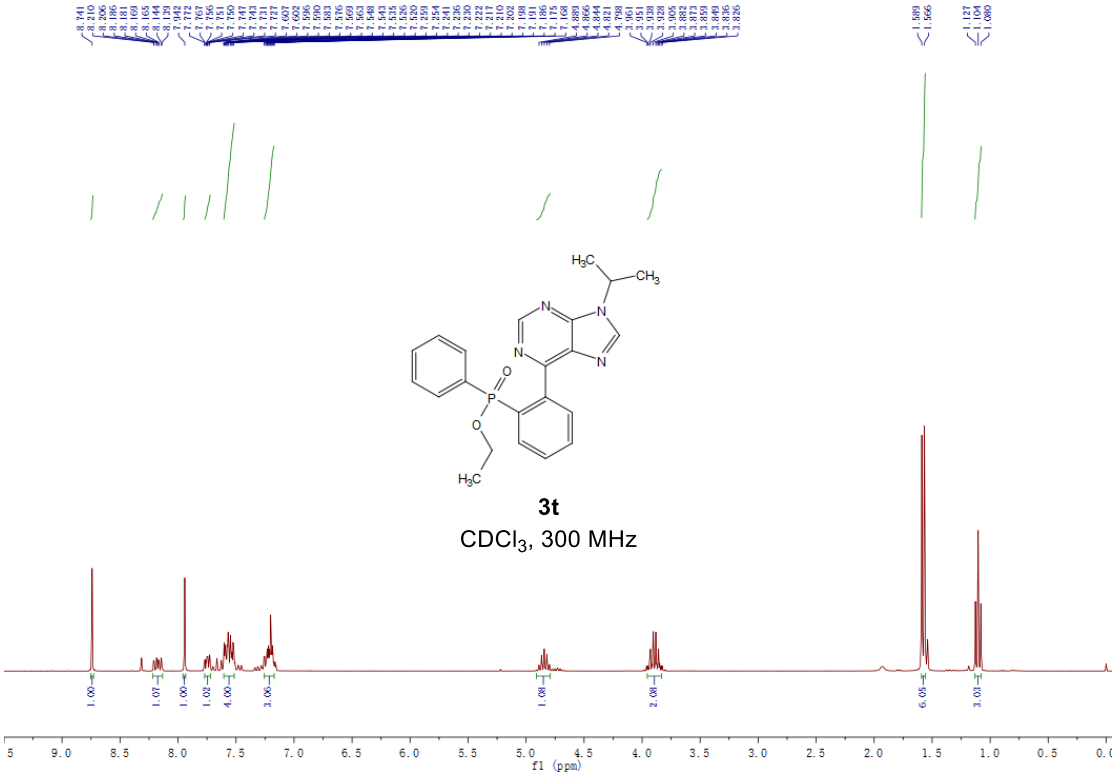
3s

$CDCl_3$, 300 MHz


173.198
156.586
156.553
151.011
150.976
143.411
143.384
141.900
139.710
139.673
139.600
135.490
135.390
132.890
132.596
132.230
132.123
131.938
131.641
131.560
131.525
129.213
129.004
128.794
127.941
126.954
126.268
126.142
77.318
77.000
76.682
47.126
21.999
H3C
CH3
N
N
N
N
O
P
3s
CDCl3, 101 MHz
f1 (ppm)

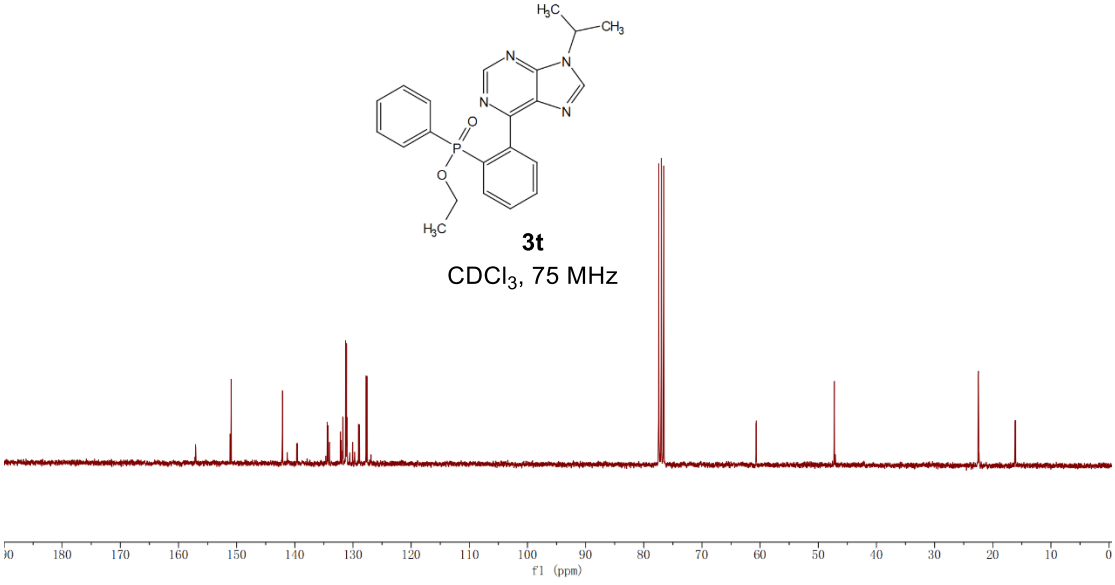

29.015
H3C
CH3
N
N
N
N
O
P
3s
CDCl3, 121 MHz
f1 (ppm)

Eethyl (2-(9-isopropyl-9H-purin-6-yl)phenyl)(phenyl)phosphinate (**3t**)



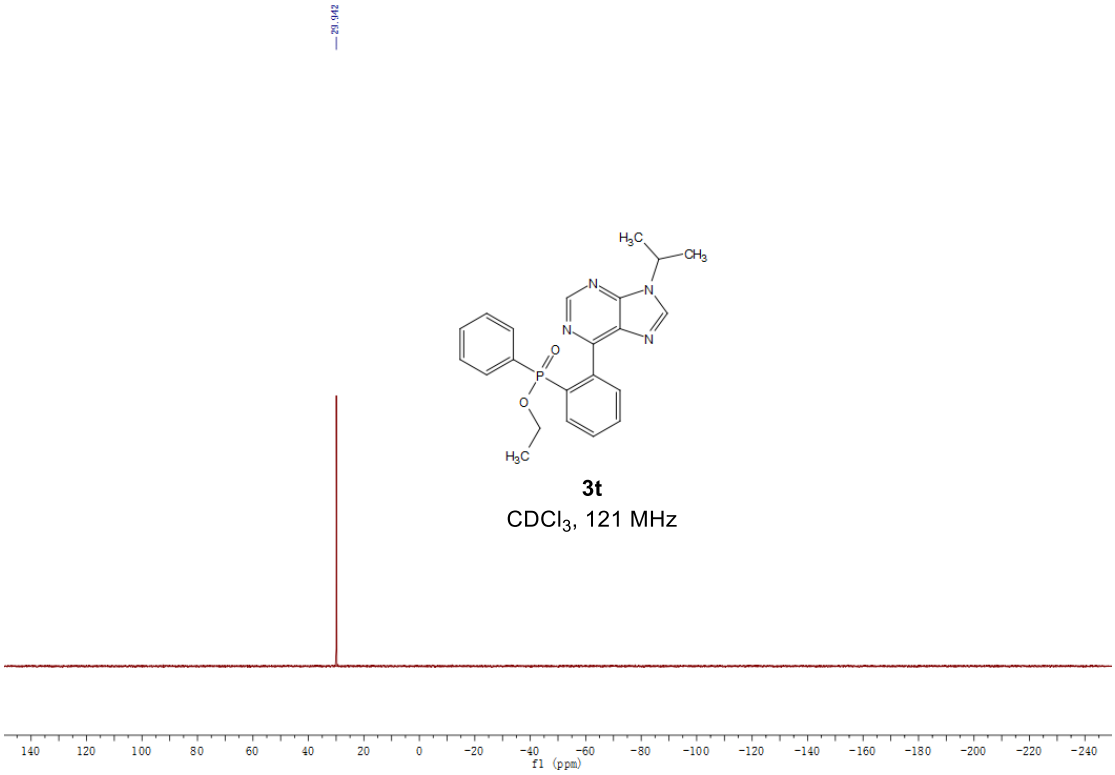
3t

$CDCl_3$, 300 MHz

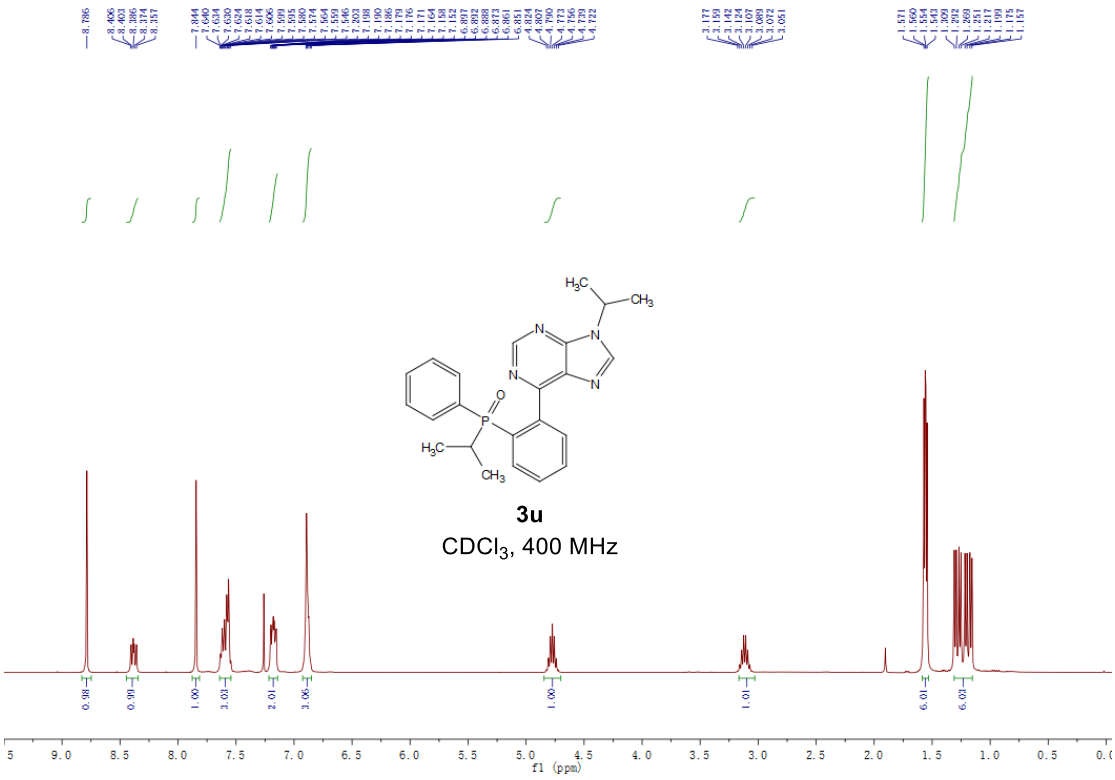


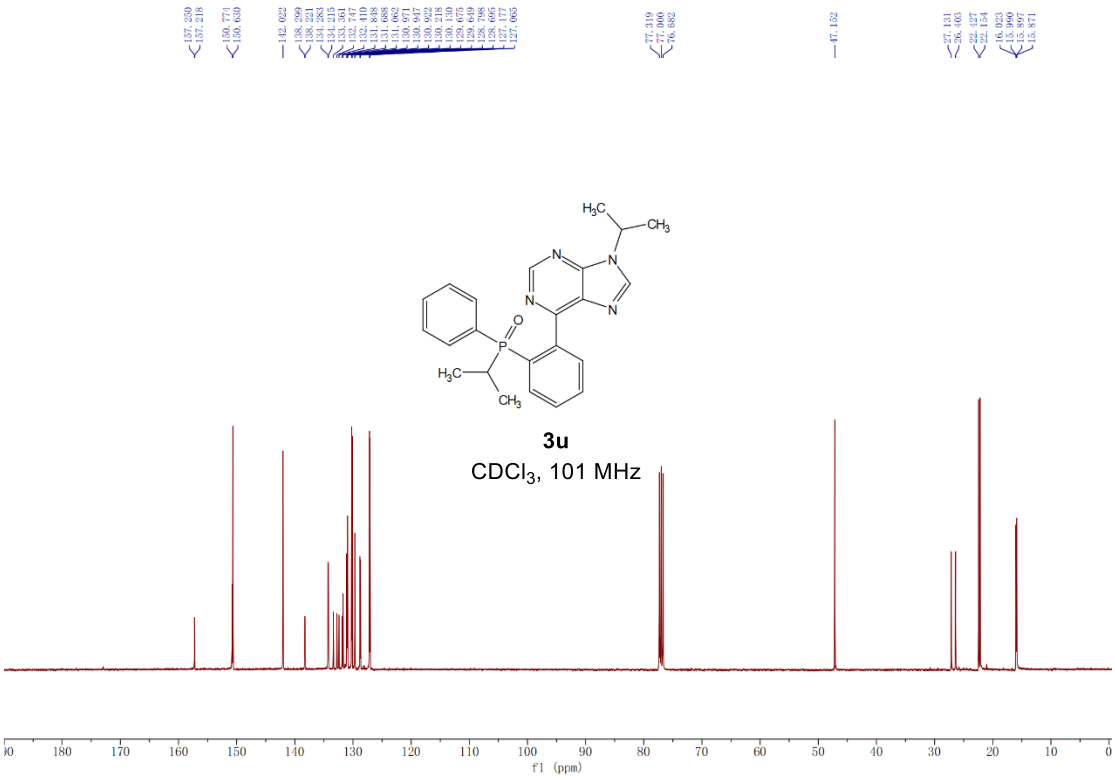
3t

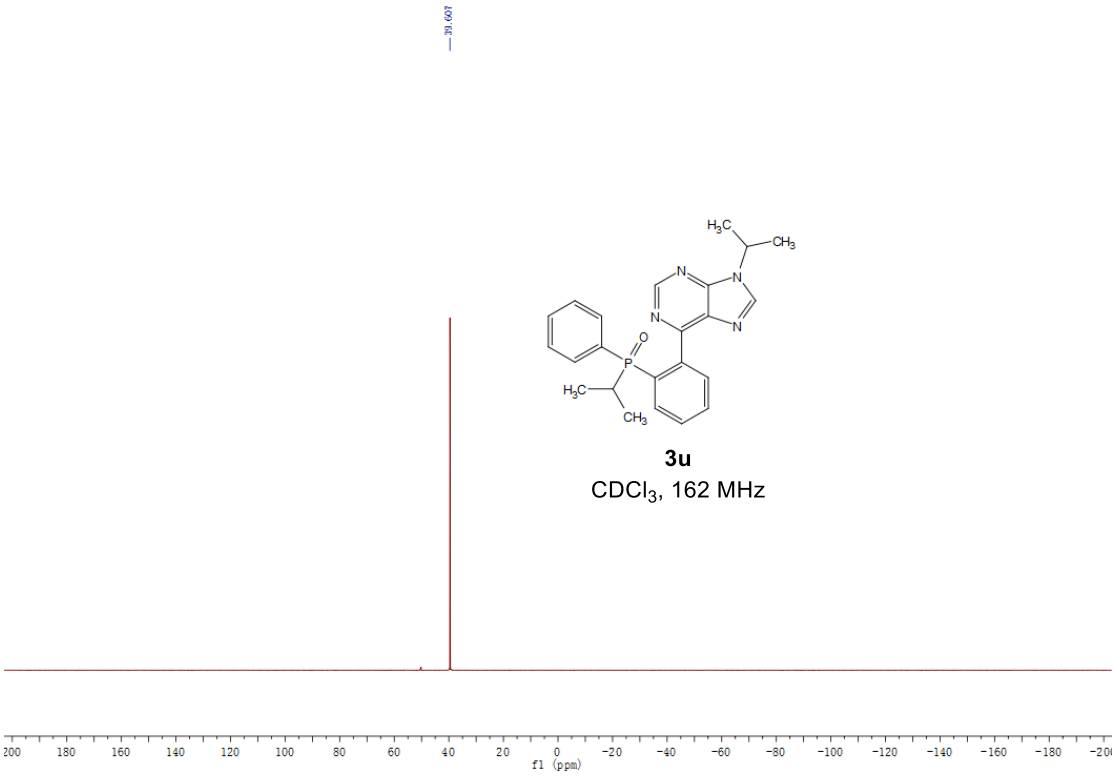
$CDCl_3$, 75 MHz



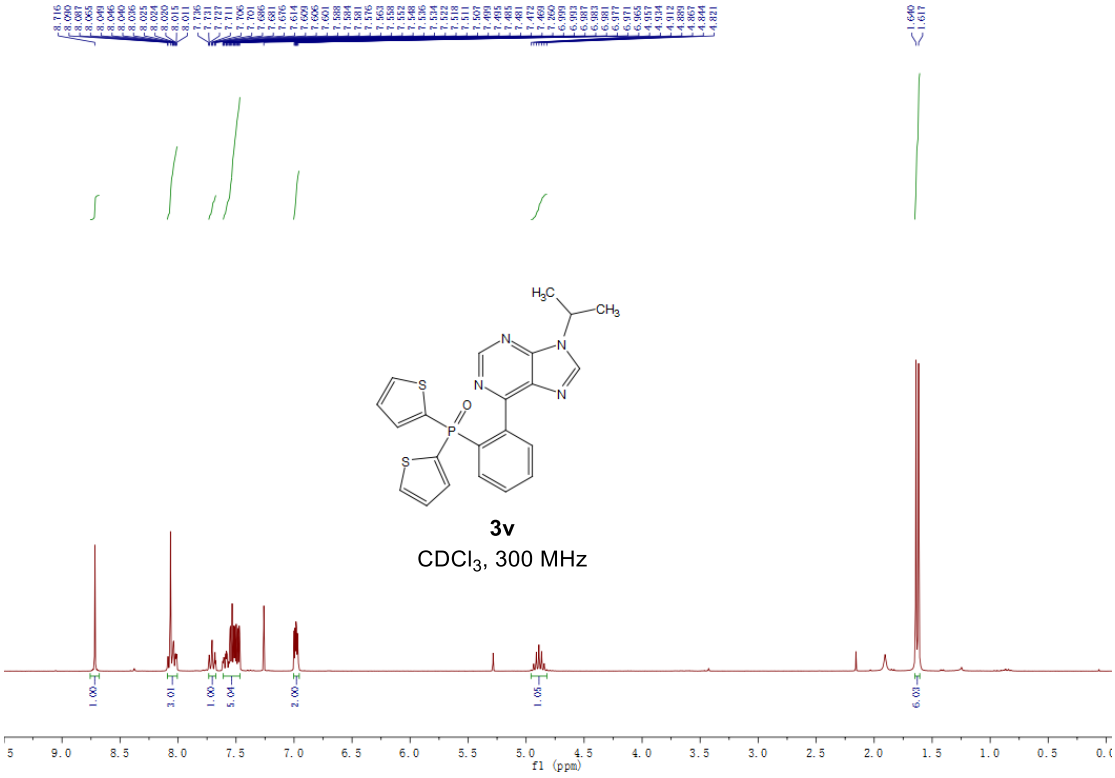
Isopropyl(2-(9-isopropyl-9H-purin-6-yl)phenyl)(phenyl)phosphine oxide (**3u**)

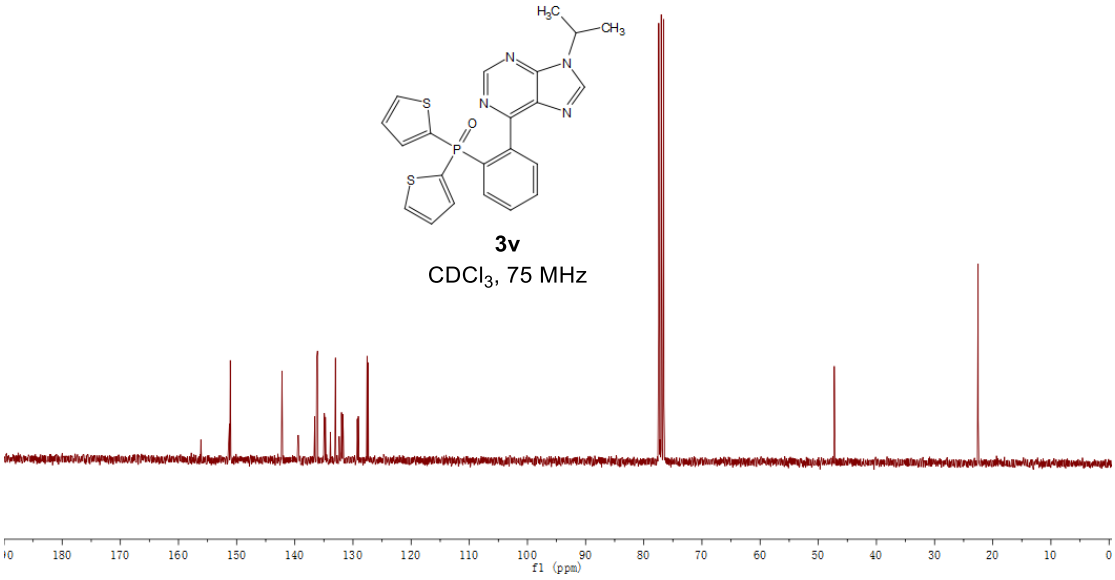


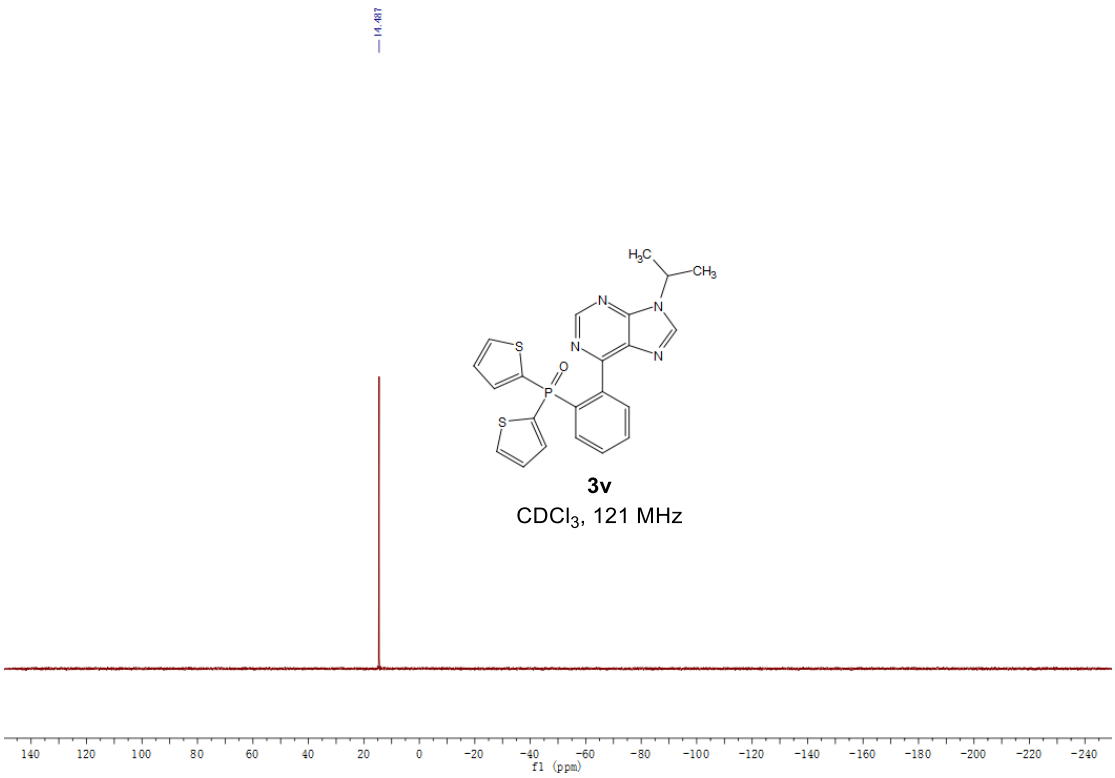

3u
CDCl3, 101 MHz
f1 (ppm)


3u
CDCl3, 162 MHz
f1 (ppm)

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)di(thiophen-2-yl)phosphine oxide (**3v**)



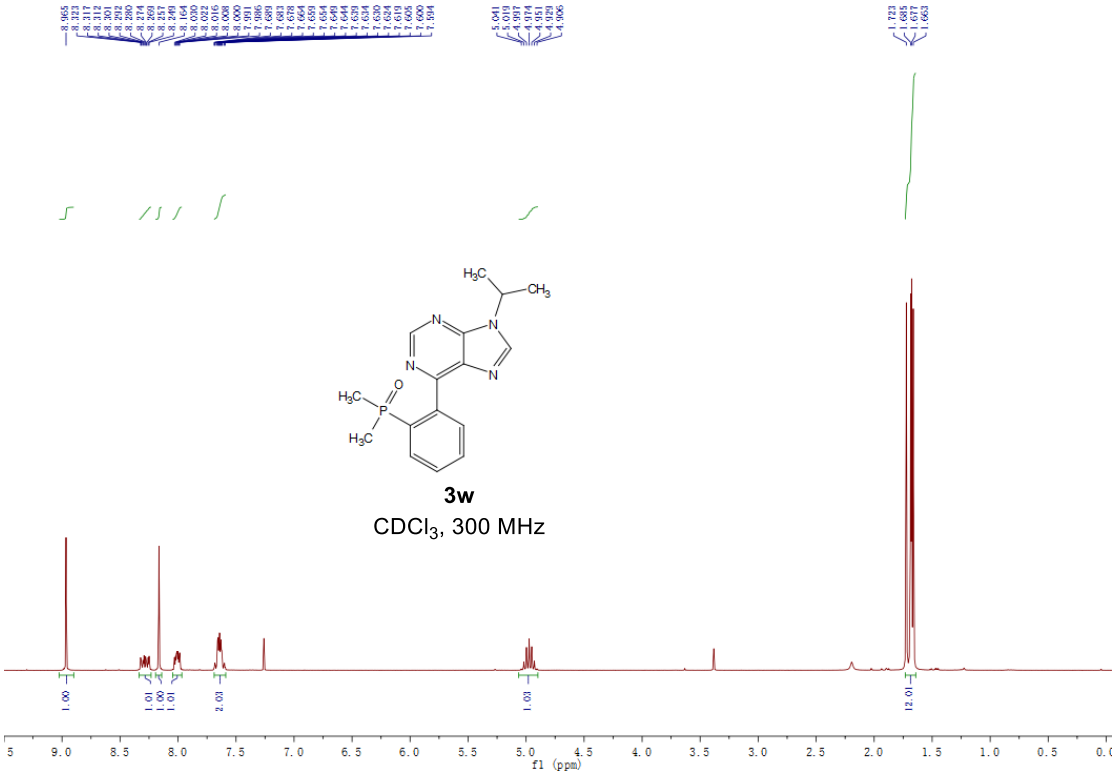




3v

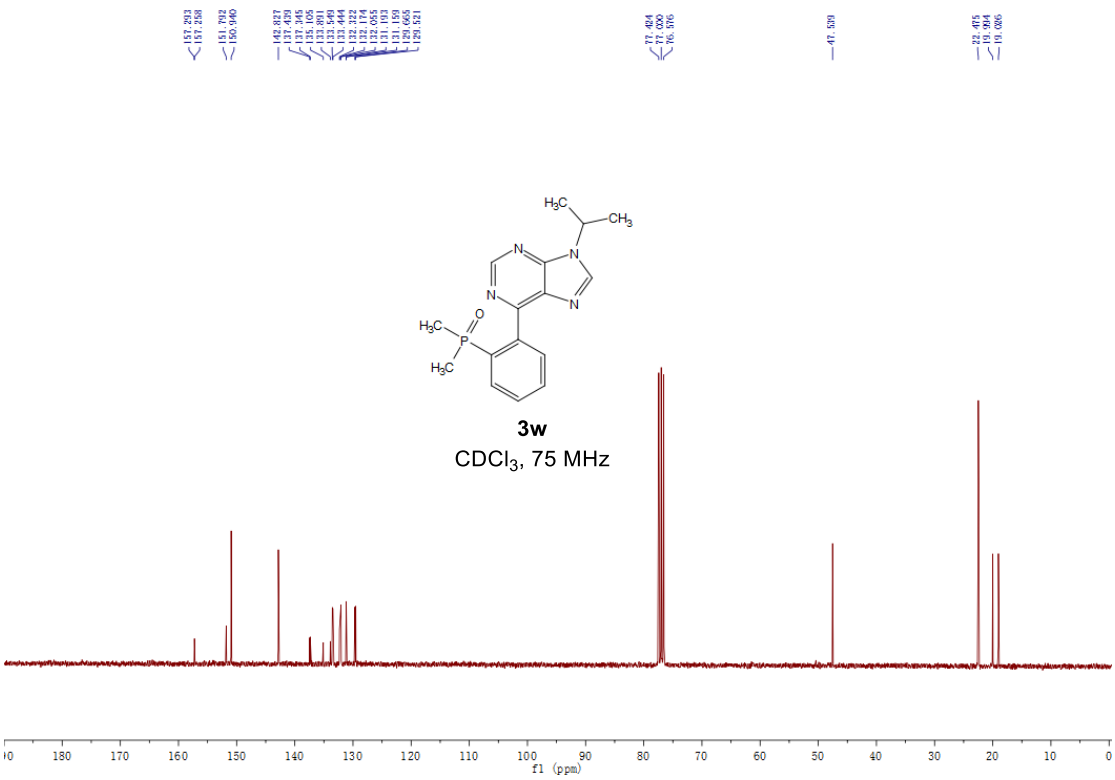
$CDCl_3$, 121 MHz

(2-(9-Isopropyl-9H-purin-6-yl)phenyl)dimethylphosphine oxide (**3w**)



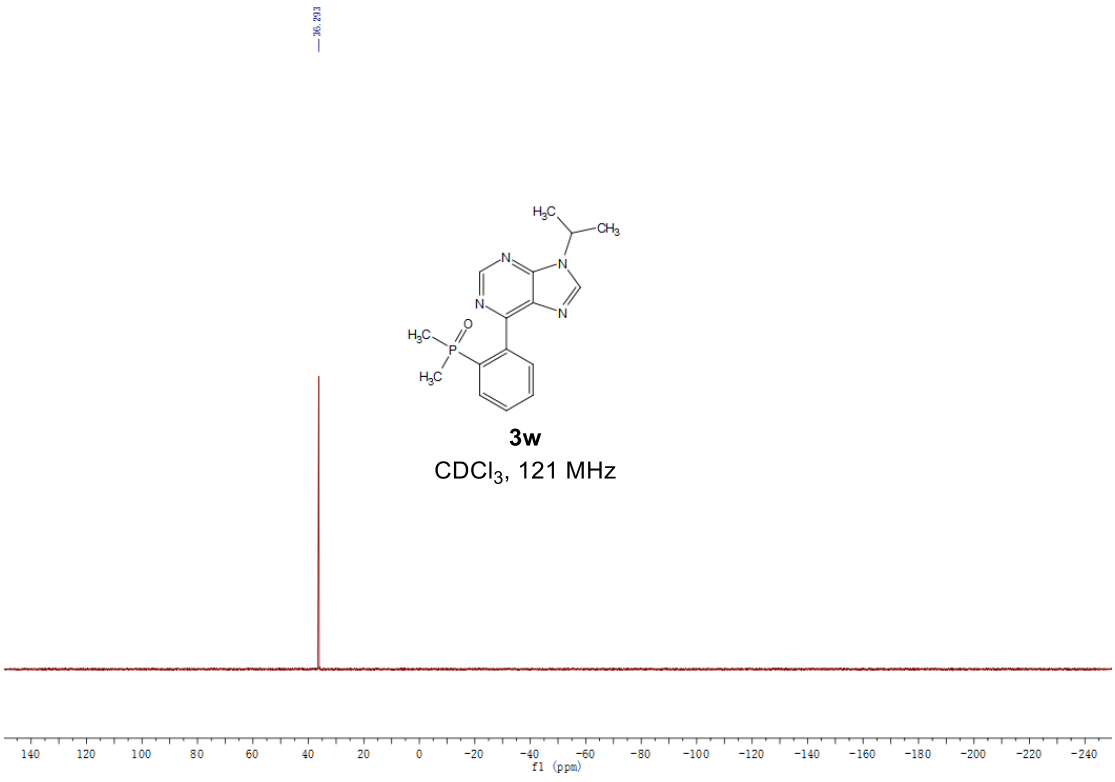
3w

$CDCl_3$, 300 MHz



3w

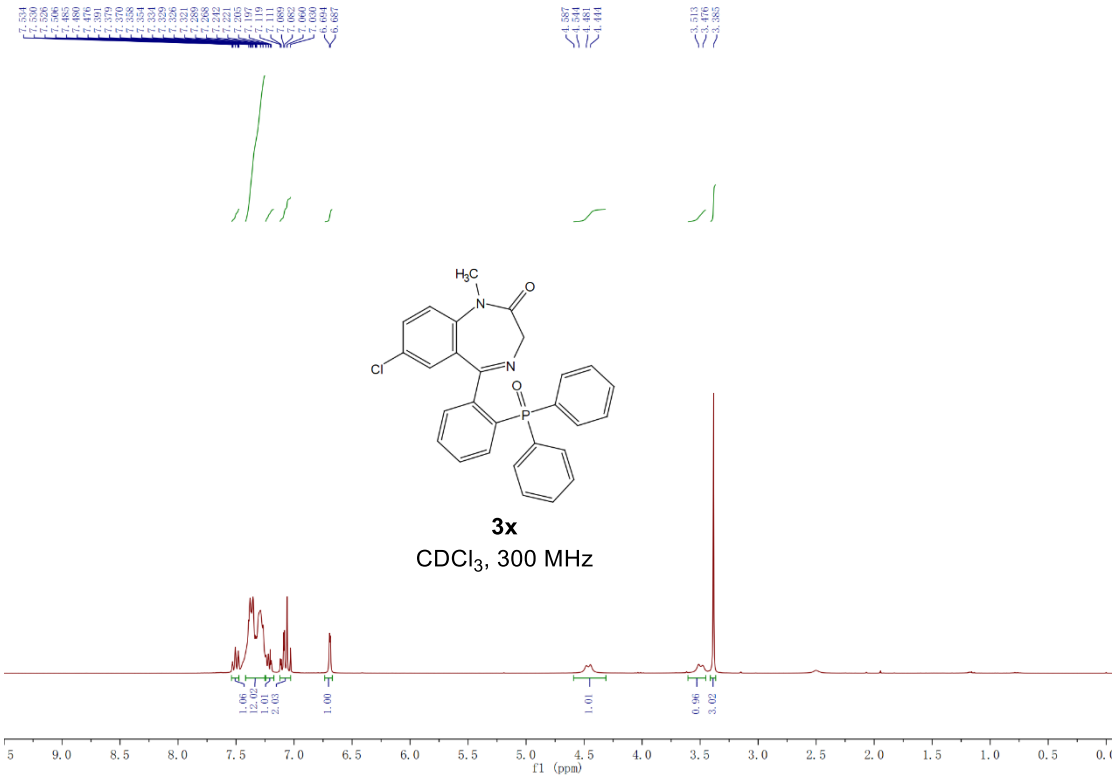
$CDCl_3$, 75 MHz

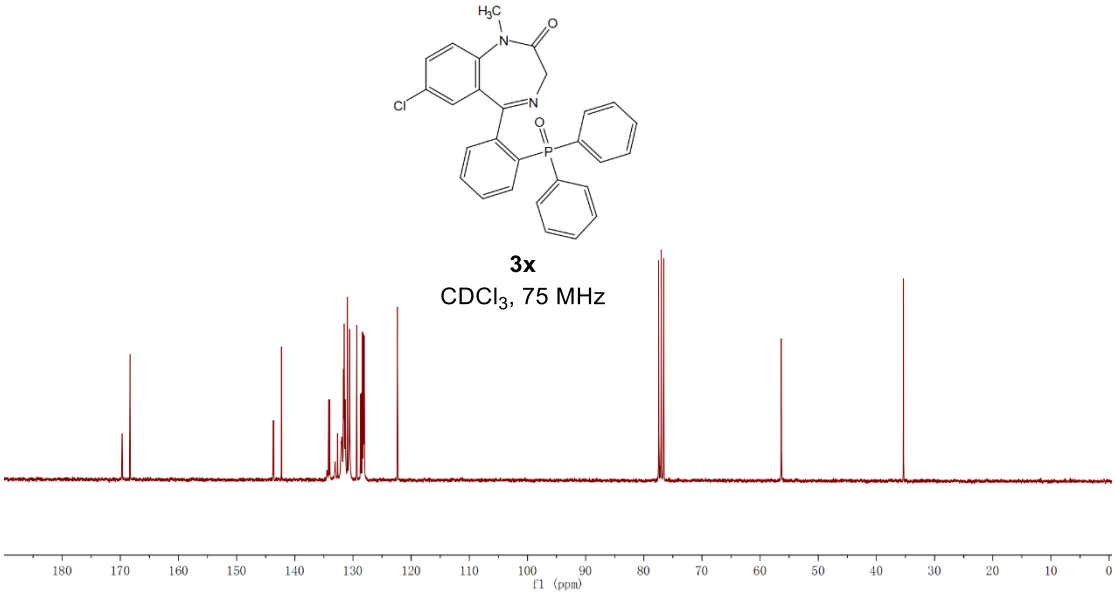


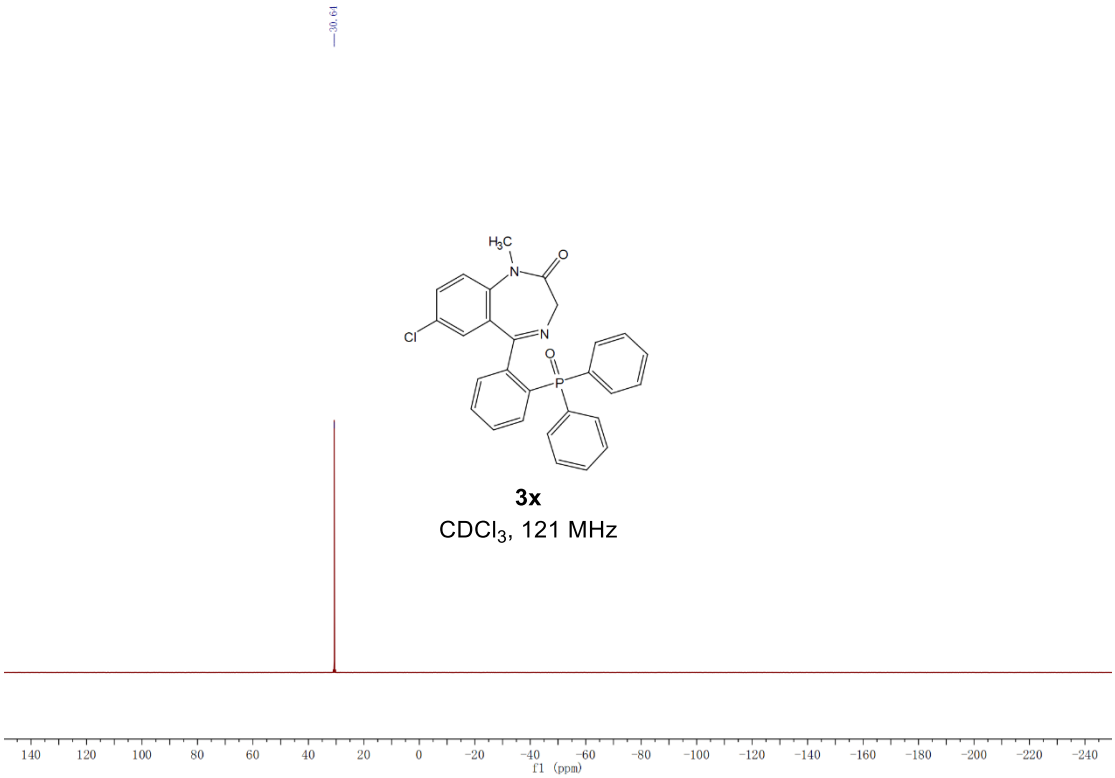
3w

$CDCl_3$, 121 MHz

7-Chloro-5-(2-(diphenylphosphoryl)phenyl)-1-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (**3x**)



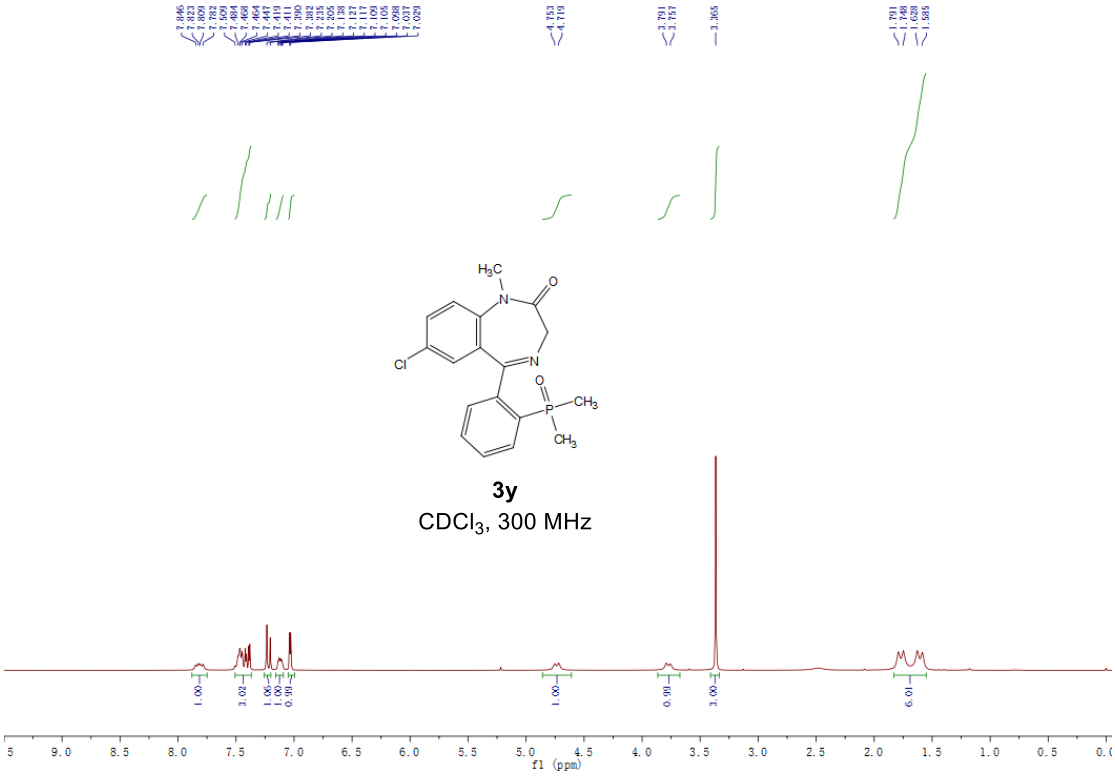




3x

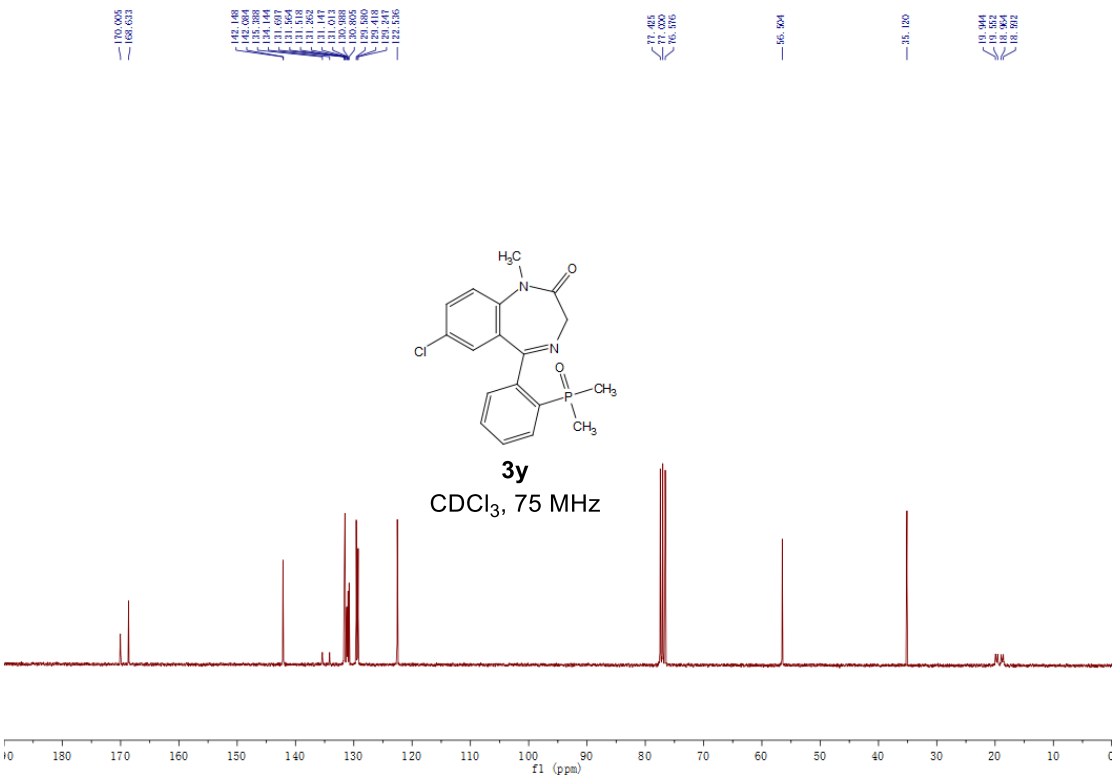
$CDCl_3$, 121 MHz

7-Chloro-5-(2-(dimethylphosphoryl)phenyl)-1-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (**3y**)



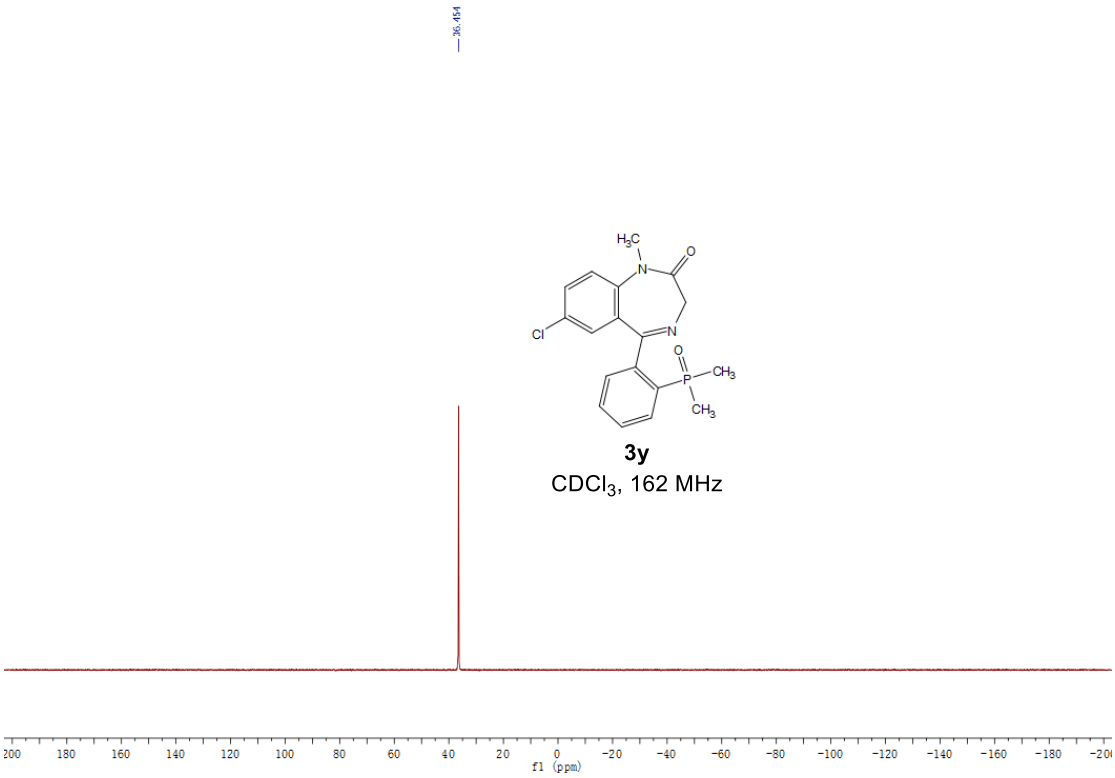
3y

$CDCl_3$, 300 MHz



3y

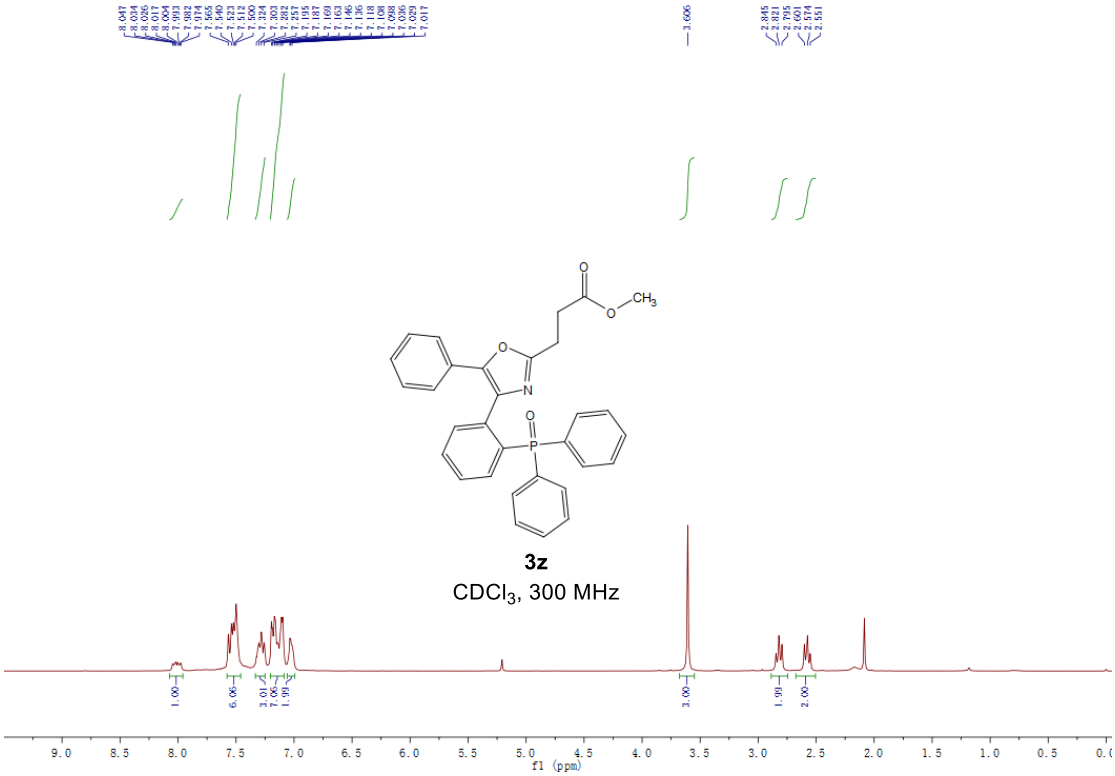
$CDCl_3$, 75 MHz

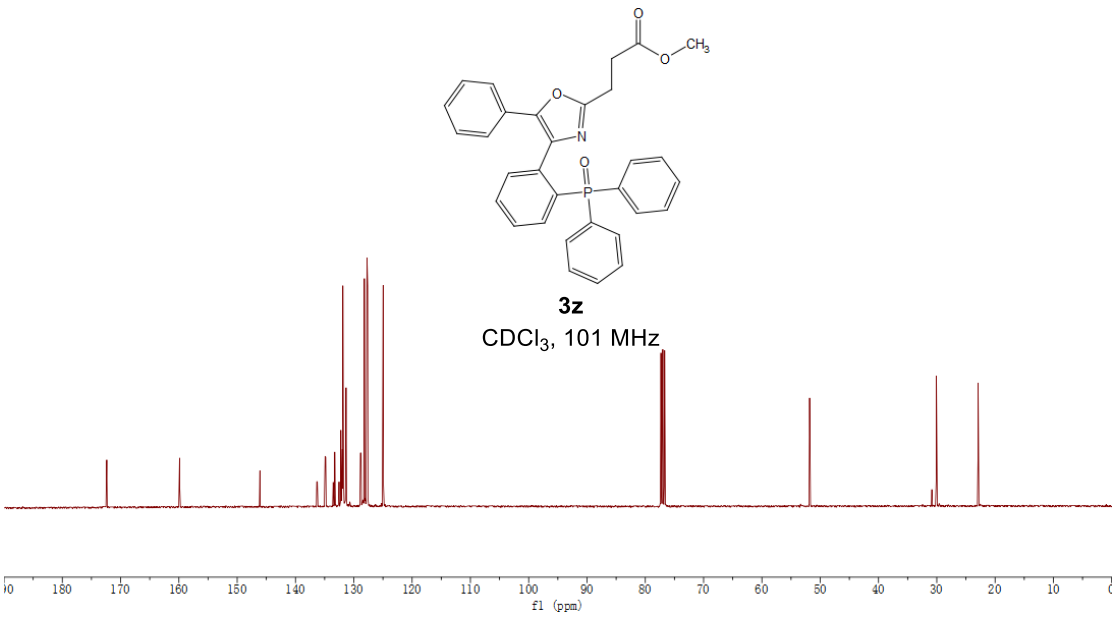


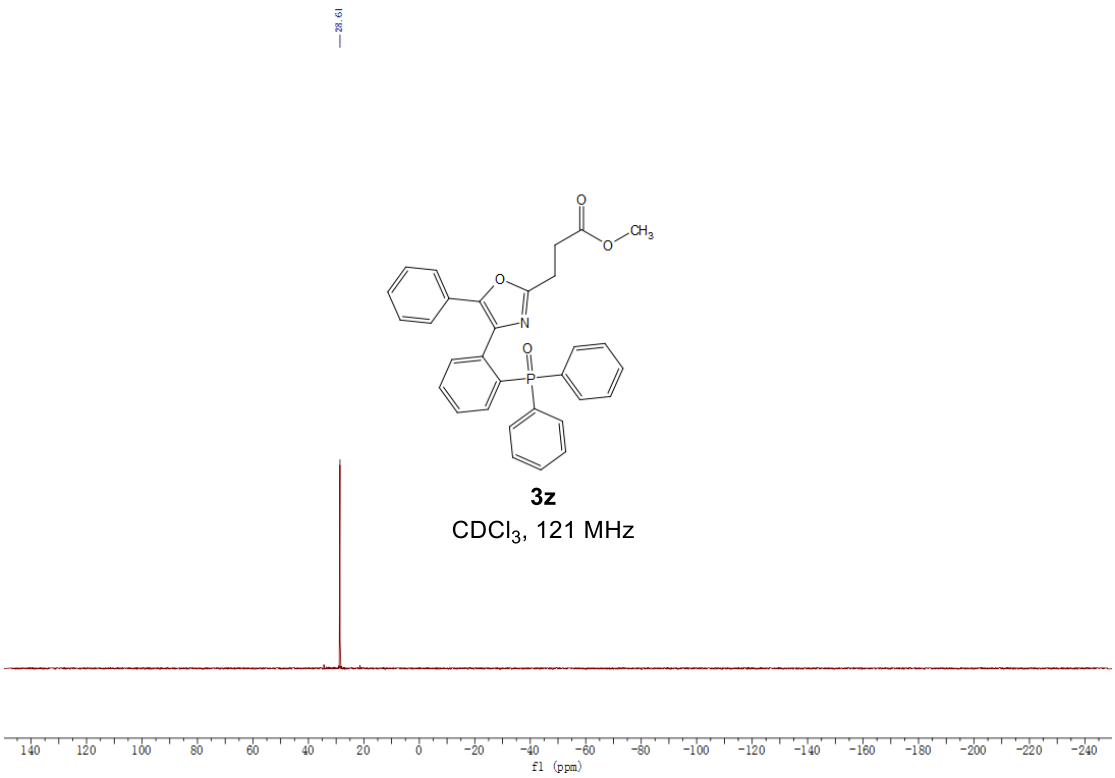
3y

$CDCl_3$, 162 MHz

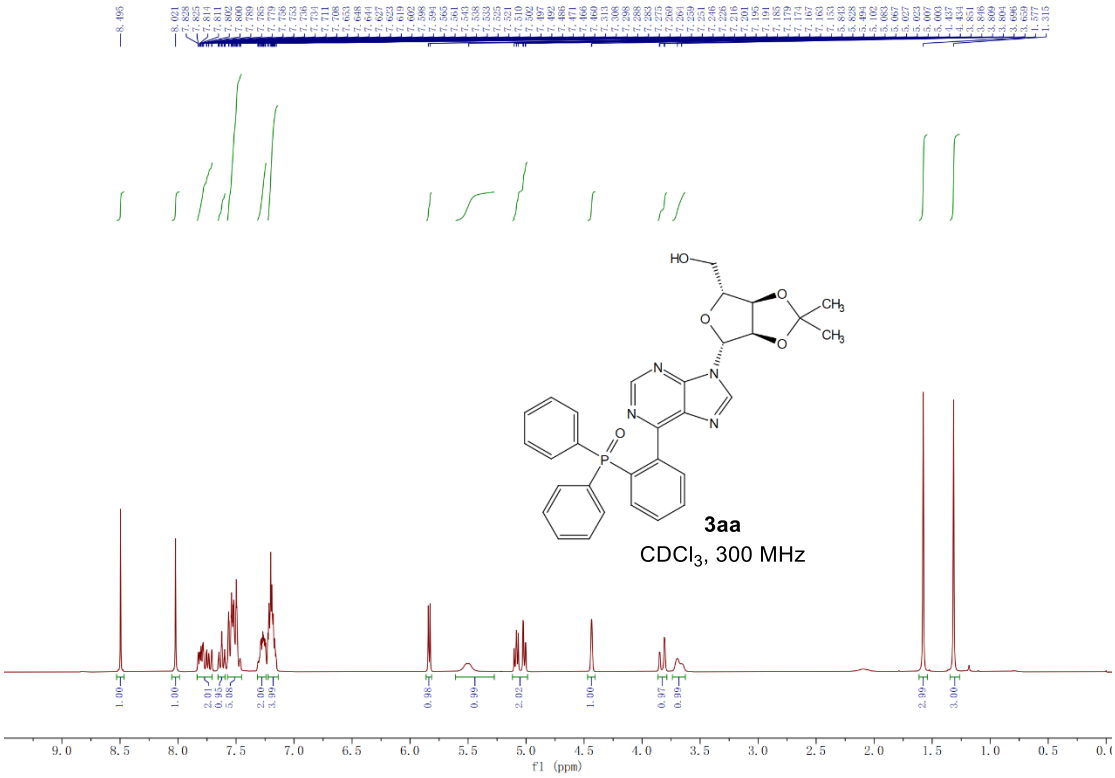
Methyl 3-(4-(2-(diphenylphosphoryl)phenyl)-5-phenyloxazol-2-yl)propanoate (**3z**)

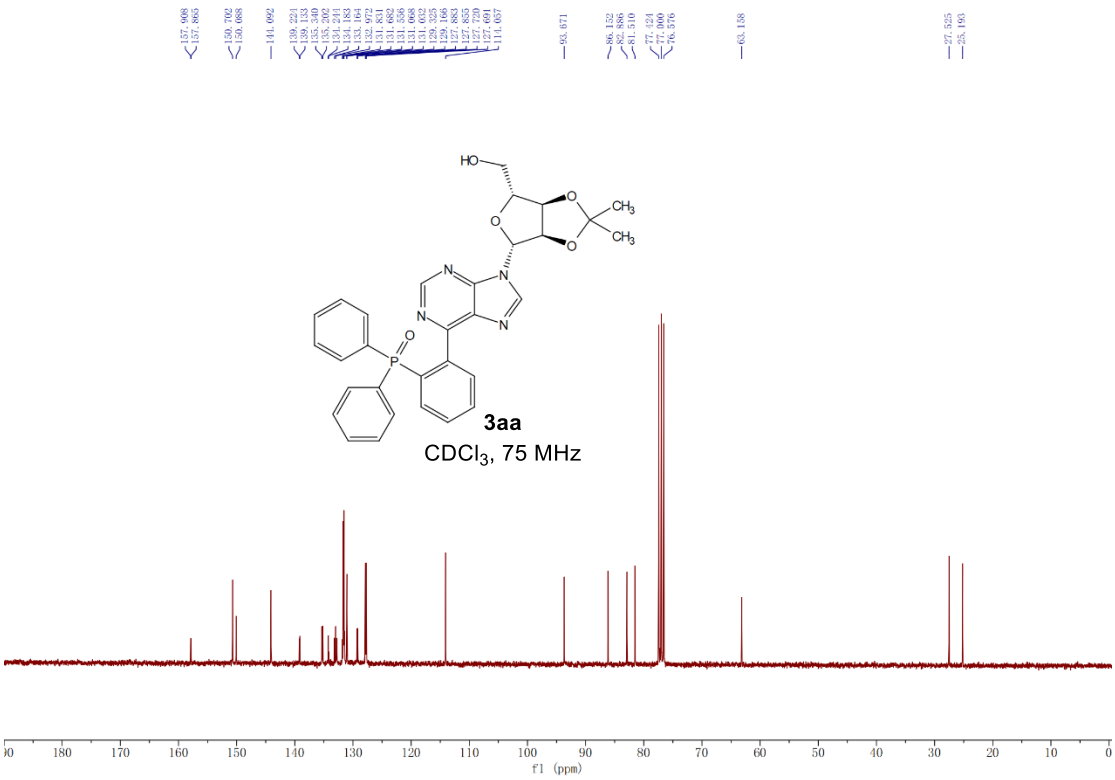


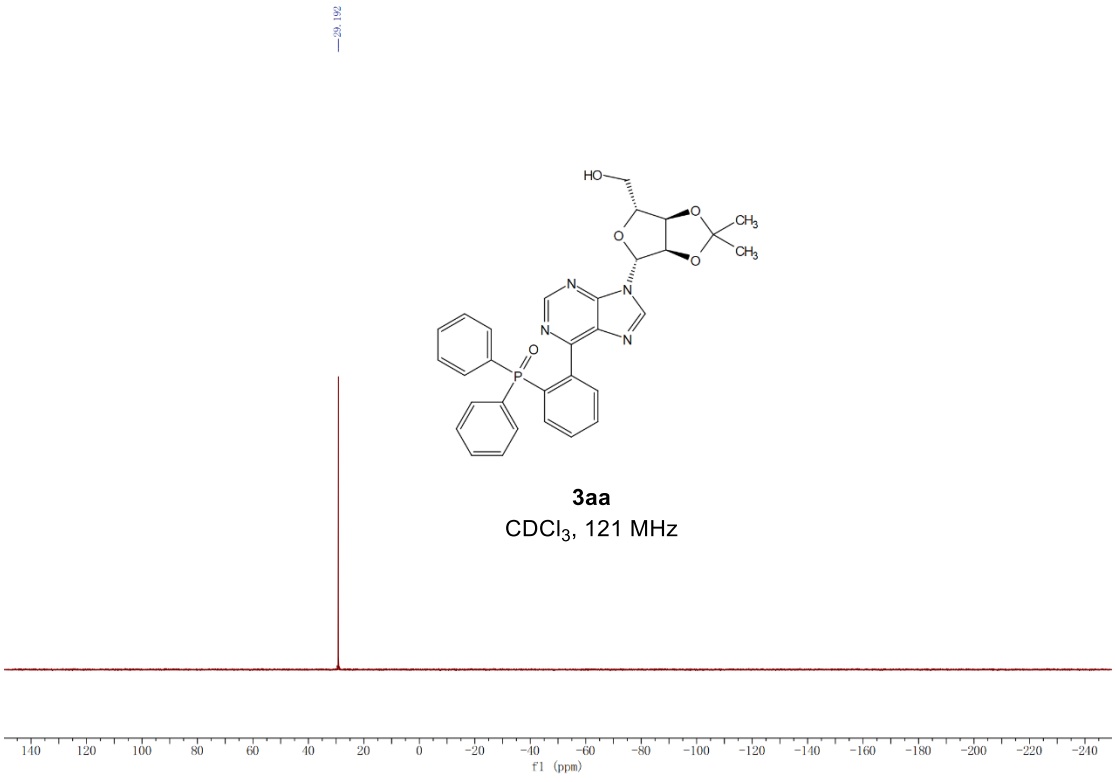




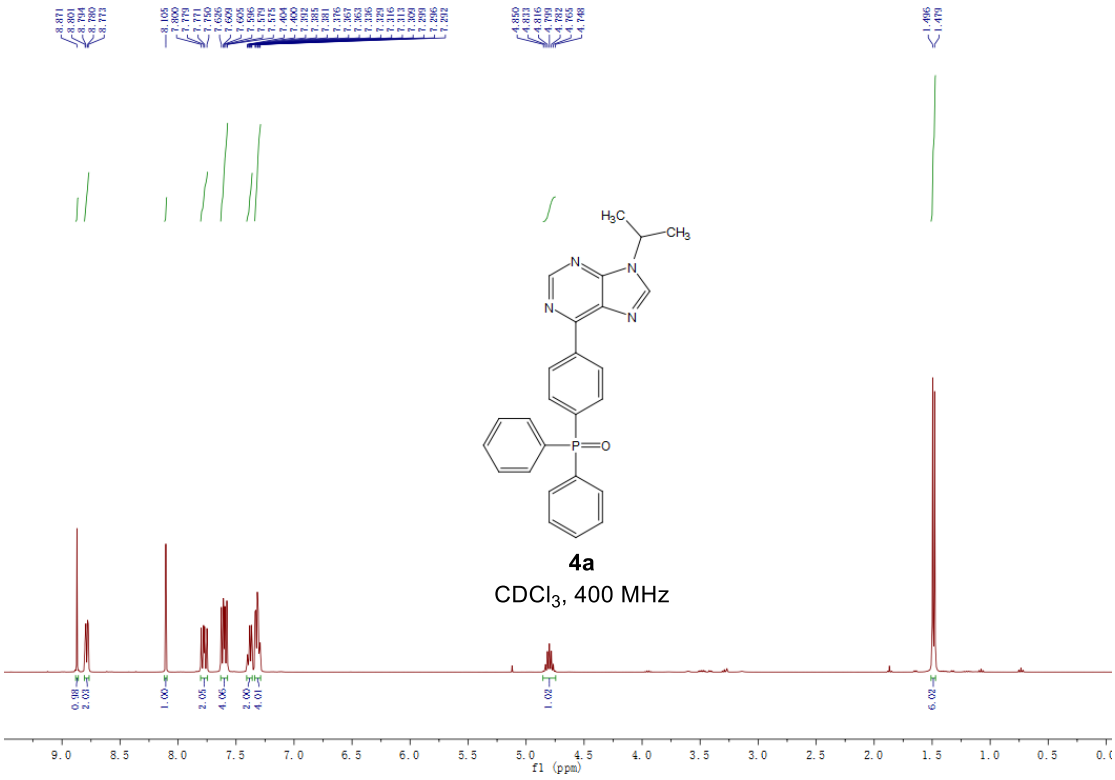
(2-(9-((3aR,4R,6R,6aR)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**3aa**)

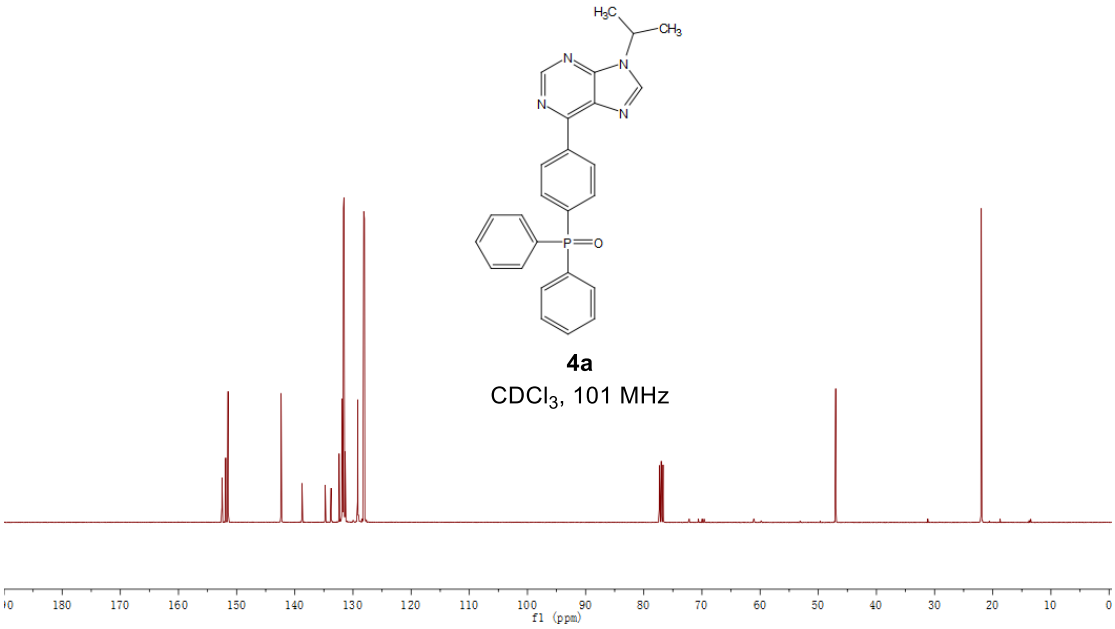


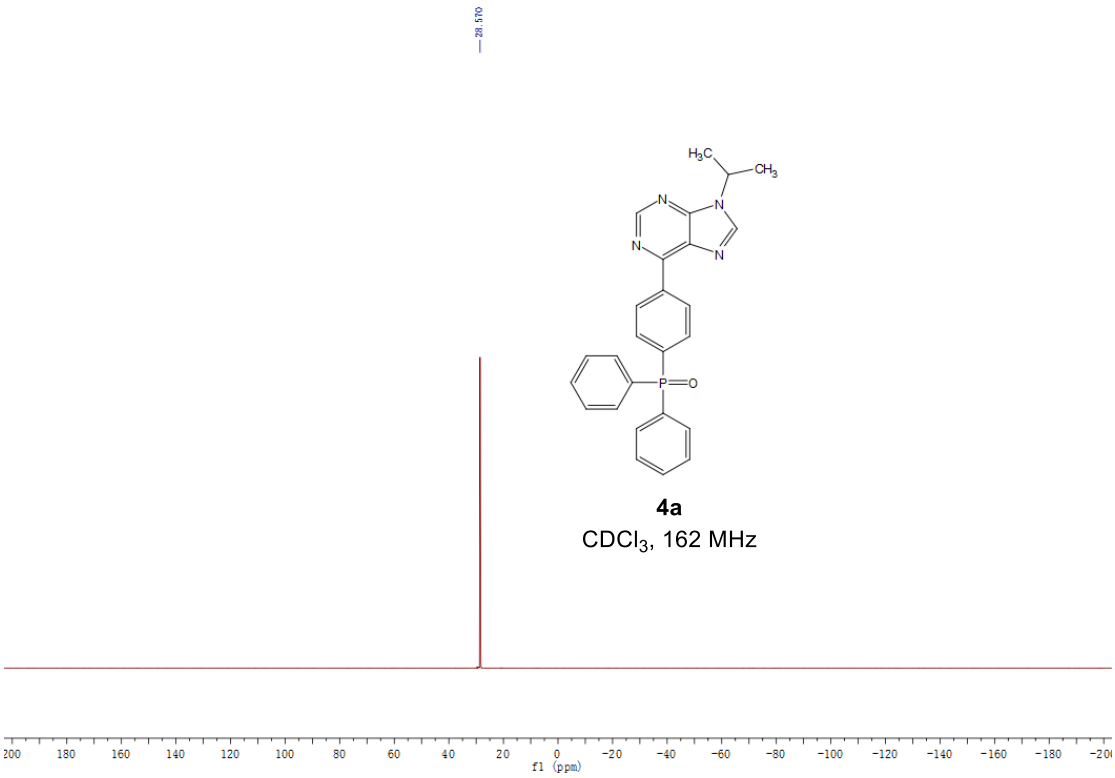

HO
O
O
O
CH3
CH3
N
N
N
N
P
O
3aa
CDCl3, 75 MHz
f1 (ppm)


HO
O
O
O
CH3
CH3
N
N
N
N
P
O
3aa
CDCl3, 121 MHz
f1 (ppm)

(4-(9-Isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4a**)



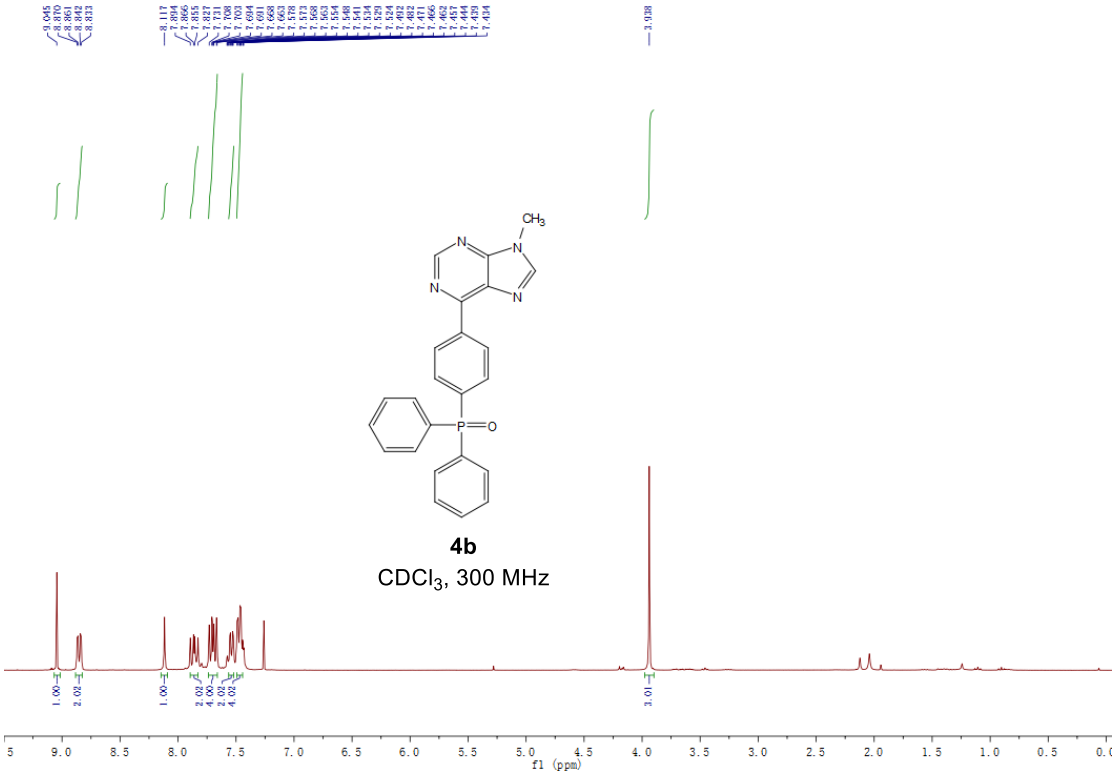




4a

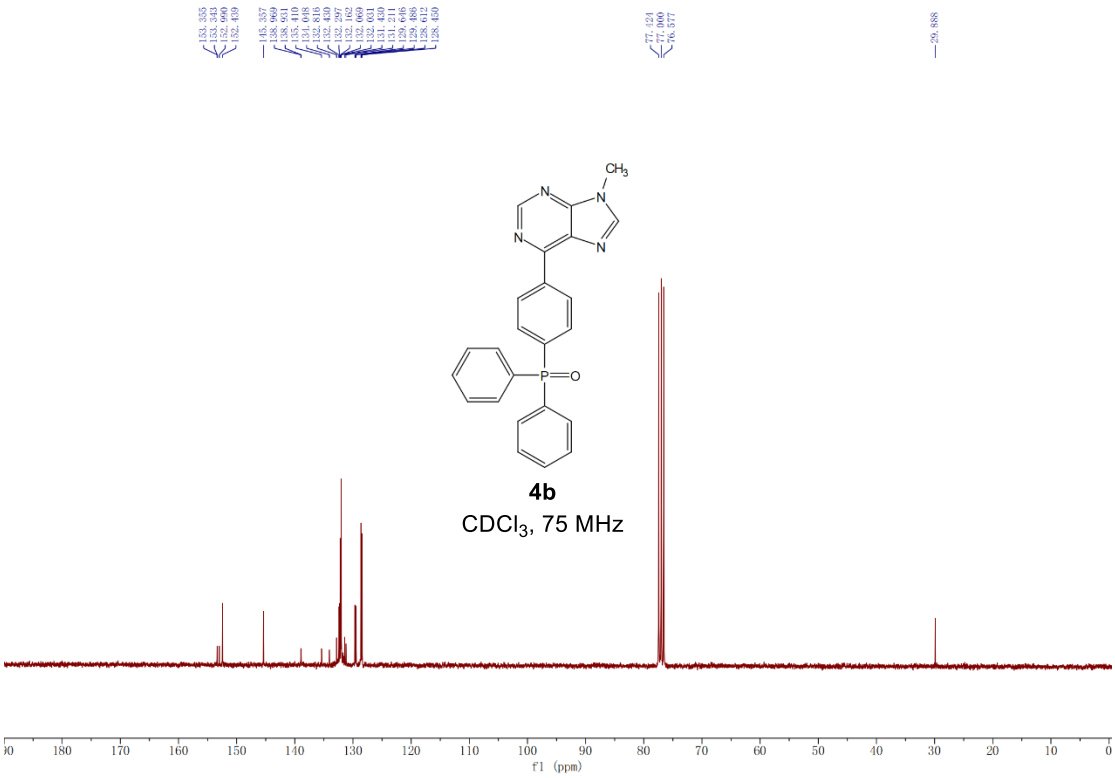
$CDCl_3$, 162 MHz

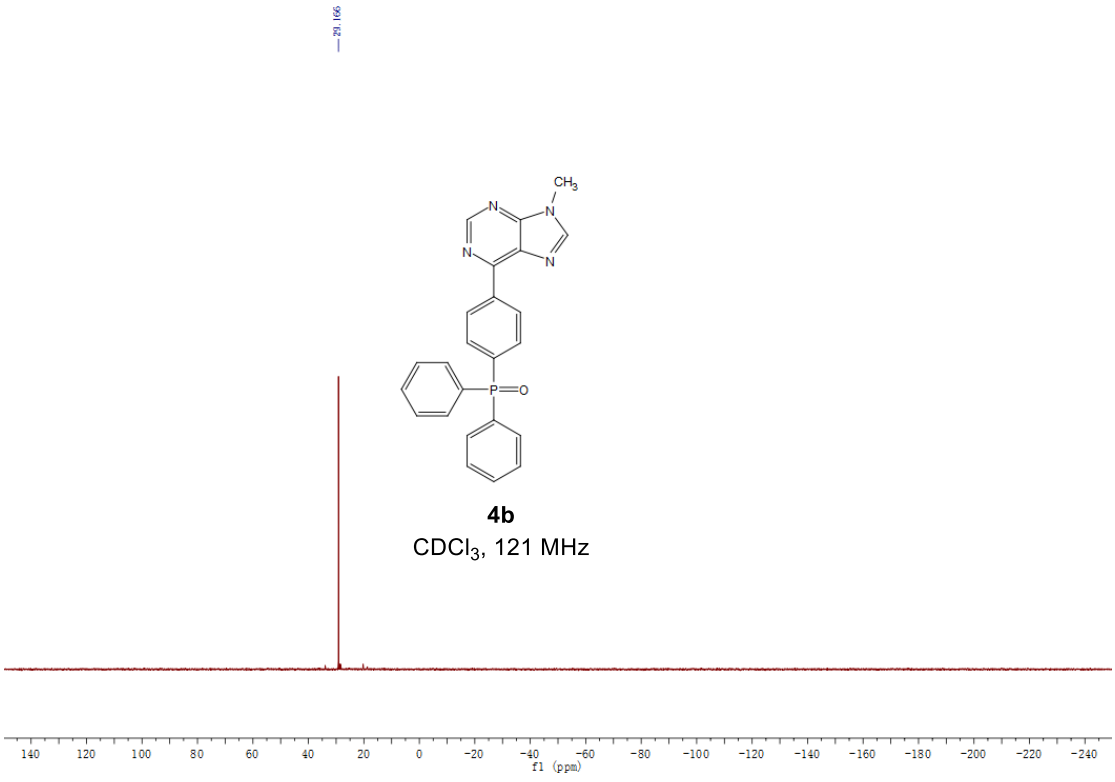
(4-(9-Methyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4b**)



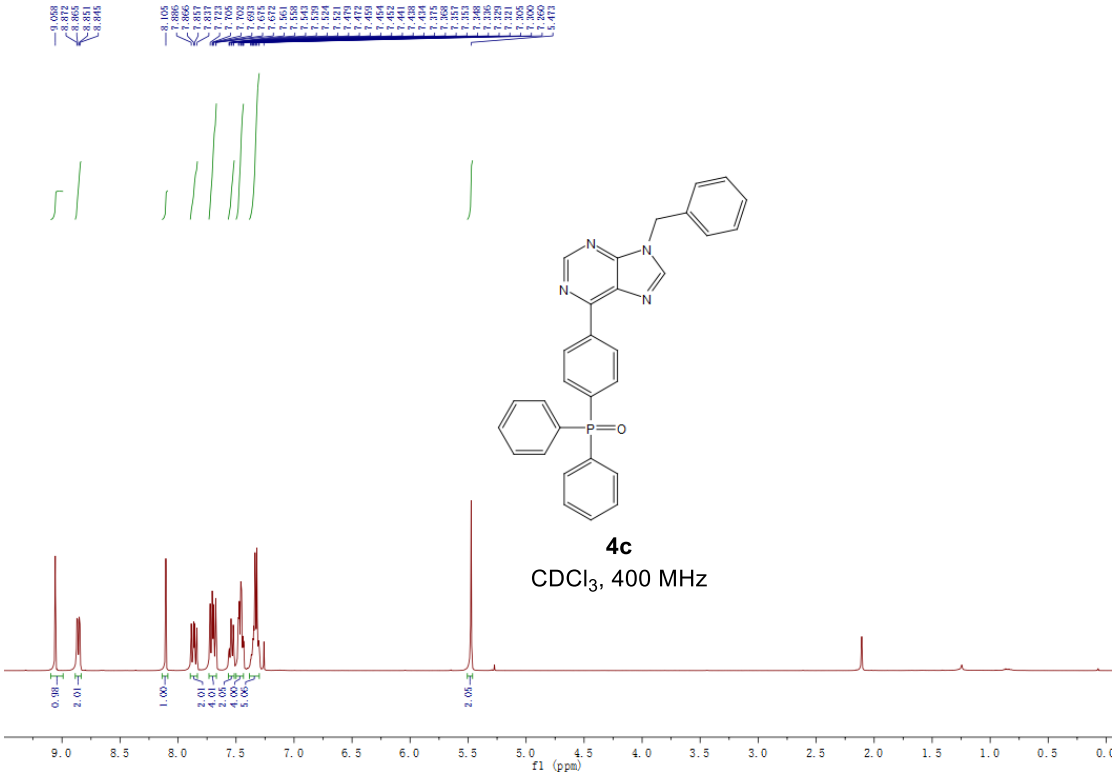
4b

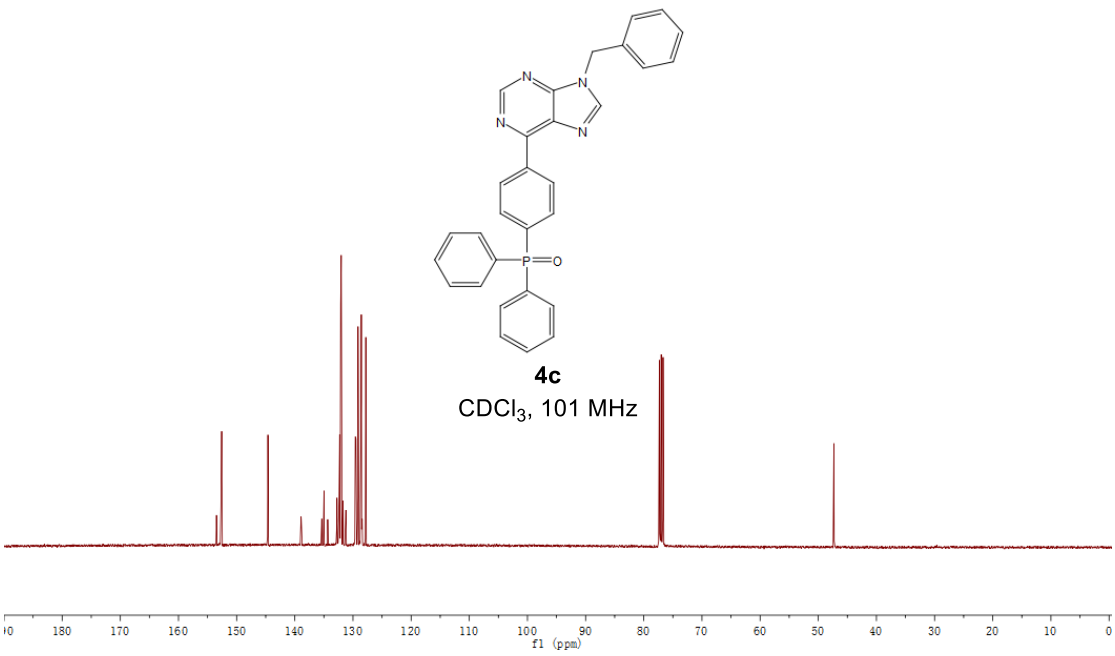
$CDCl_3$, 300 MHz

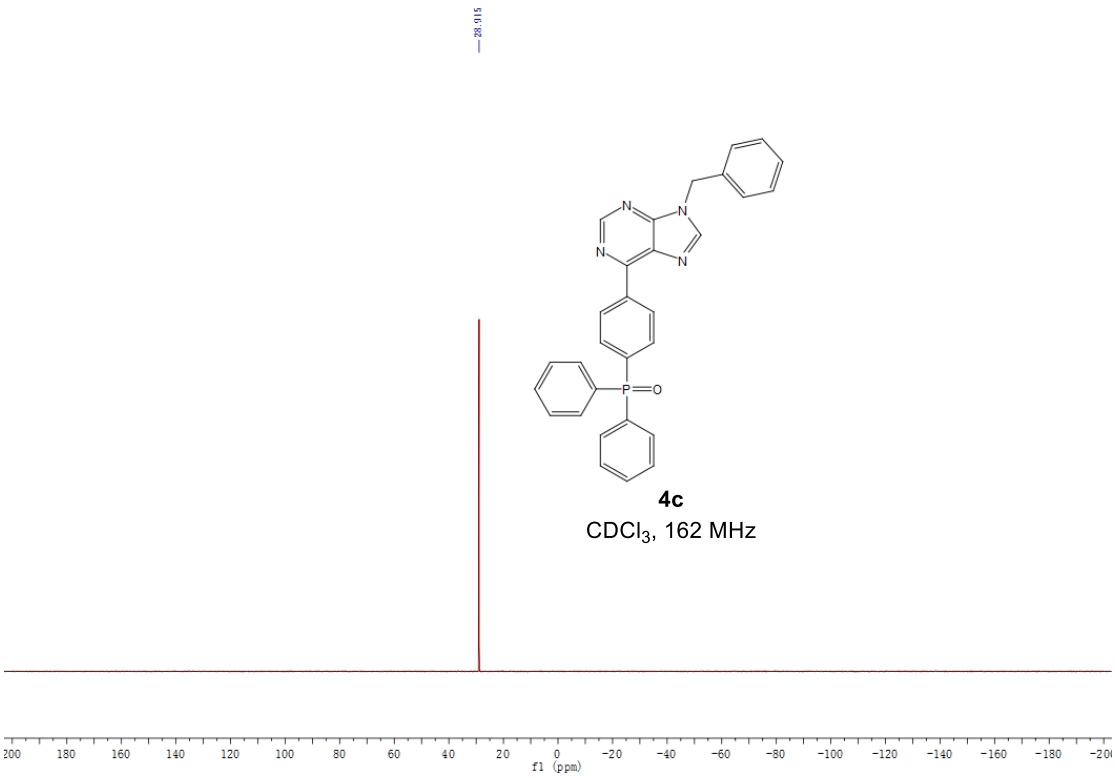

153.355
153.343
152.460
152.439
145.357
138.969
138.951
135.410
131.048
132.816
132.430
132.397
132.162
132.069
132.031
131.410
131.311
129.646
129.486
128.612
128.450
77.424
77.000
76.577
29.888
CH3
N
N
N
N
P=O
4b
CDCl3, 75 MHz
f1 (ppm)


29.166
CH3
N
N
N
N
P=O
4b
CDCl3, 121 MHz
f1 (ppm)

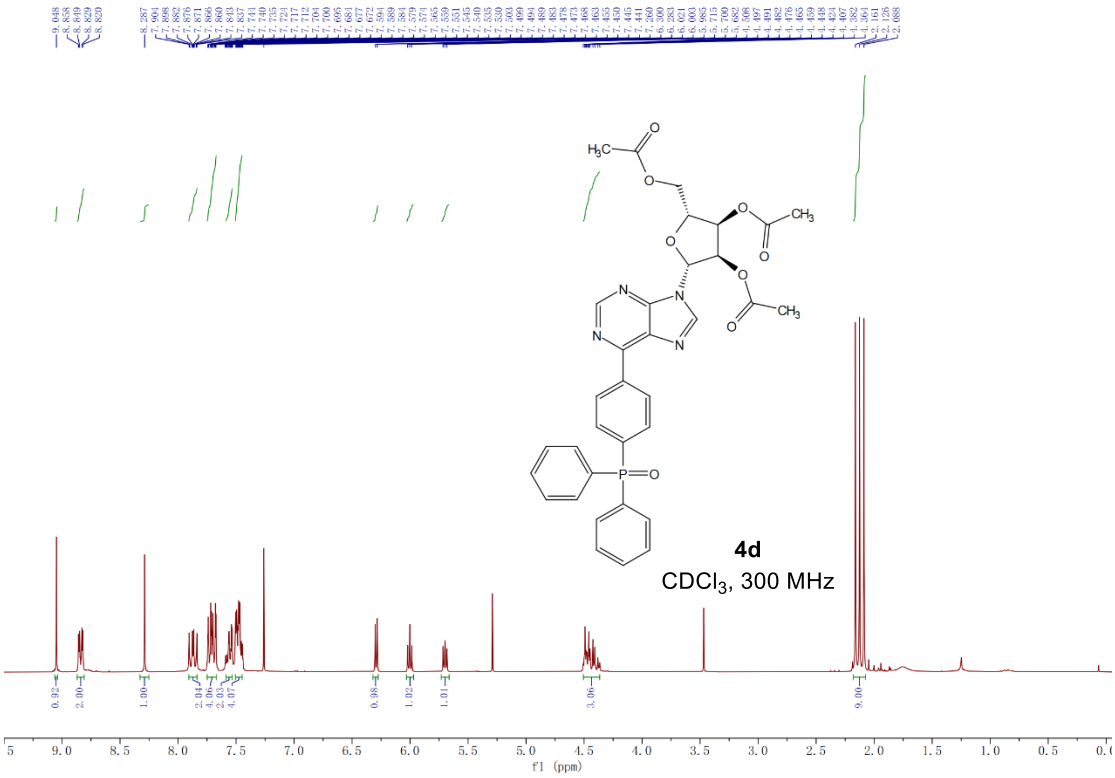
(4-(9-Benzyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4c**)

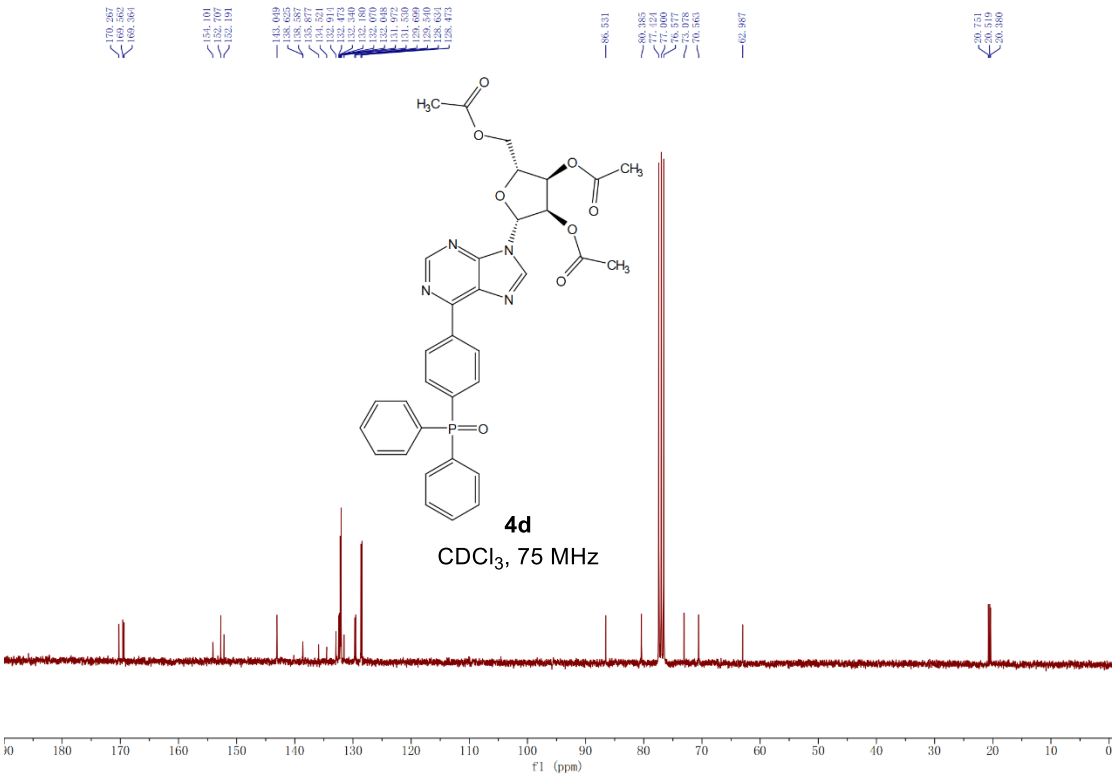


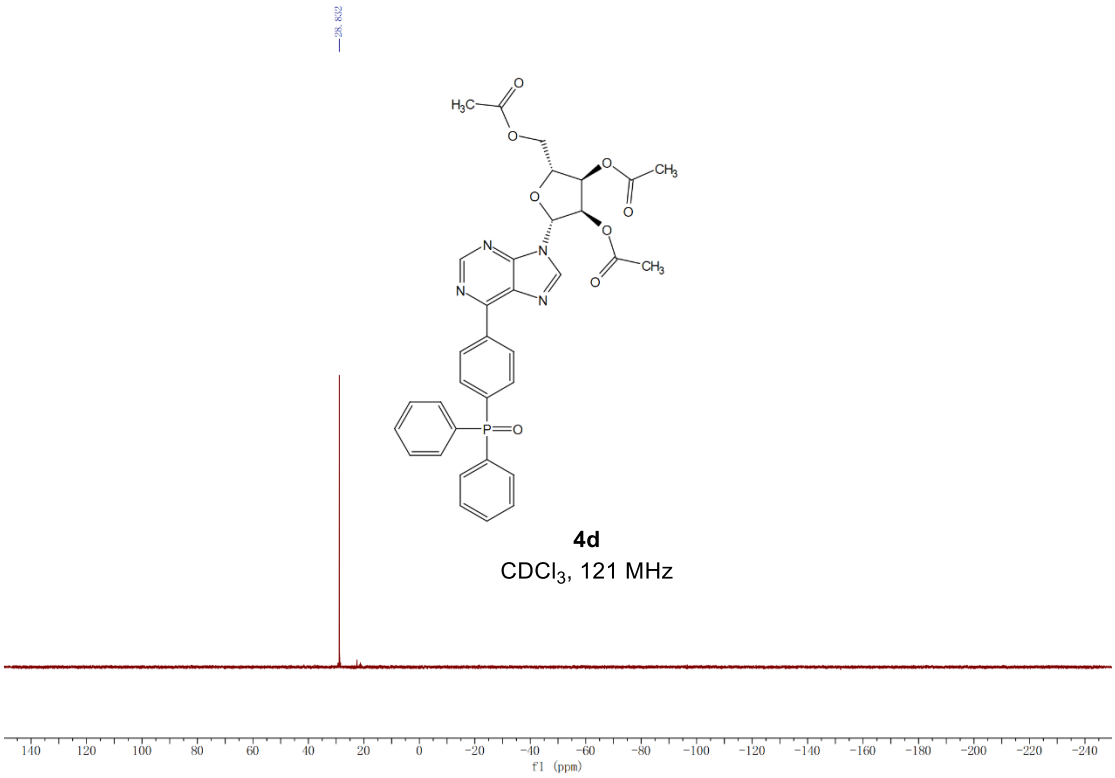




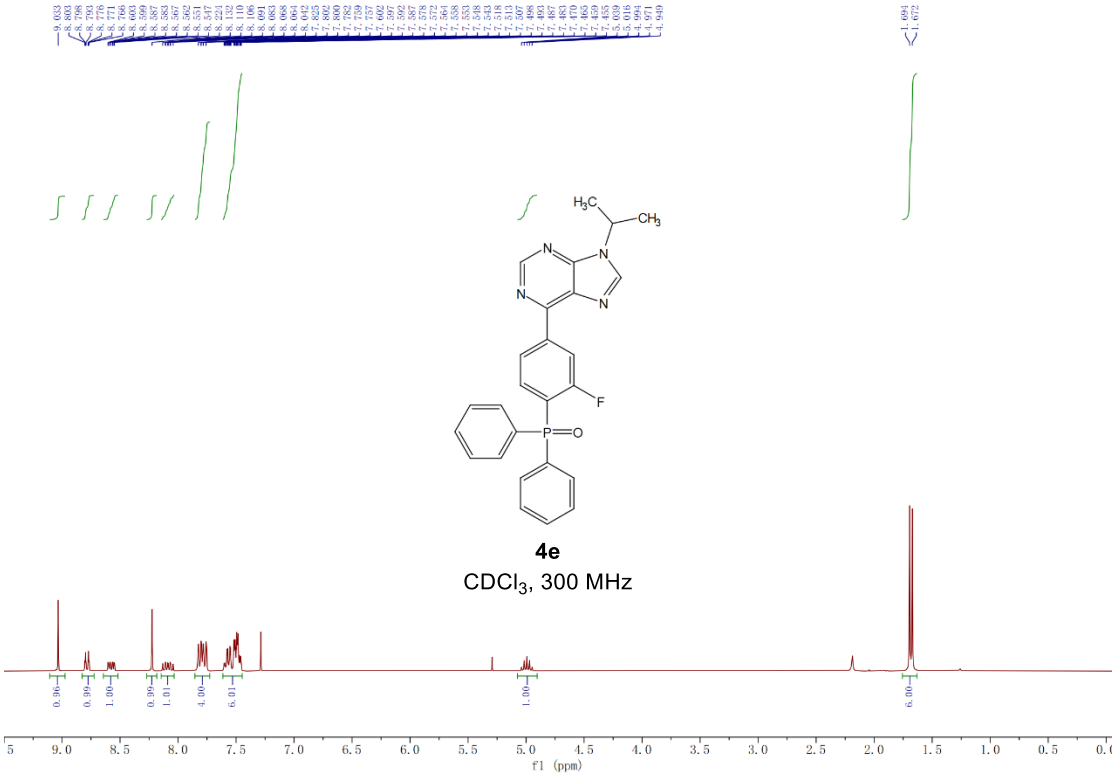
(2R,3R,4R,5R)-2-(Acetoxymethyl)-5-(6-(4-(diphenylphosphoryl)phenyl)-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate (**4d**)

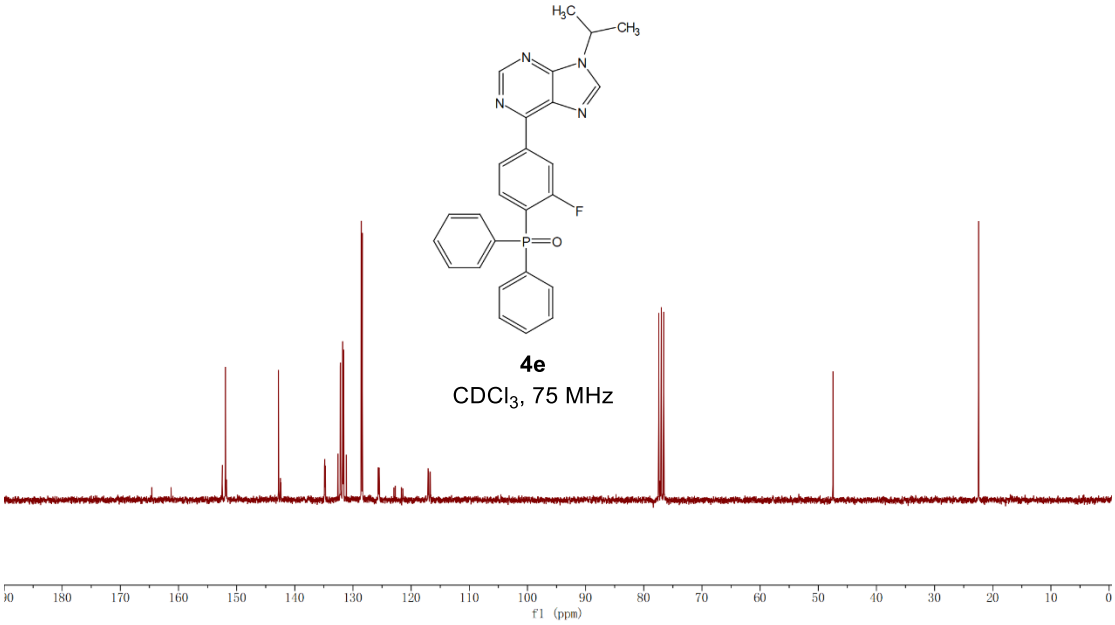


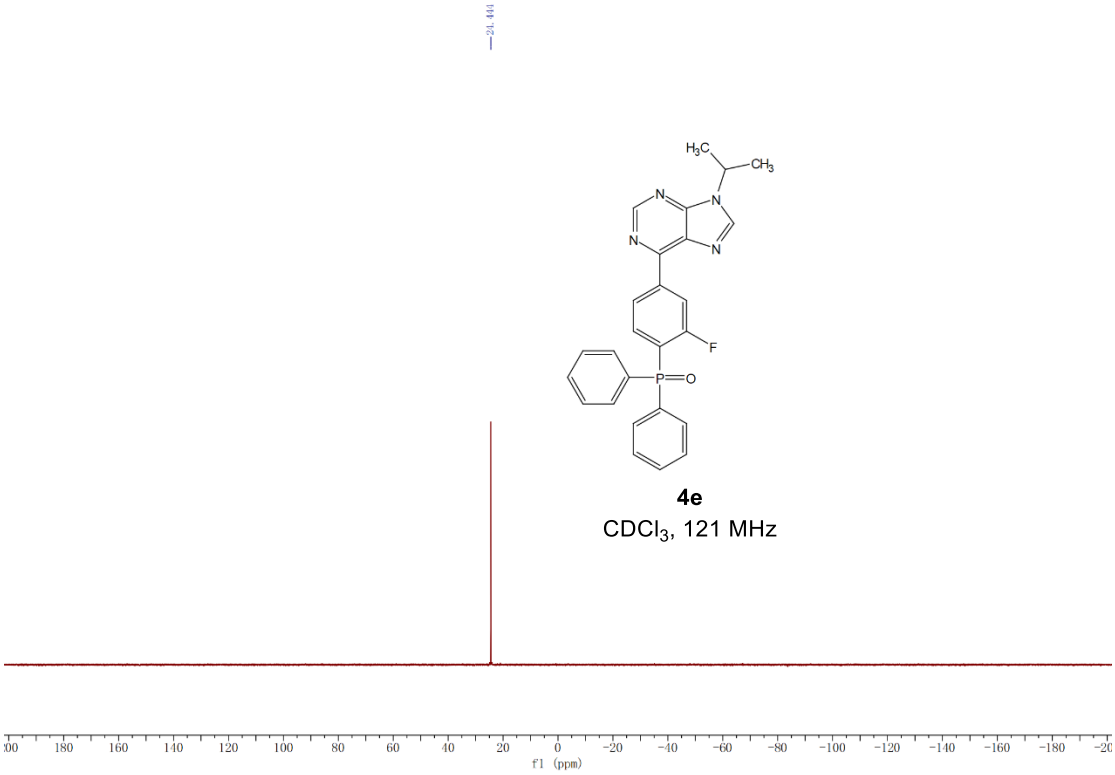

170.267
169.562
169.364
154.101
152.707
152.191
143.049
138.625
138.387
135.877
134.521
132.911
132.473
132.348
132.180
132.070
132.048
131.677
131.539
129.699
129.540
128.631
128.413
86.531
80.385
77.124
77.000
76.877
75.178
70.863
62.987
20.751
20.519
20.380
4d
CDCl3, 75 MHz
f1 (ppm)


28.832
4d
CDCl3, 121 MHz
f1 (ppm)

(2-Fluoro-4-(9-isopropyl-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4e**)

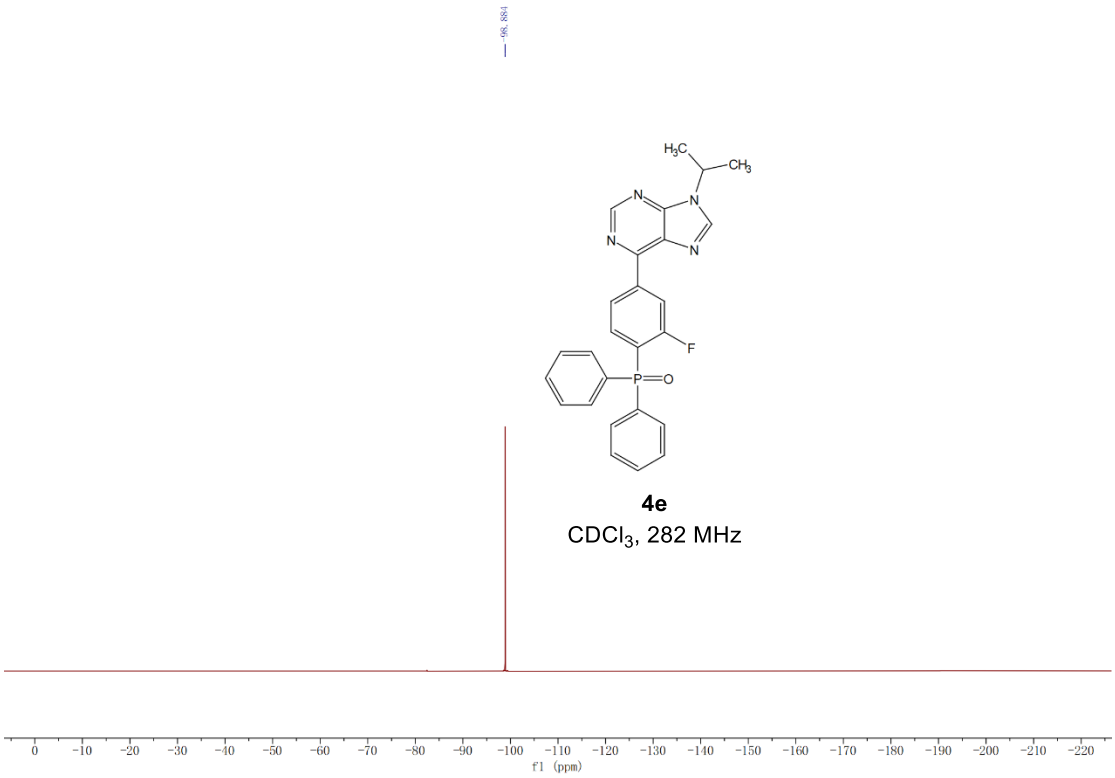






4e

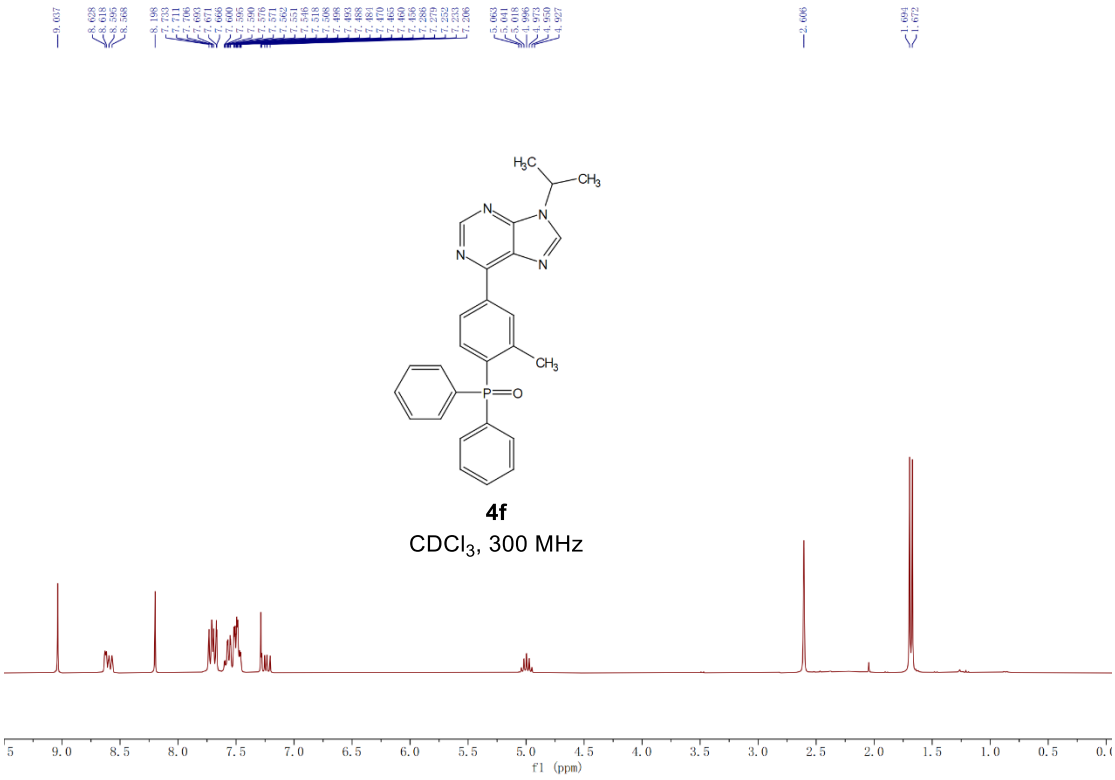
$CDCl_3$, 121 MHz

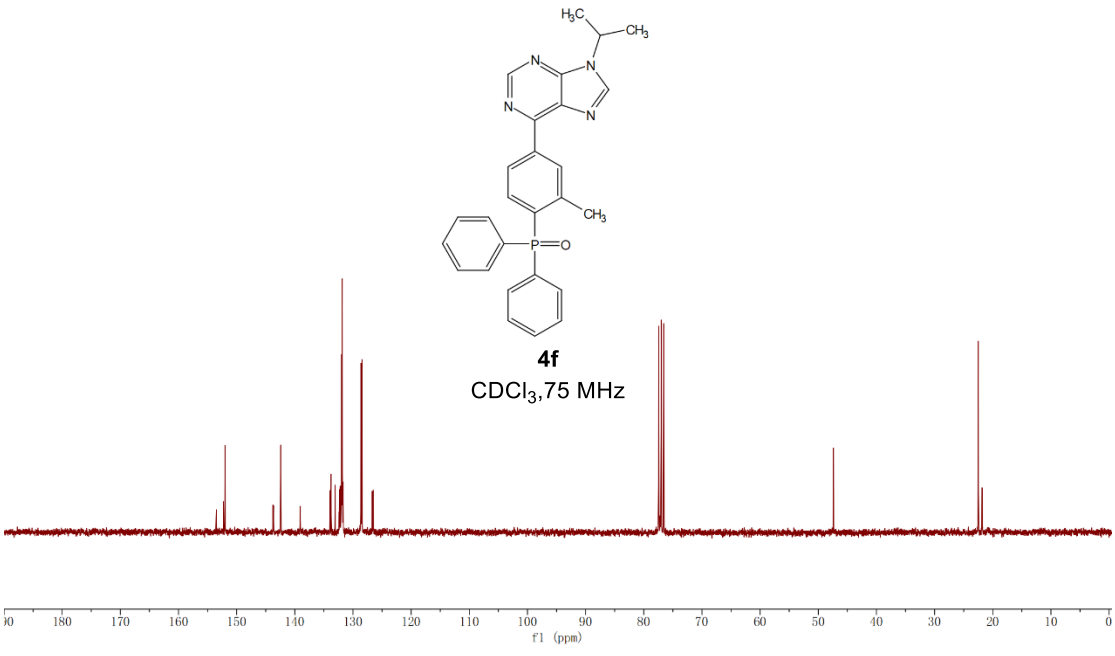


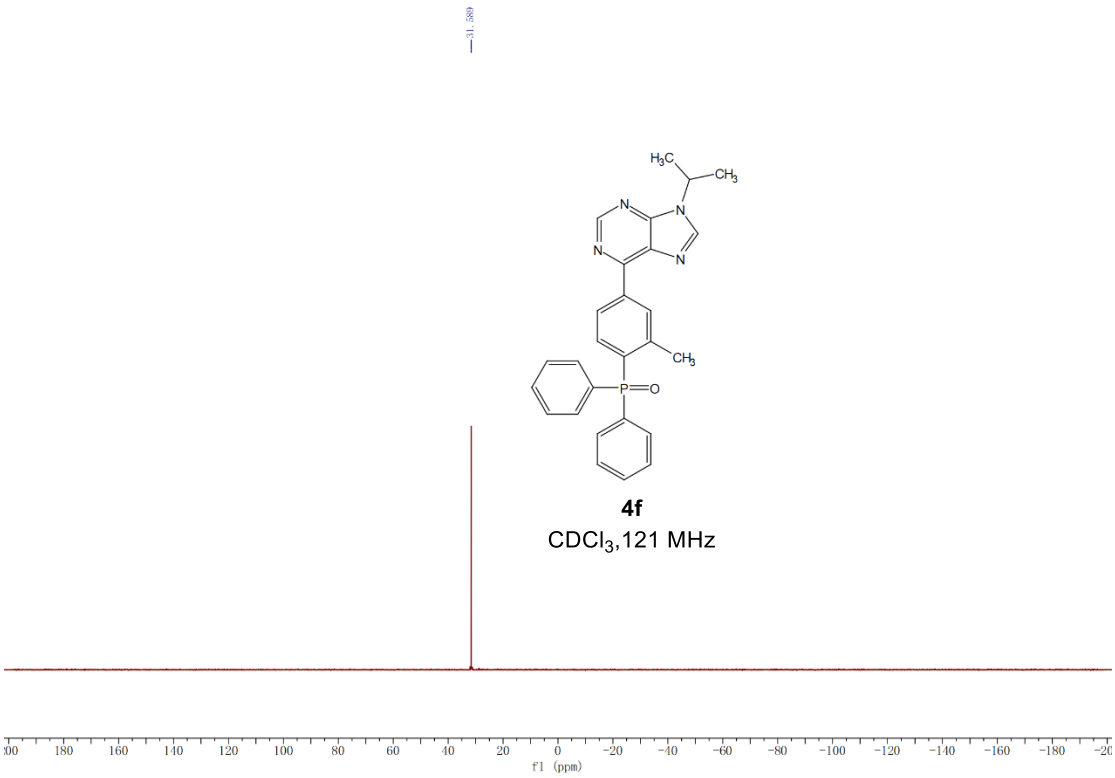
4e

$CDCl_3$, 282 MHz

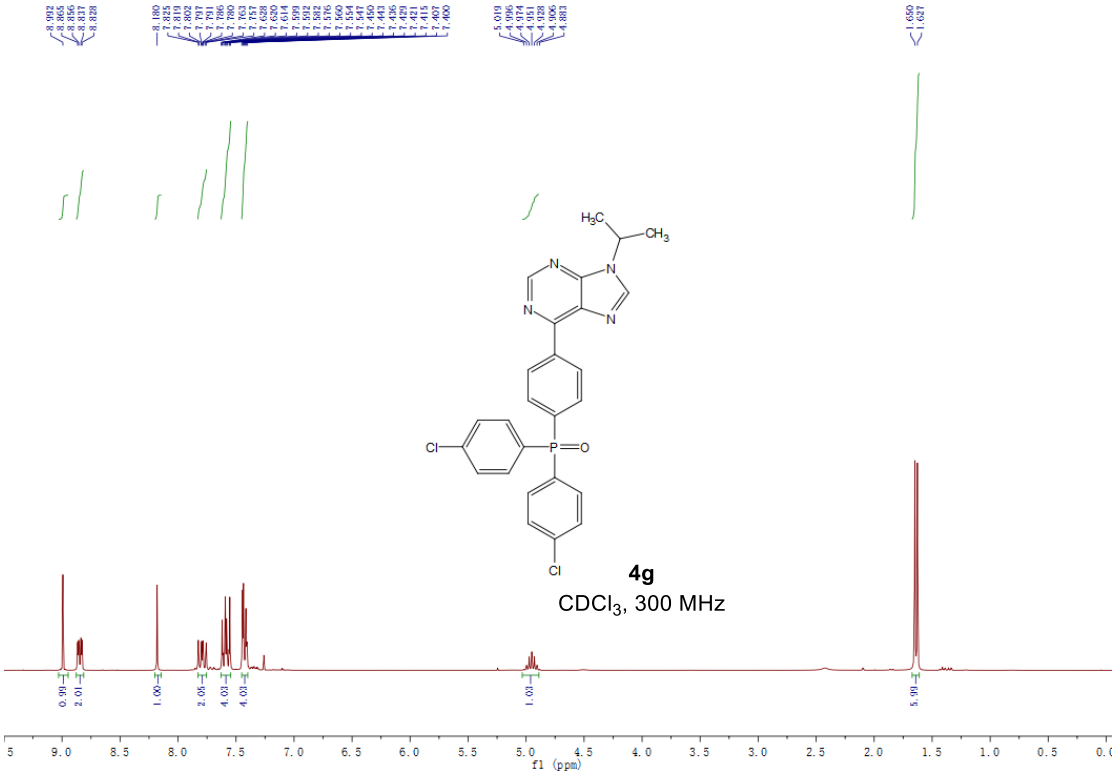
(4-(9-Isopropyl-9H-purin-6-yl)-2-methylphenyl)diphenylphosphine oxide (**4f**)

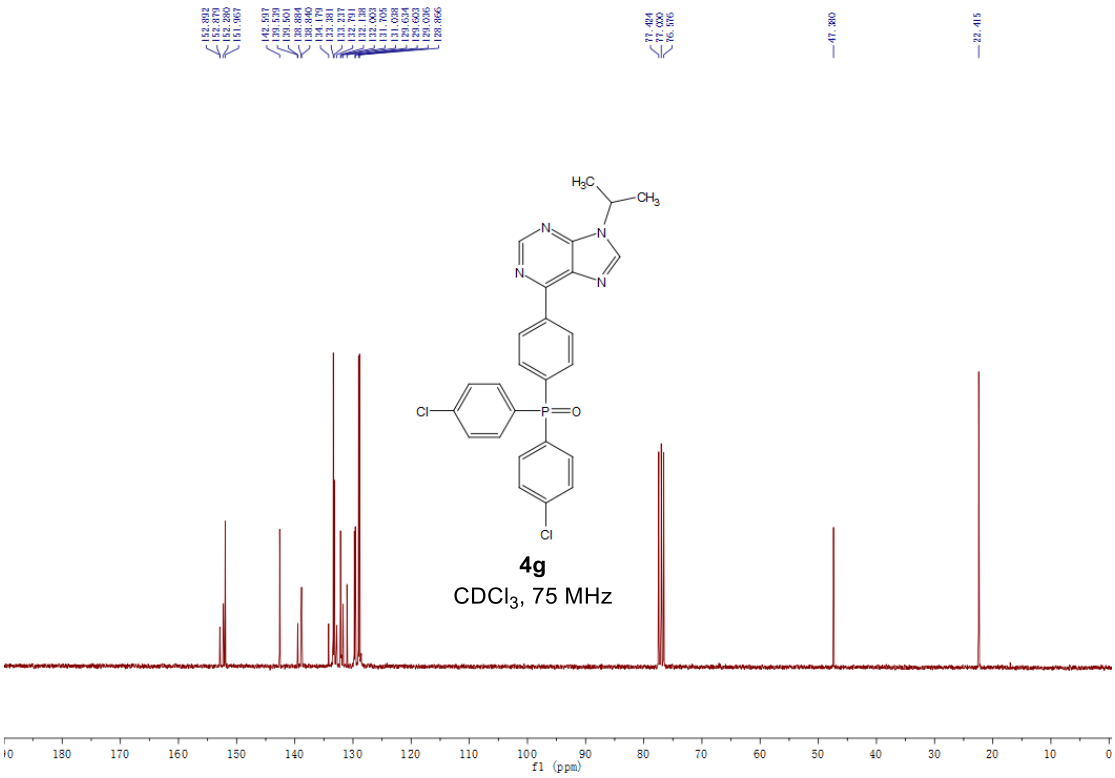






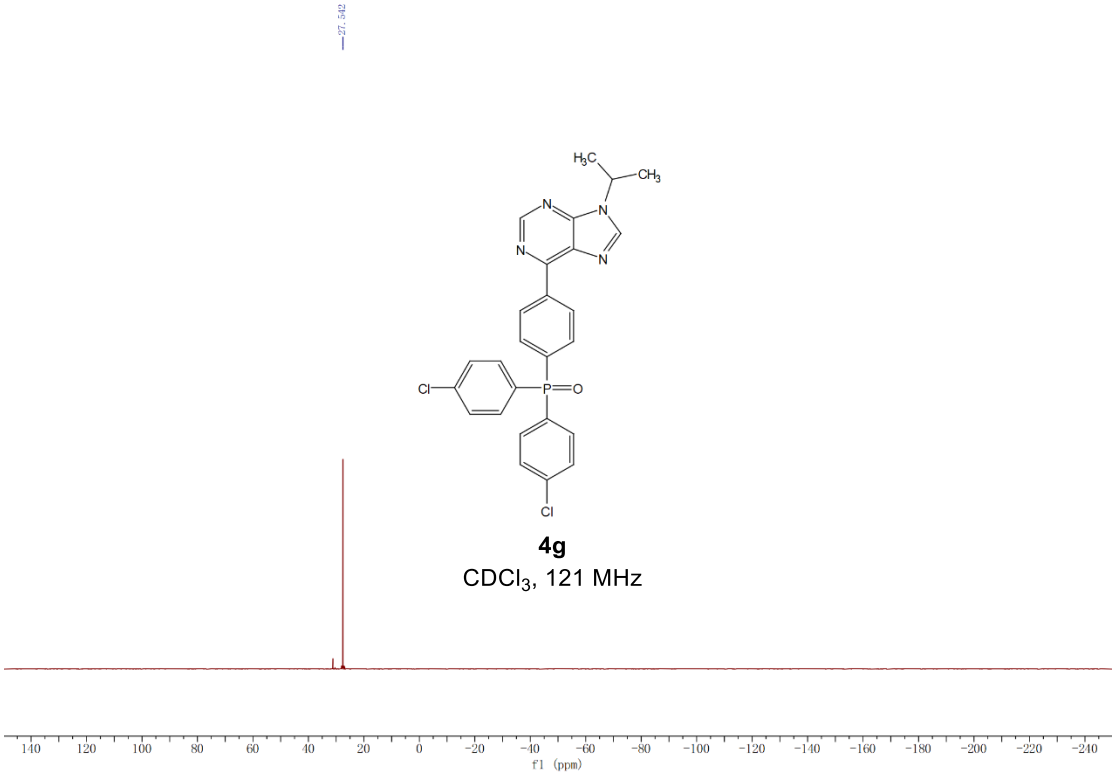
Bis(4-chlorophenyl)(4-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**4g**)





4g

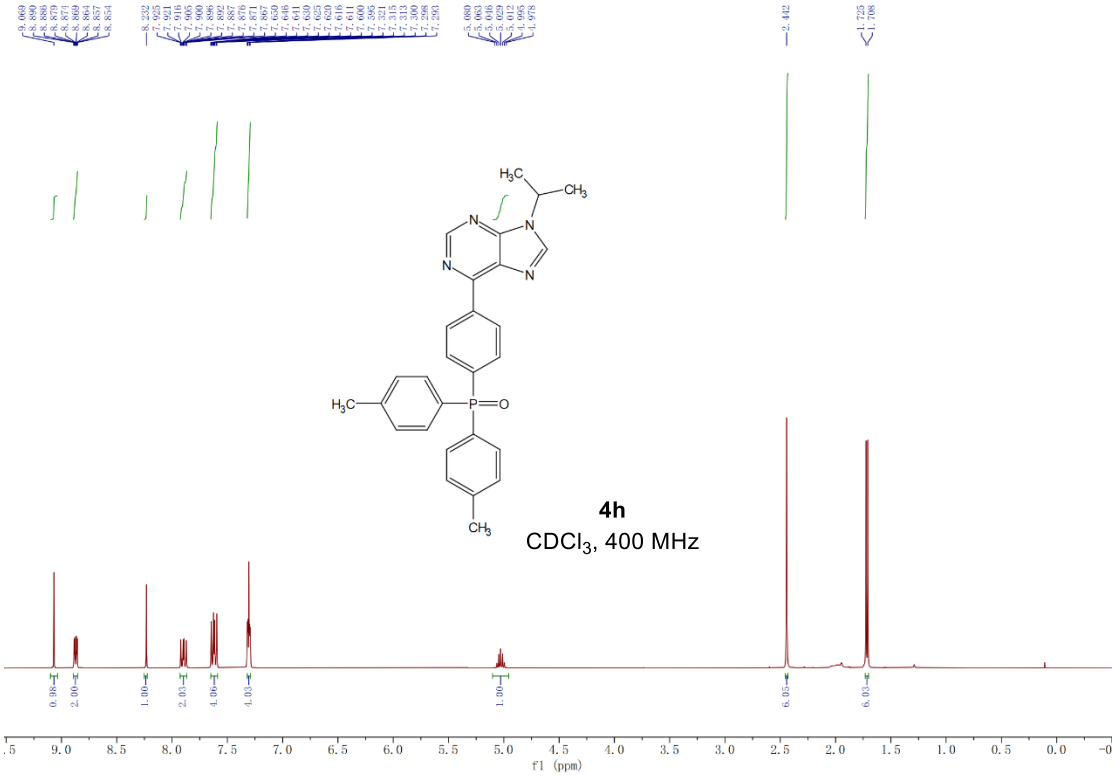
$CDCl_3$, 75 MHz

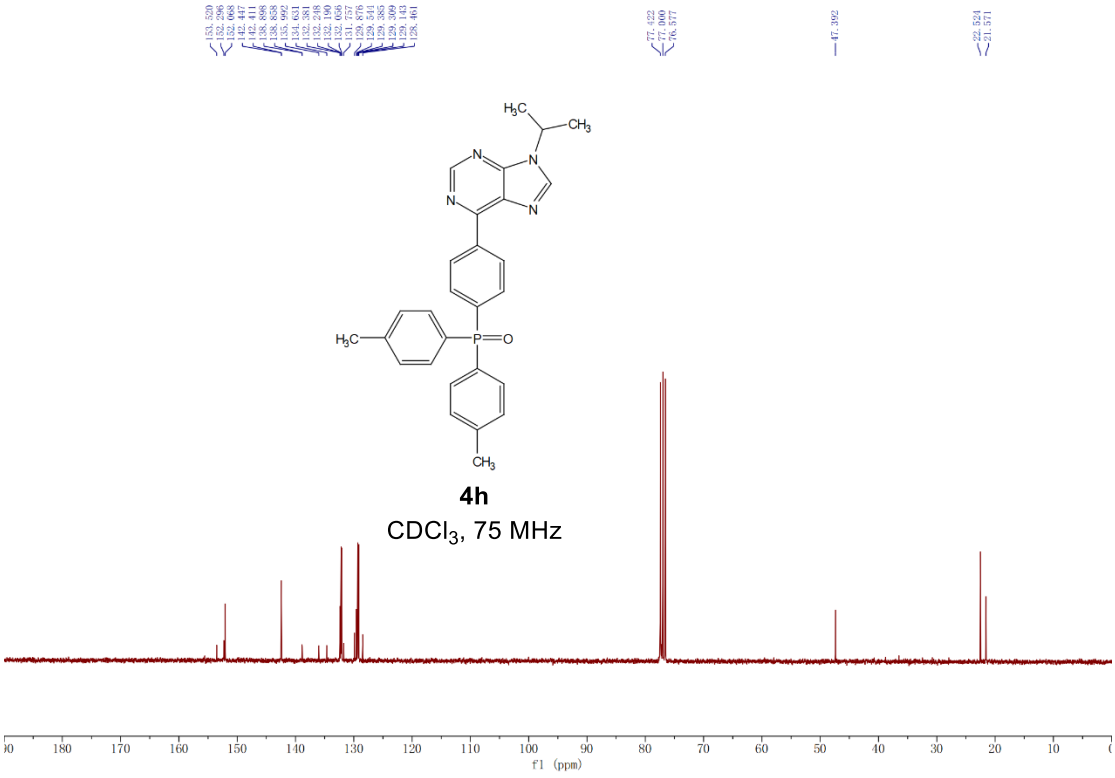


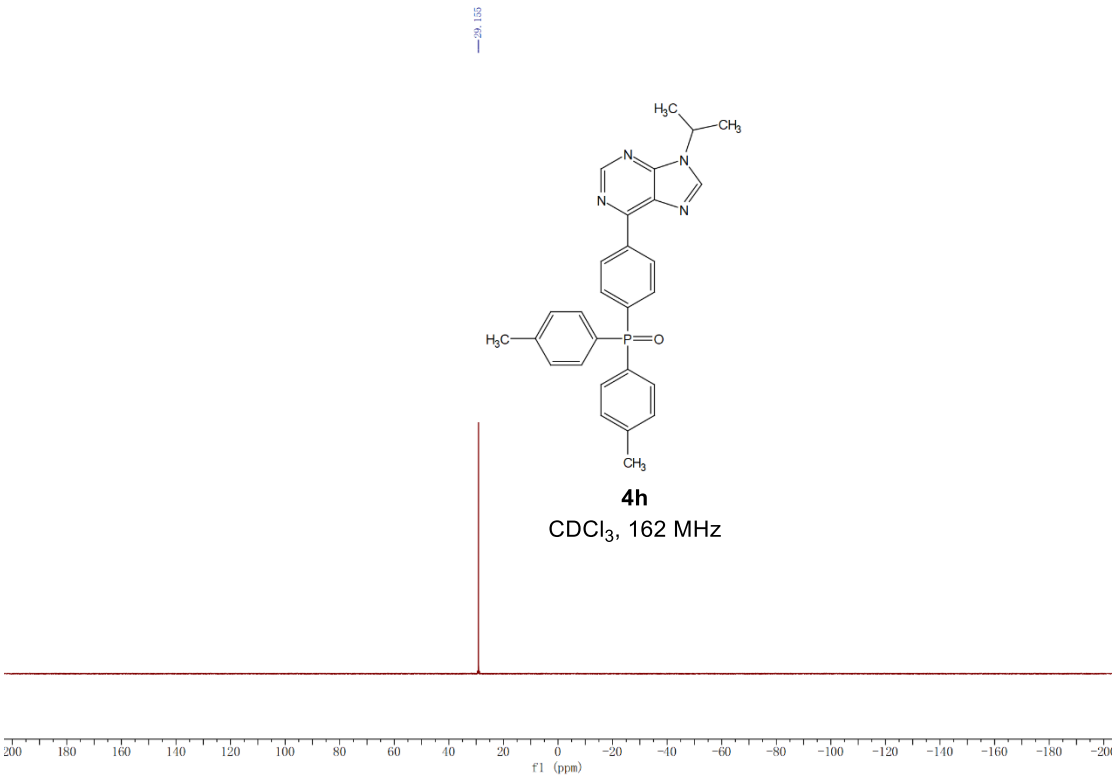
4g

$CDCl_3$, 121 MHz

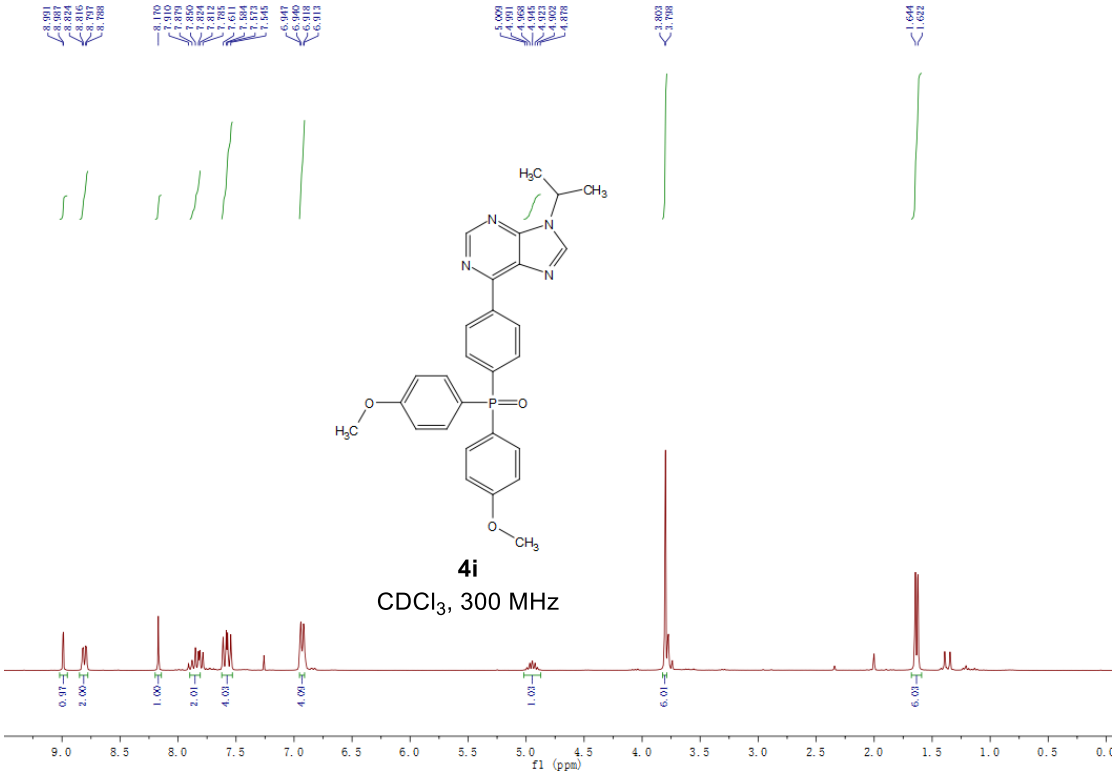
(4-(9-Isopropyl-9H-purin-6-yl)phenyl)di-p-tolylphosphine oxide (**4h**)

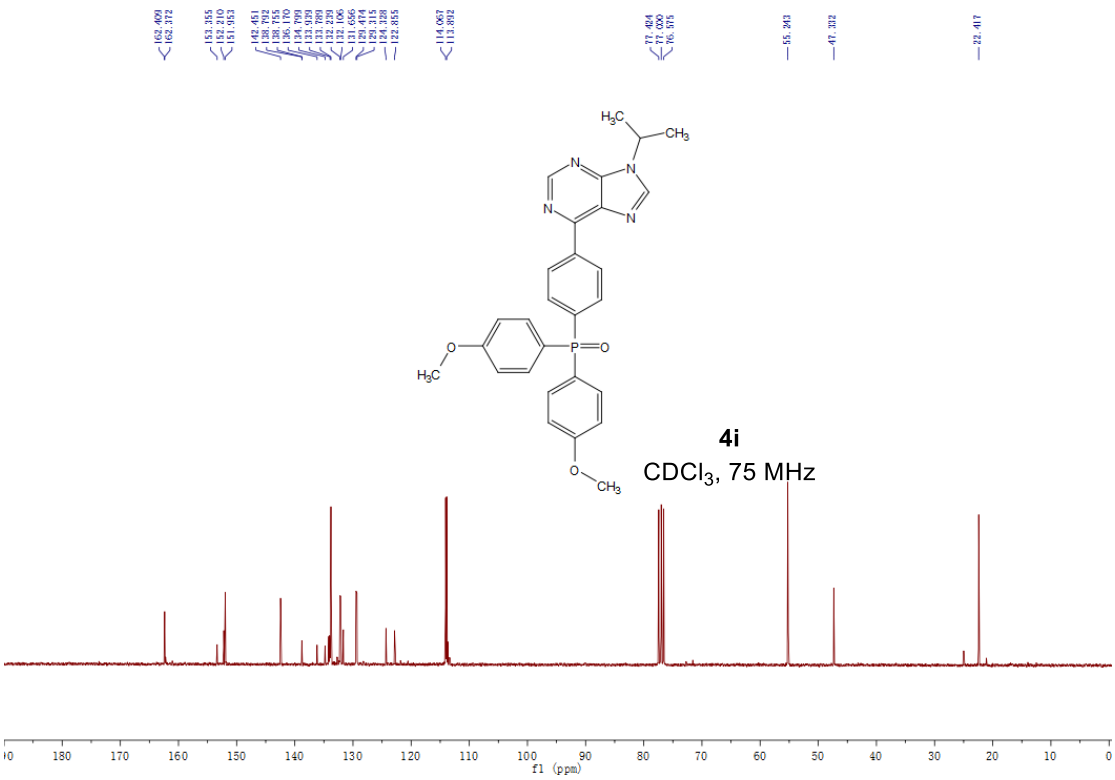


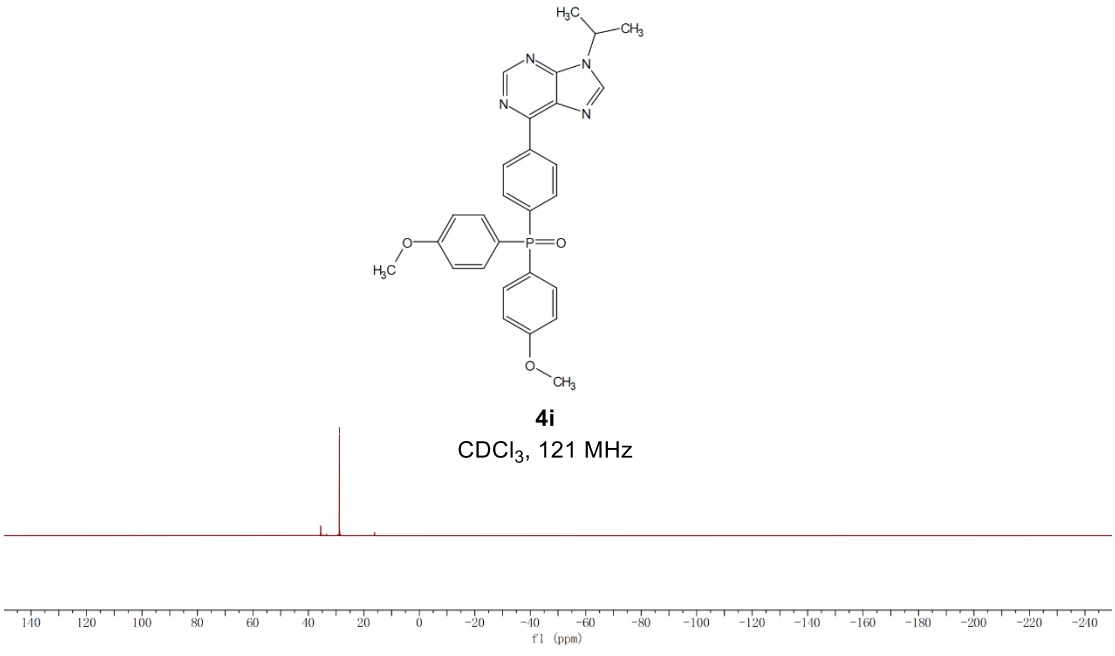




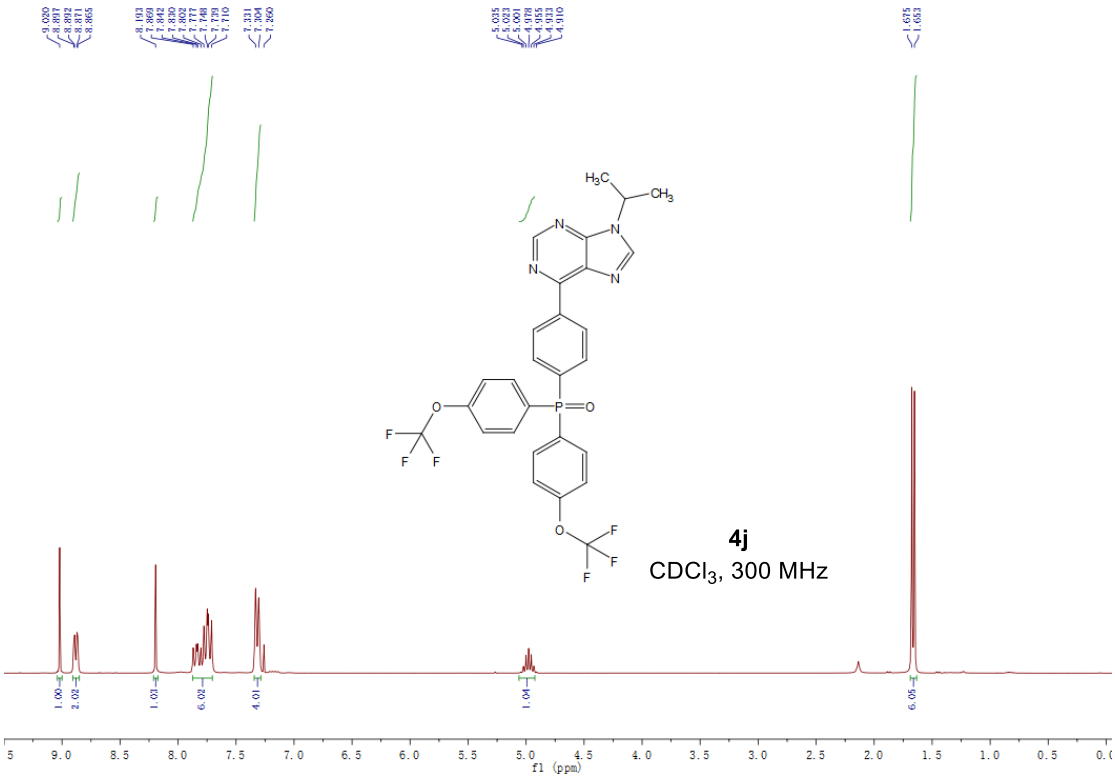
(4-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-methoxyphenyl)phosphine oxide (**4i**)

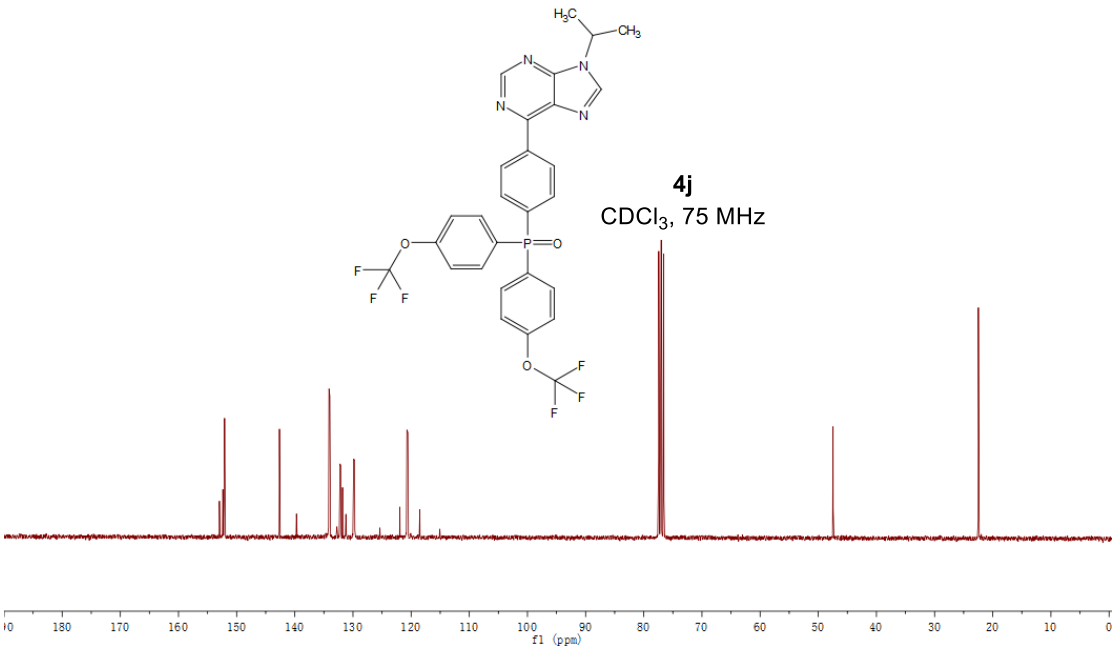


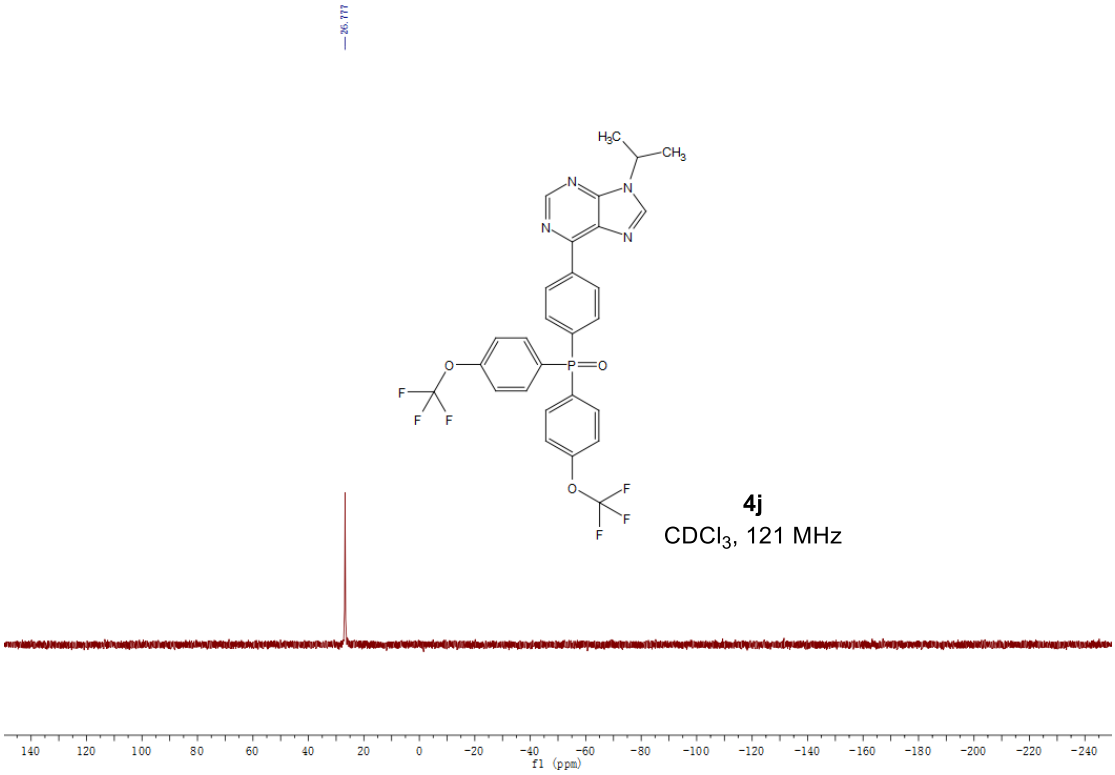

4i
CDCl3, 75 MHz
f1 (ppm)


4i
CDCl3, 121 MHz
f1 (ppm)

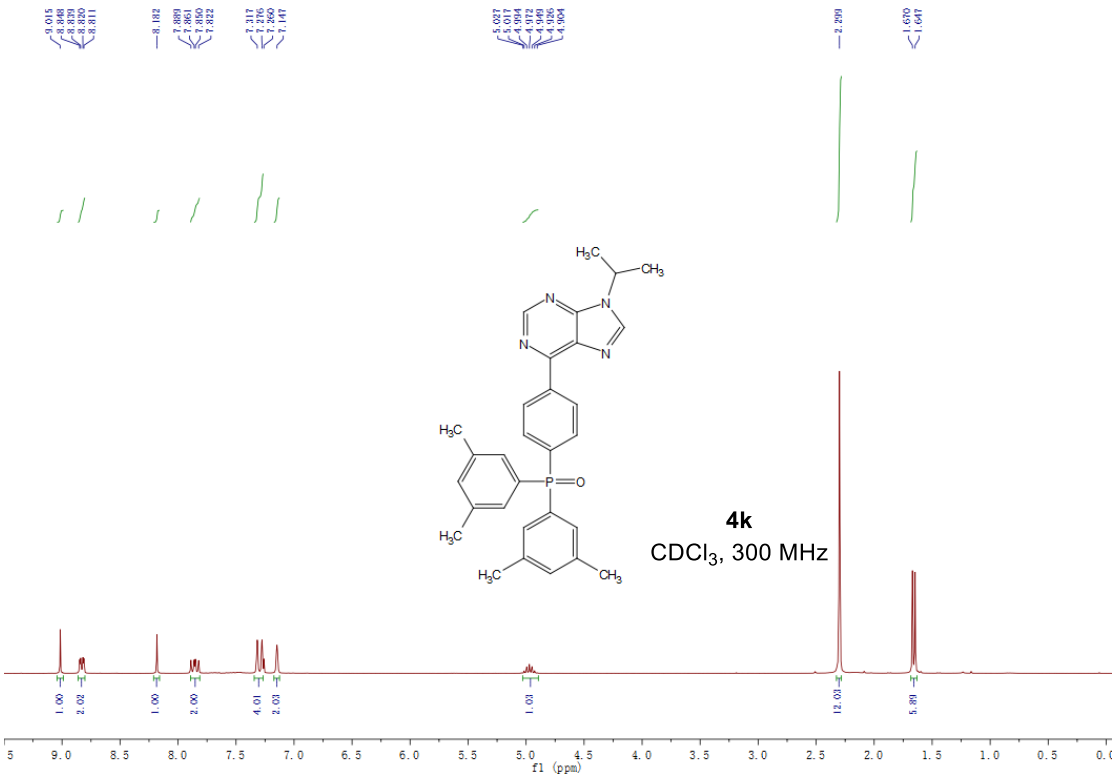
(4-(9-Isopropyl-9H-purin-6-yl)phenyl)bis(4-(trifluoromethoxy)phenyl)phosphine oxide (**4j**)

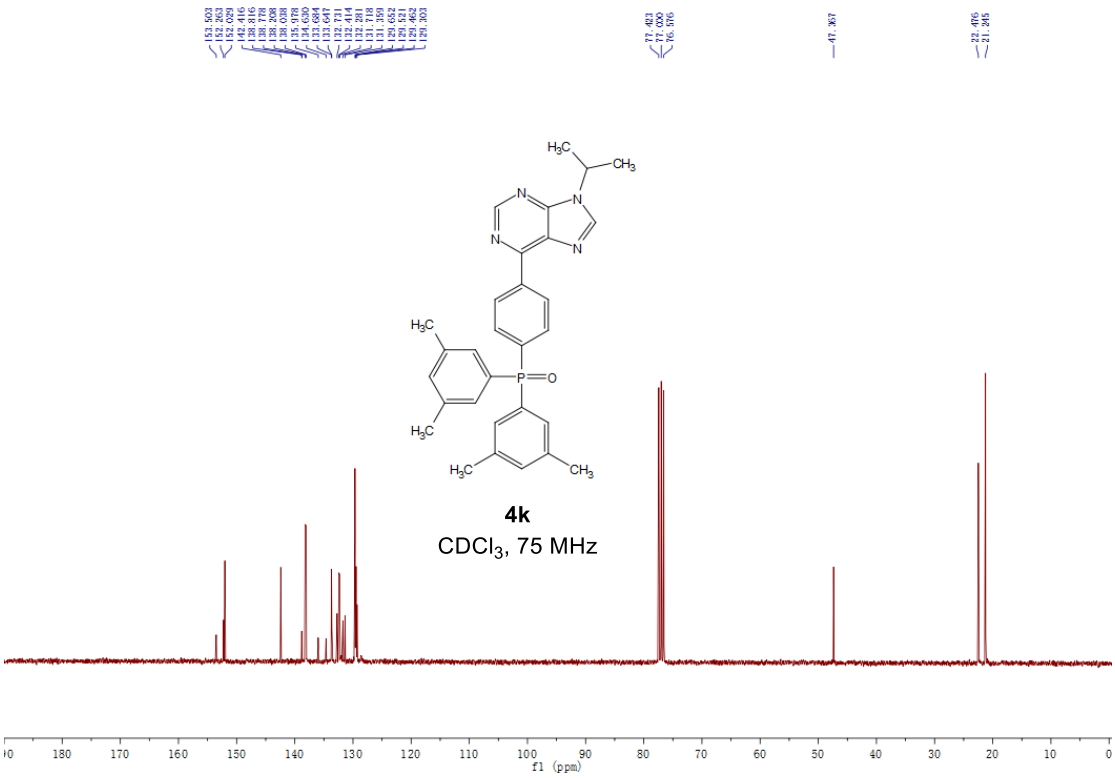


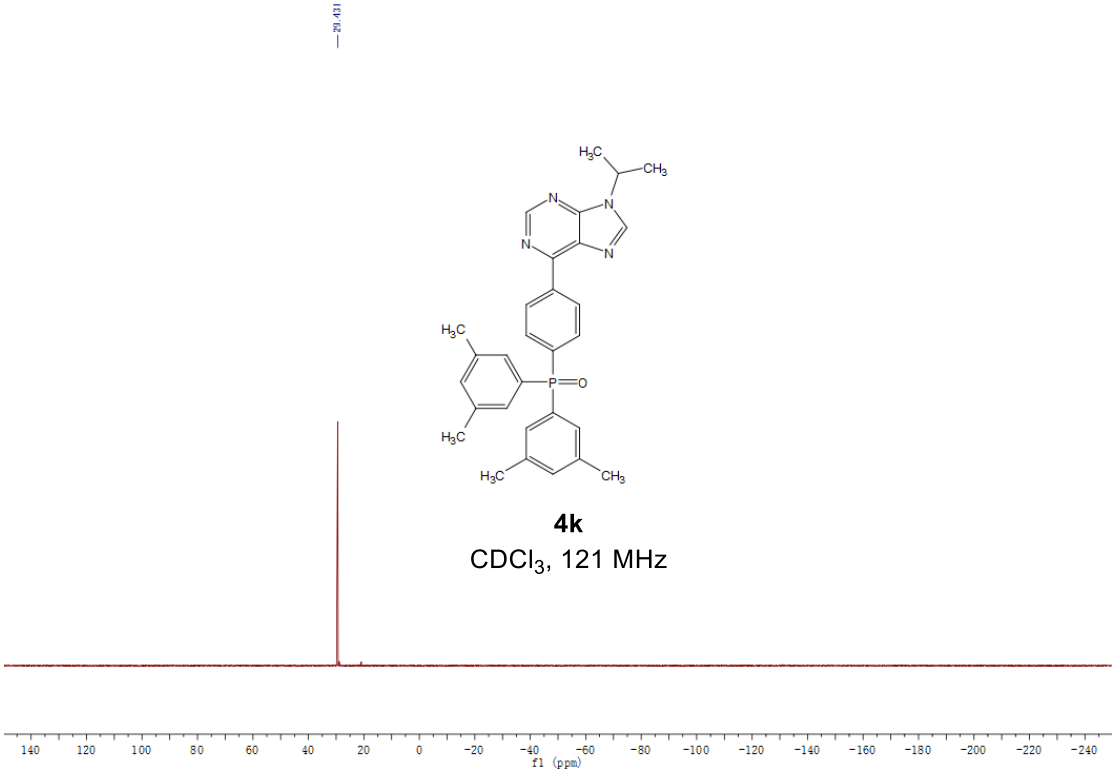




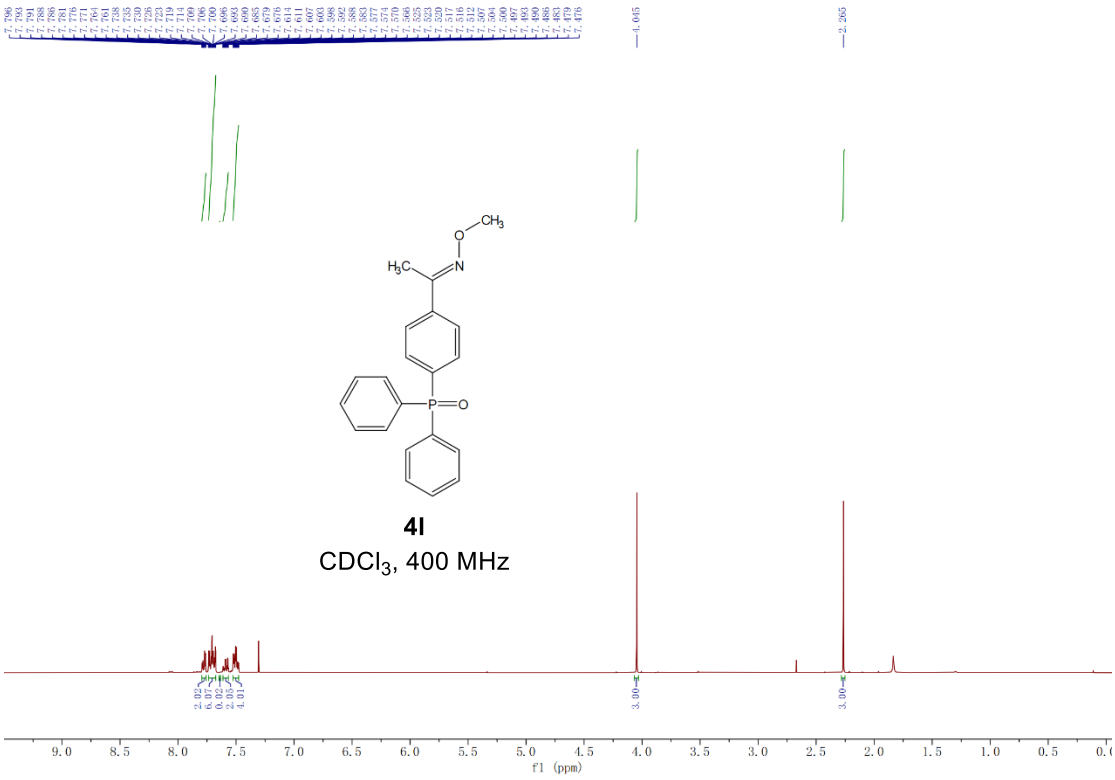
Bis(3,5-dimethylphenyl)(4-(9-isopropyl-9H-purin-6-yl)phenyl)phosphine oxide (**4k**)

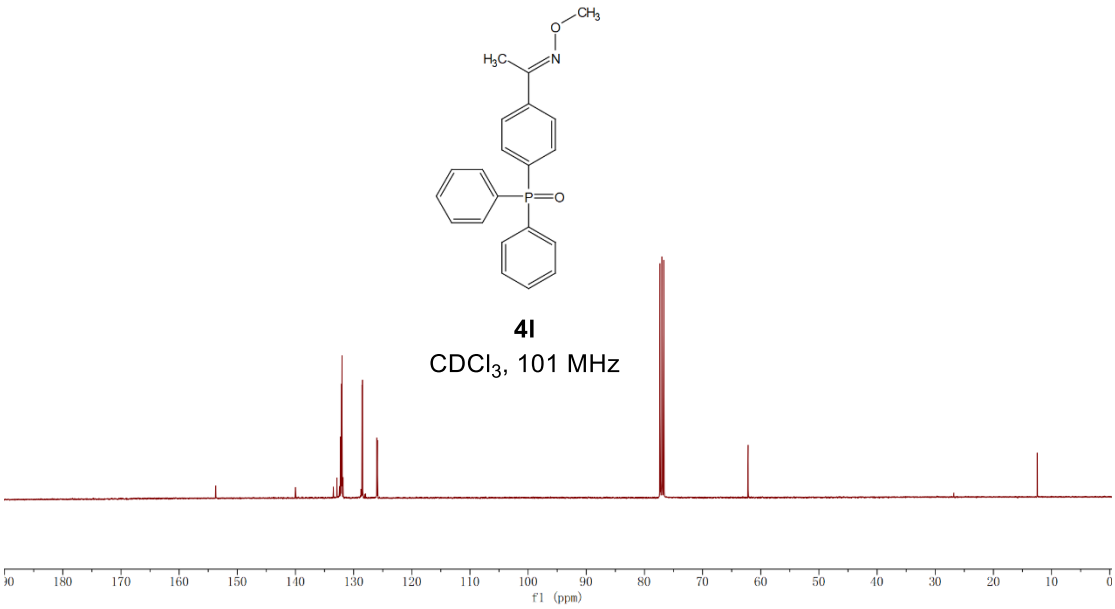


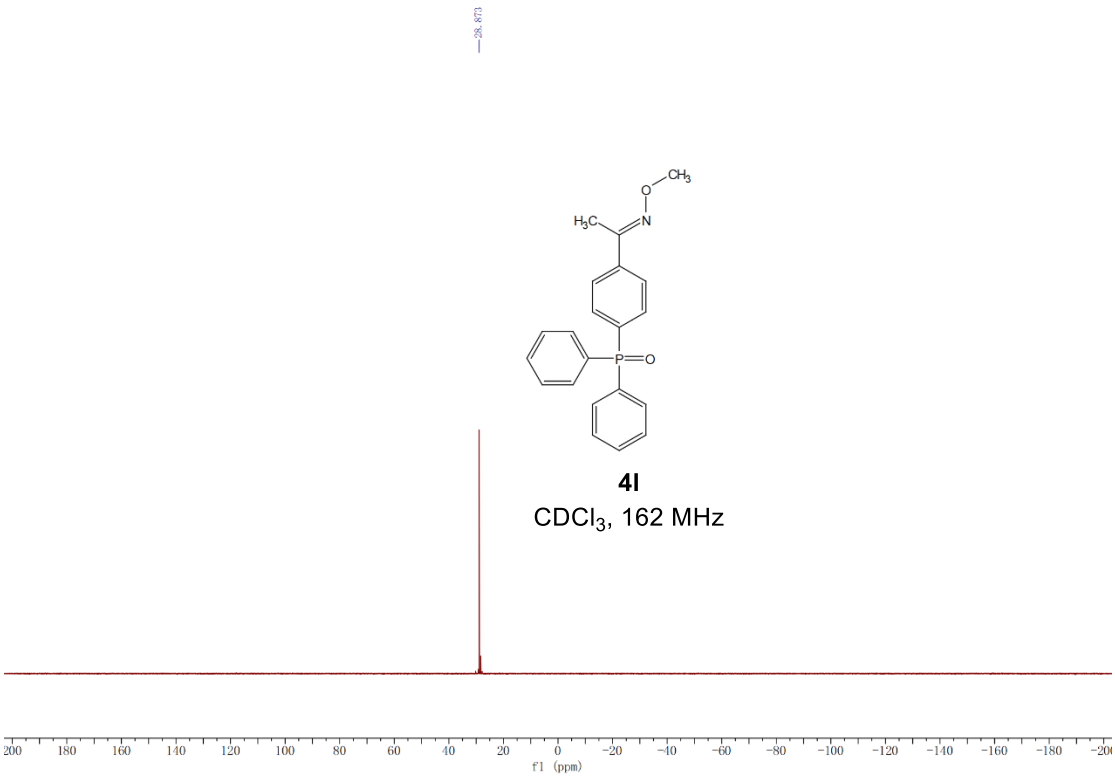

153.503
152.263
152.029
142.416
142.146
138.178
138.028
135.978
134.630
133.694
133.647
132.414
132.281
131.718
131.393
129.652
129.521
129.462
129.303
77.423
77.000
76.576
47.367
22.476
21.345
4k
CDCl3, 75 MHz
f1 (ppm)


29.431
4k
CDCl3, 121 MHz
f1 (ppm)

(E)-(4-(1-(Methoxyimino)ethyl)phenyl)diphenylphosphine oxide (**4l**)



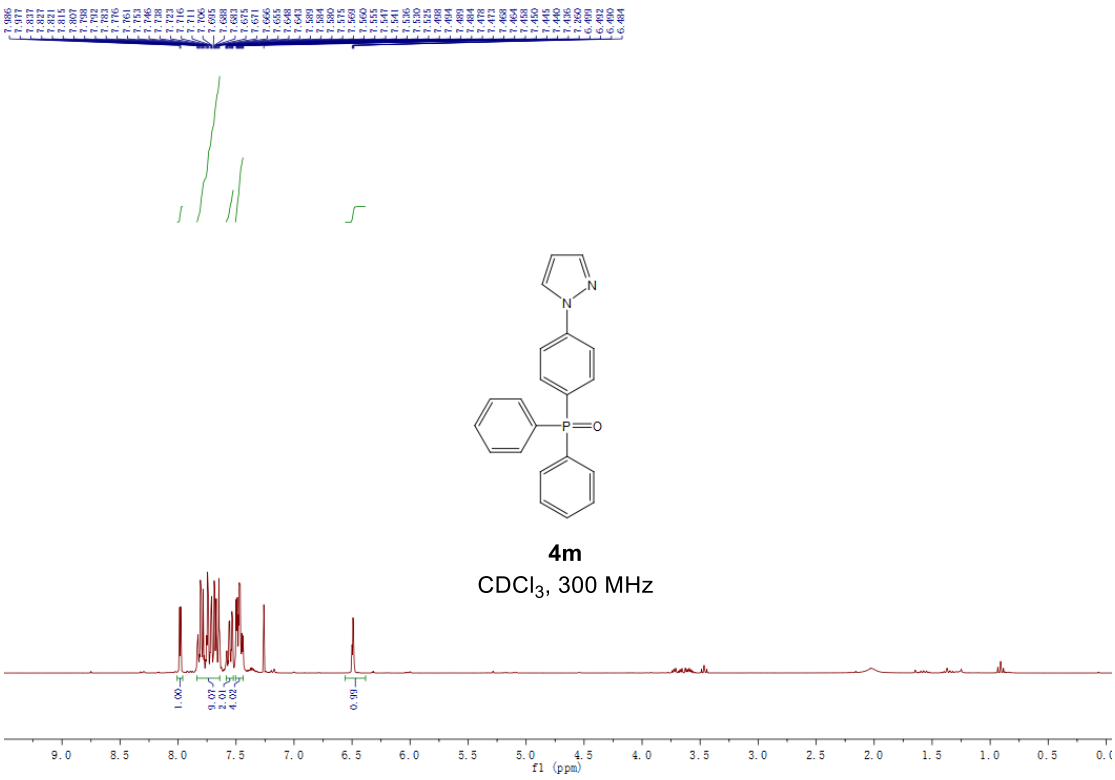




4l

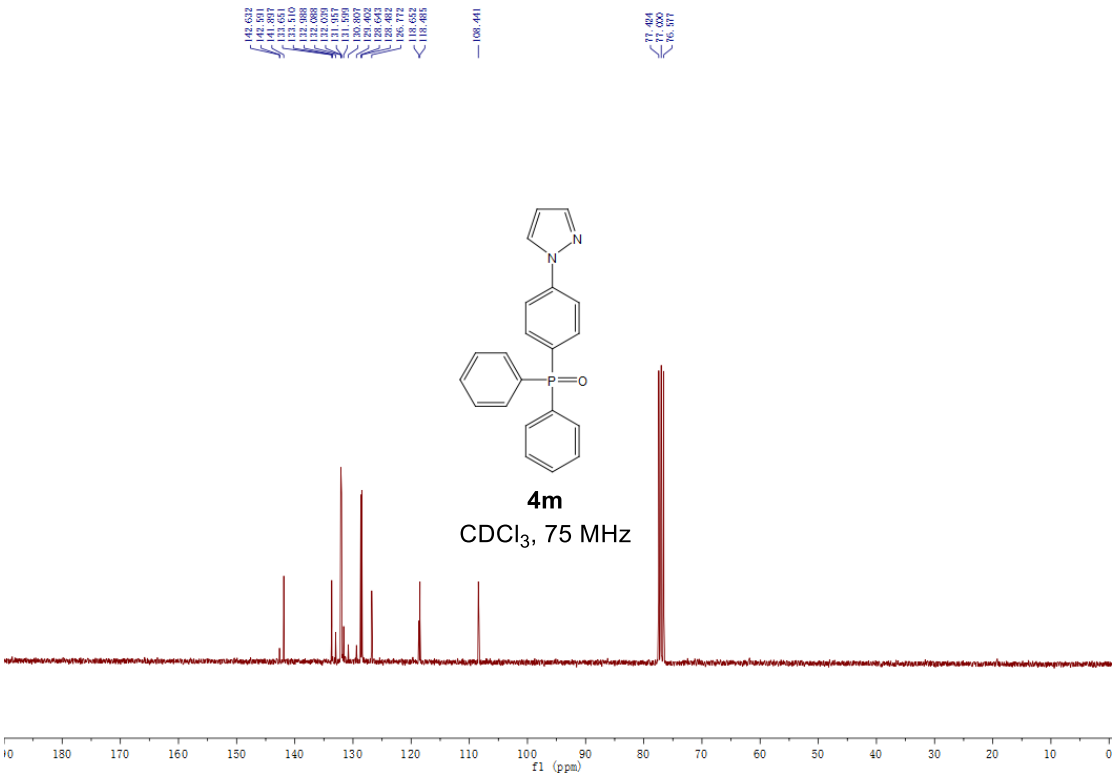
$CDCl_3$, 162 MHz

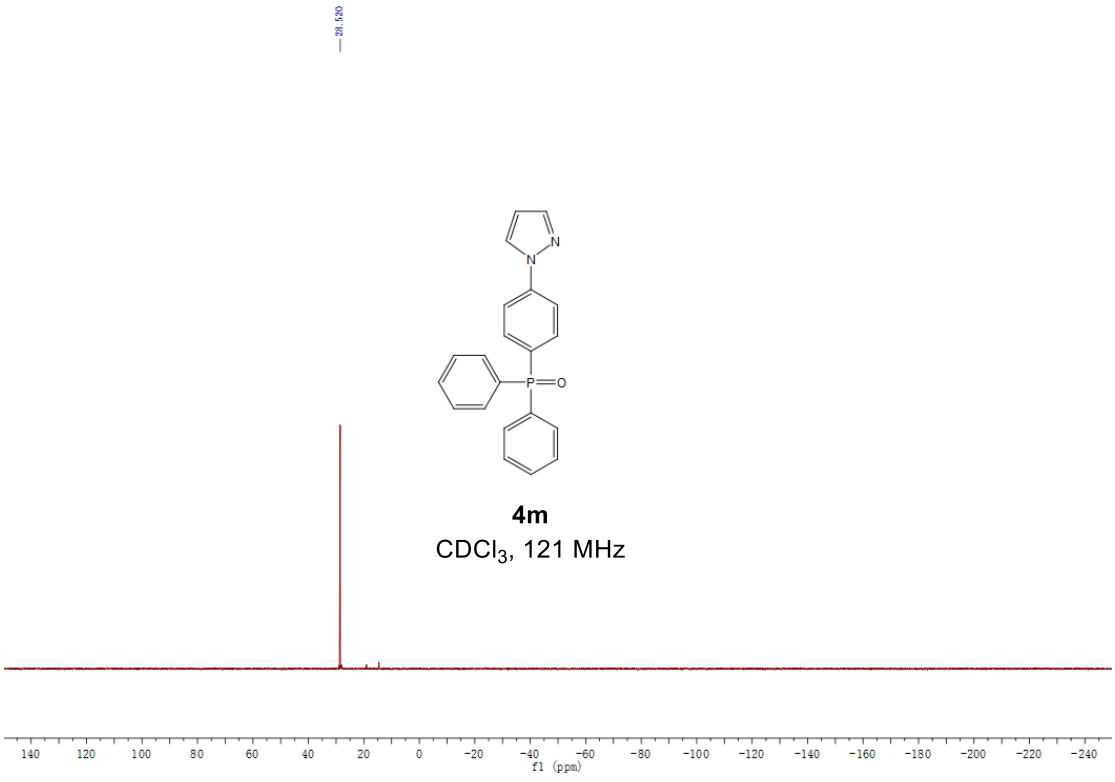
(4-(1H-pyrazol-1-yl)phenyl)diphenylphosphine oxide (**4m**)

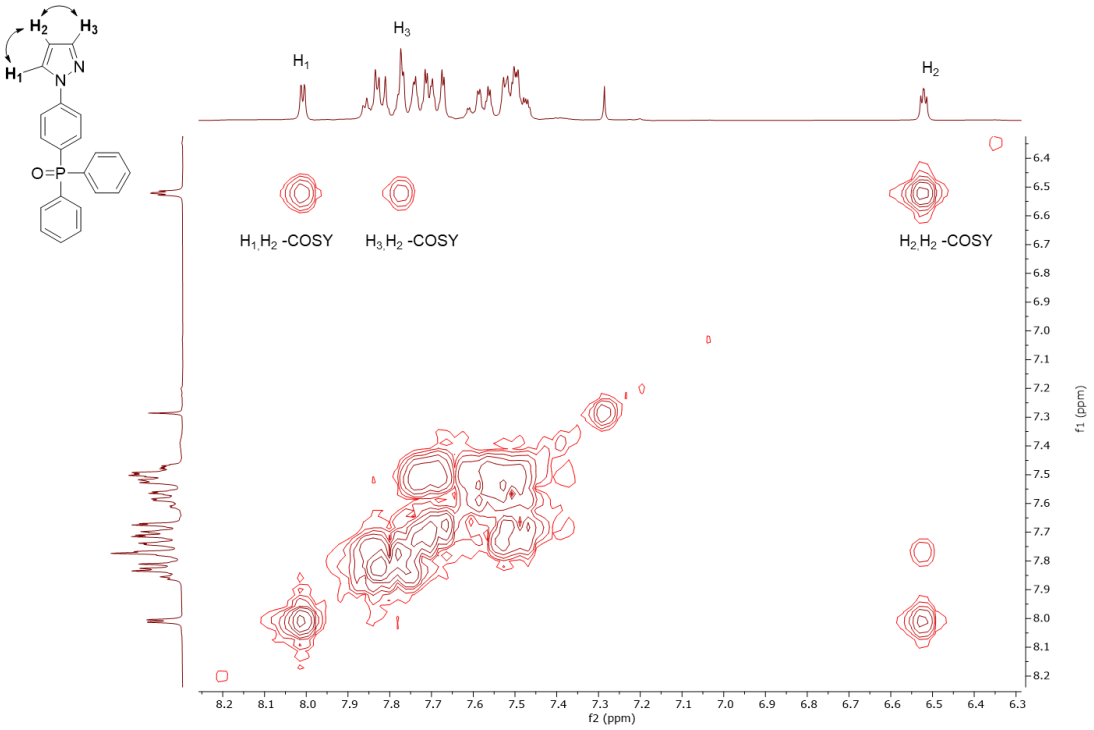


4m

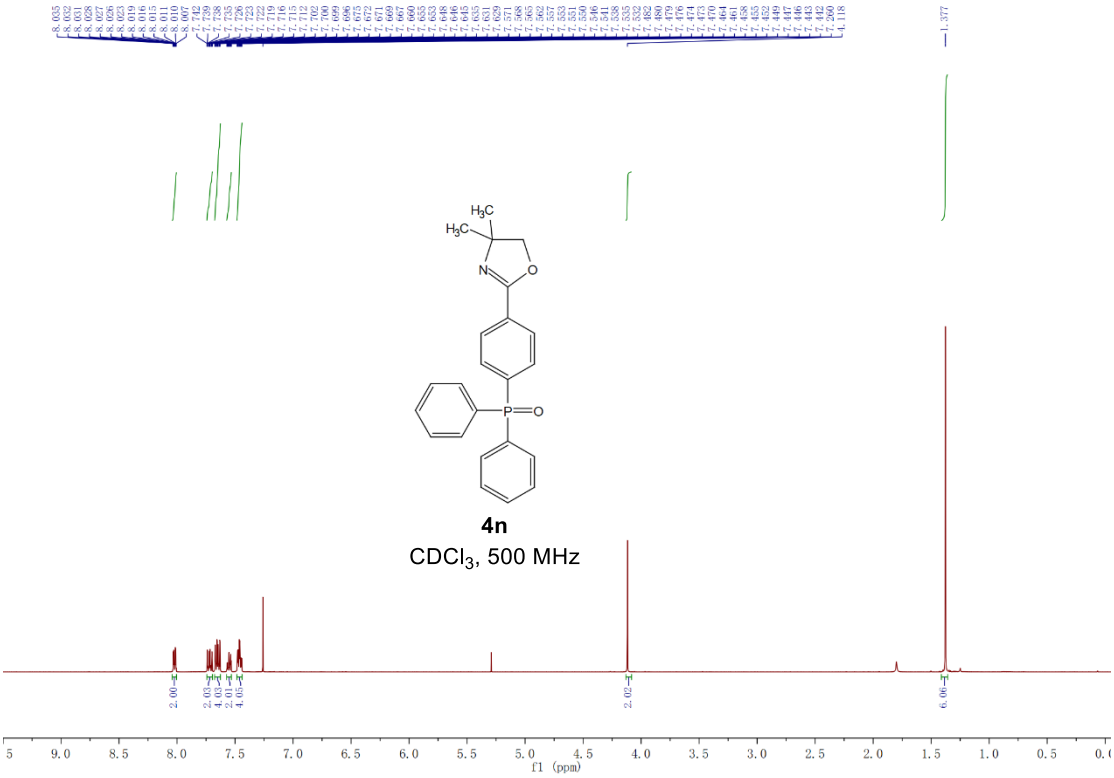
$CDCl_3$, 300 MHz

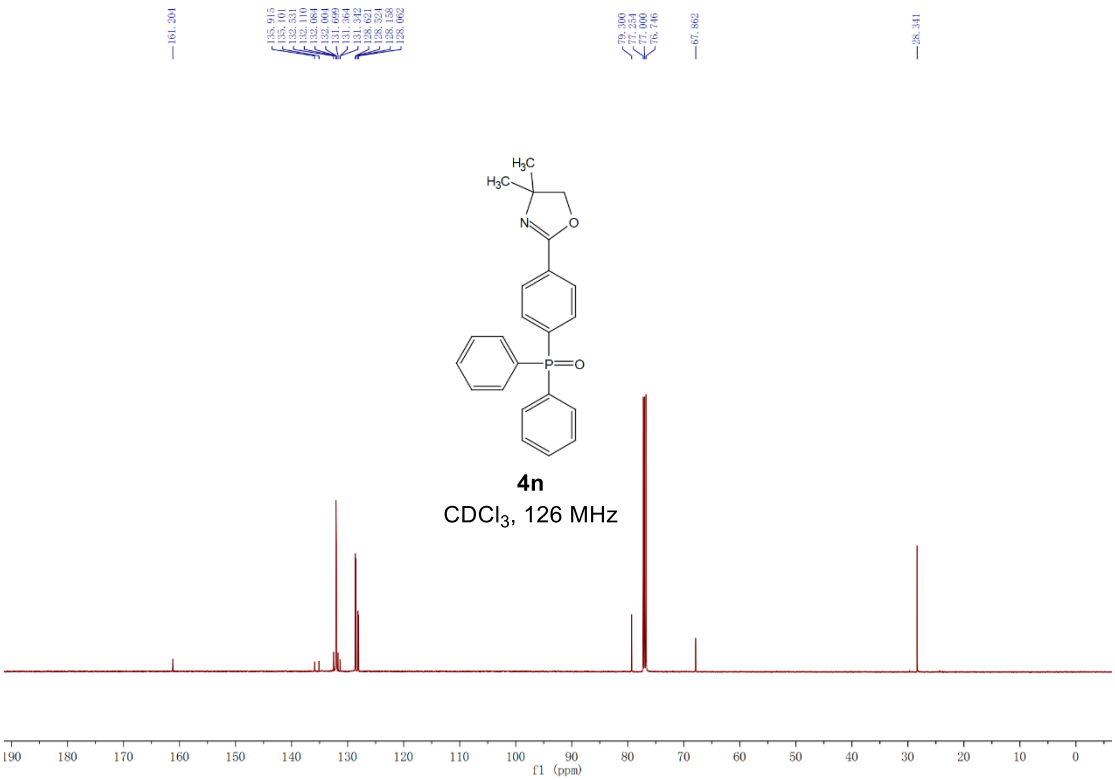

142.632
142.591
141.897
133.641
133.510
132.988
132.088
131.957
131.599
130.807
129.402
128.643
128.482
126.772
118.652
118.485
108.441
77.404
77.000
76.977
N
N
P=O
4m
CDCl3, 75 MHz
f1 (ppm)

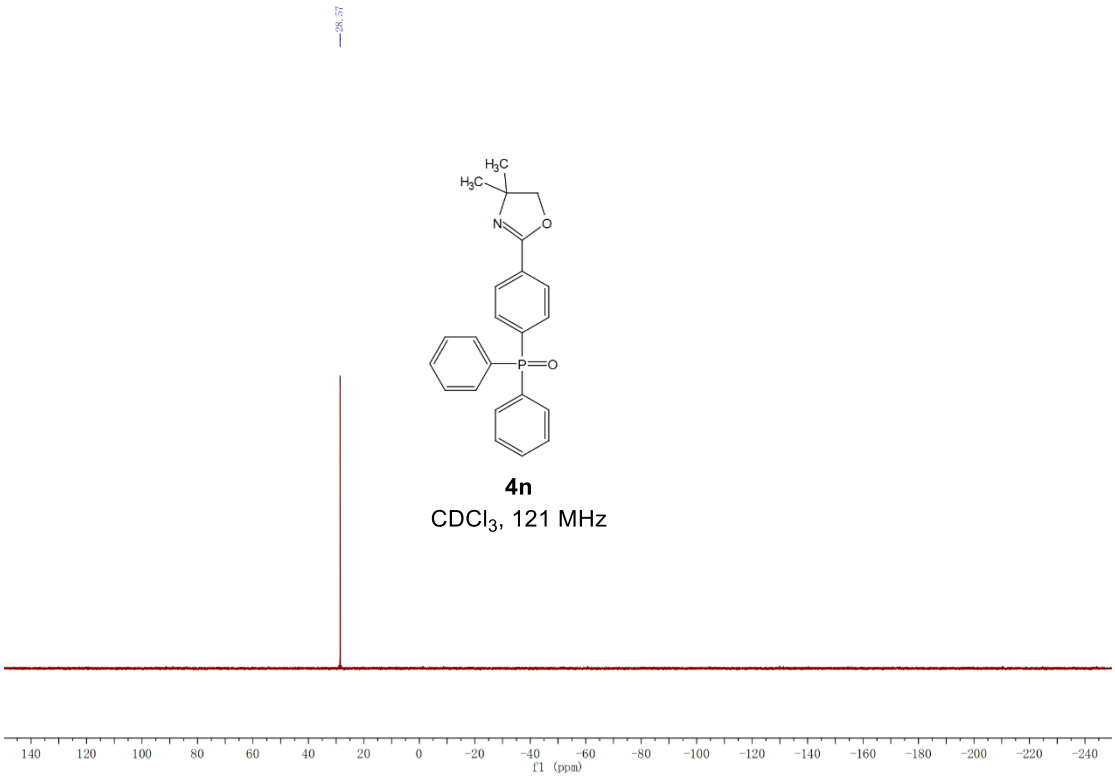

28.520
N
N
P=O
4m
CDCl3, 121 MHz
f1 (ppm)



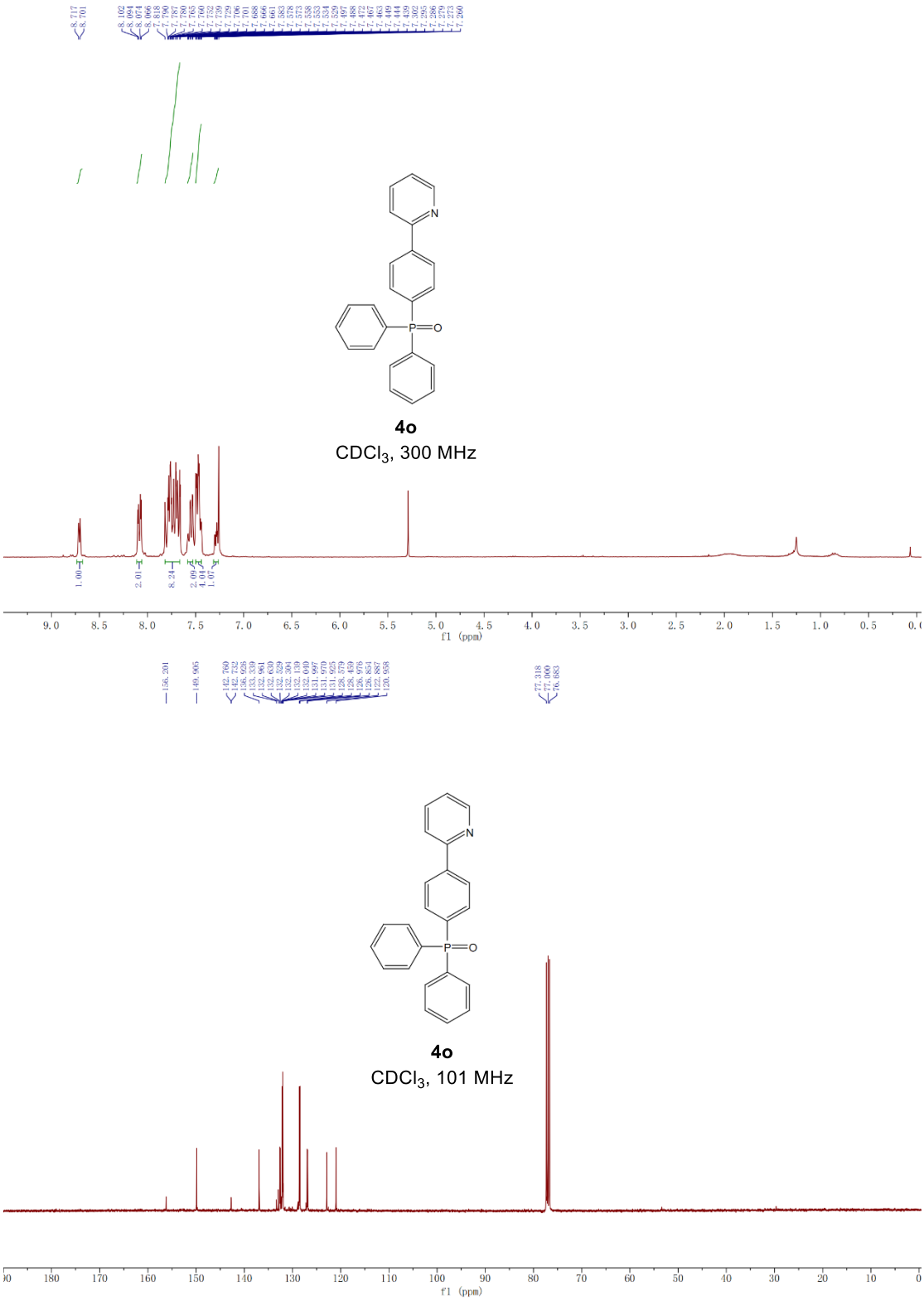
(4-(4,4-Dimethyl-4,5-dihydrooxazol-2-yl)phenyl)diphenylphosphine oxide (**4n**)

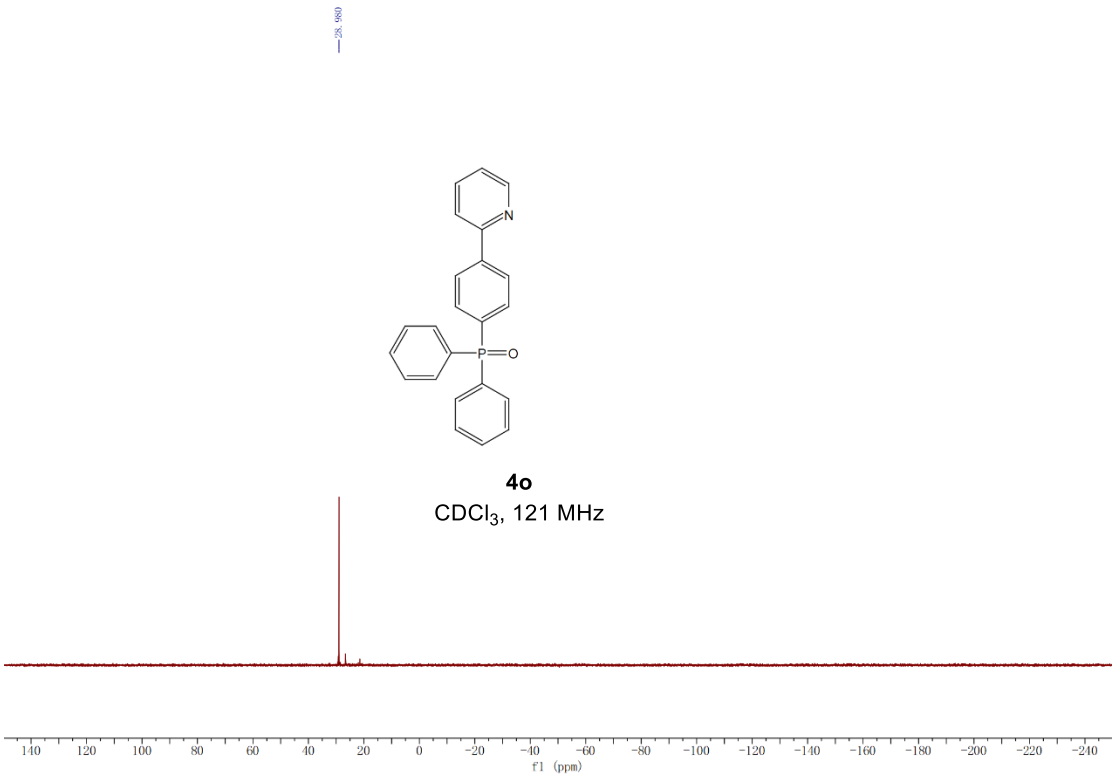



161.204
135.915
135.101
132.533
132.110
132.084
132.004
131.696
131.364
131.342
128.621
128.254
128.138
128.062
79.300
77.254
77.000
76.746
67.862
28.341
H3C
H3C
N
O
P=O
4n
CDCl3, 126 MHz
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

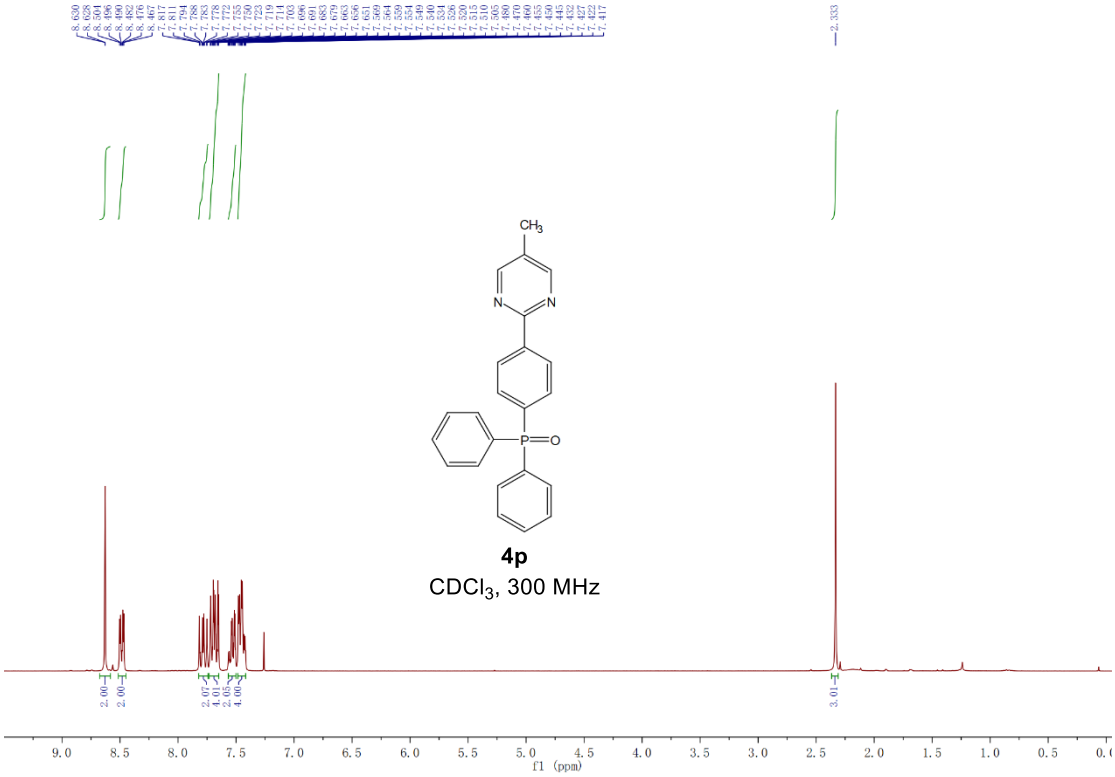

28.57
H3C
H3C
N
O
P=O
4n
CDCl3, 121 MHz
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)

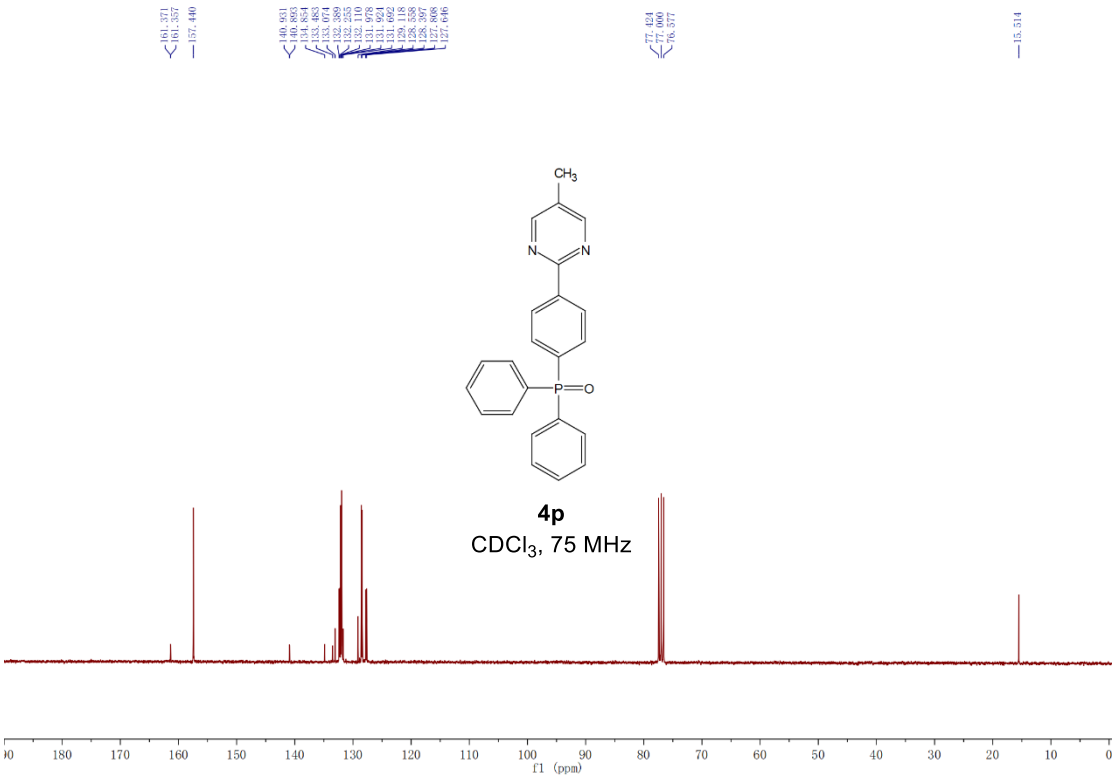
Diphenyl(4-(pyridin-2-yl)phenyl)phosphine oxide (**4o**)

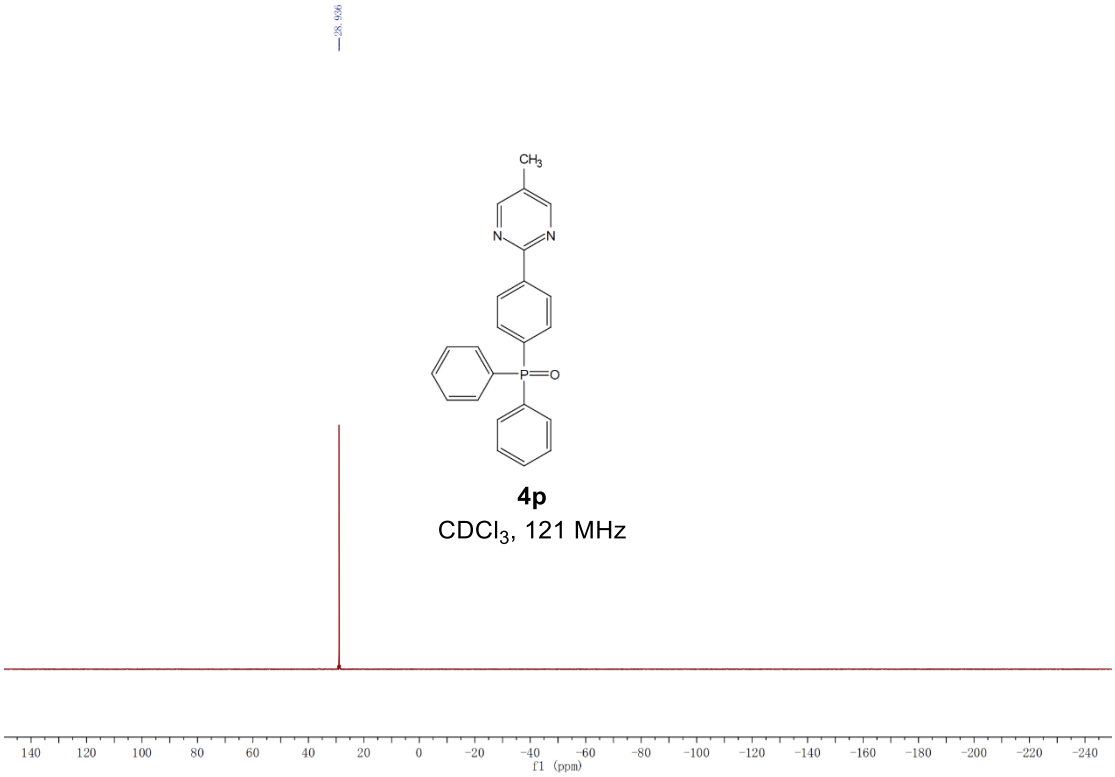




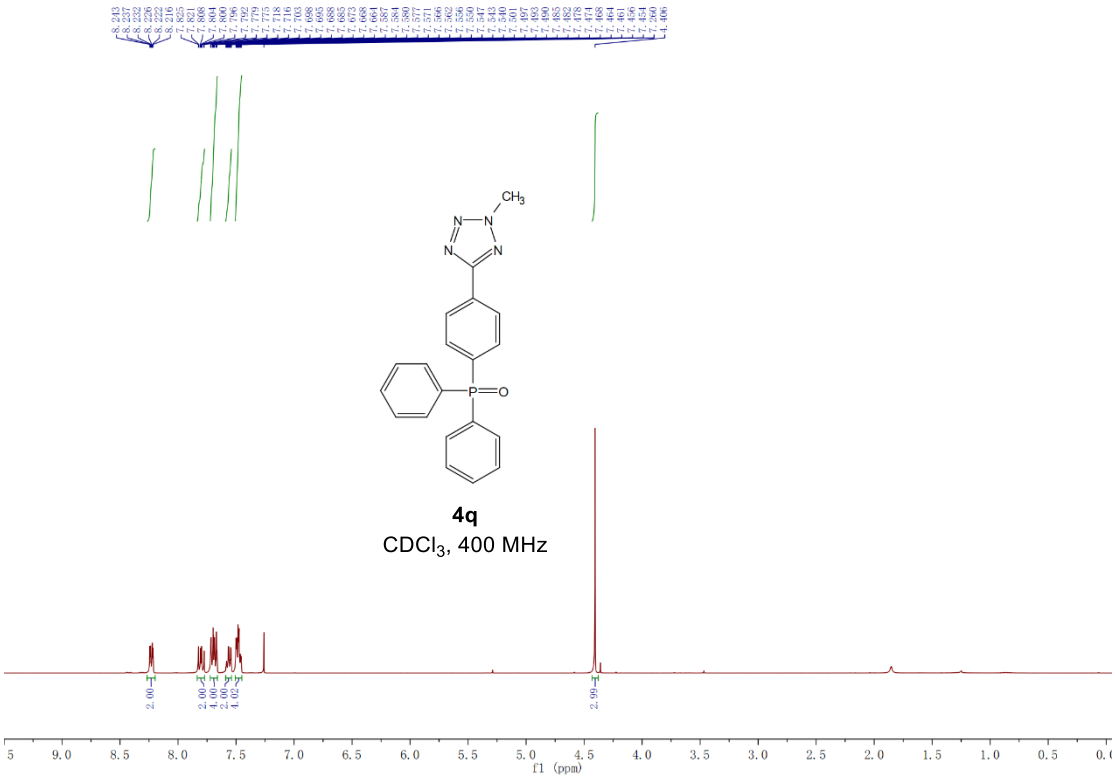
(4-(5-Methylpyrimidin-2-yl)phenyl)diphenylphosphine oxide (**4p**)

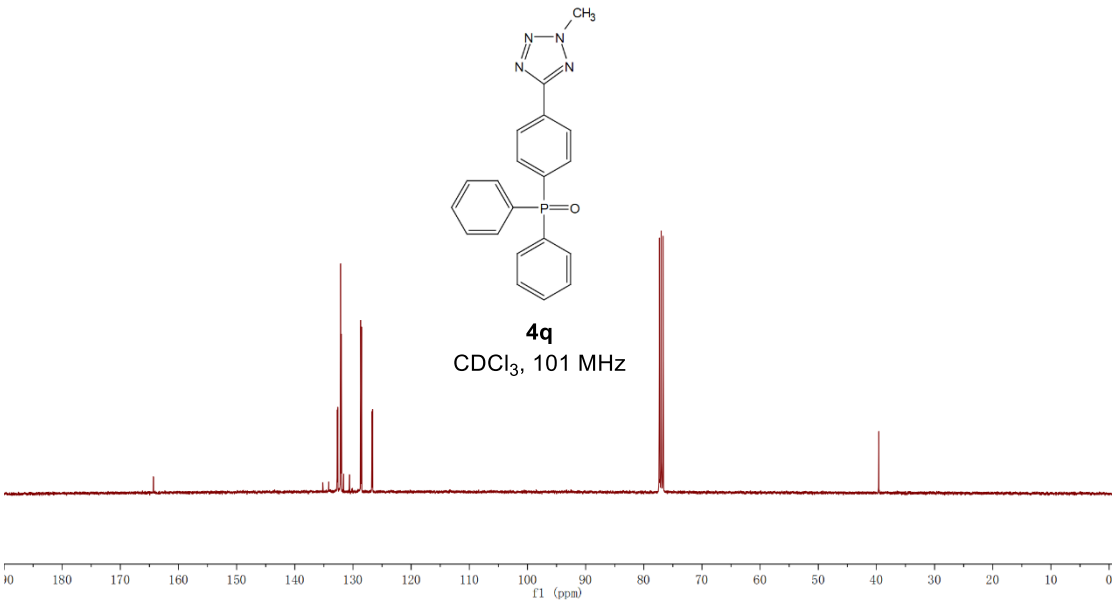


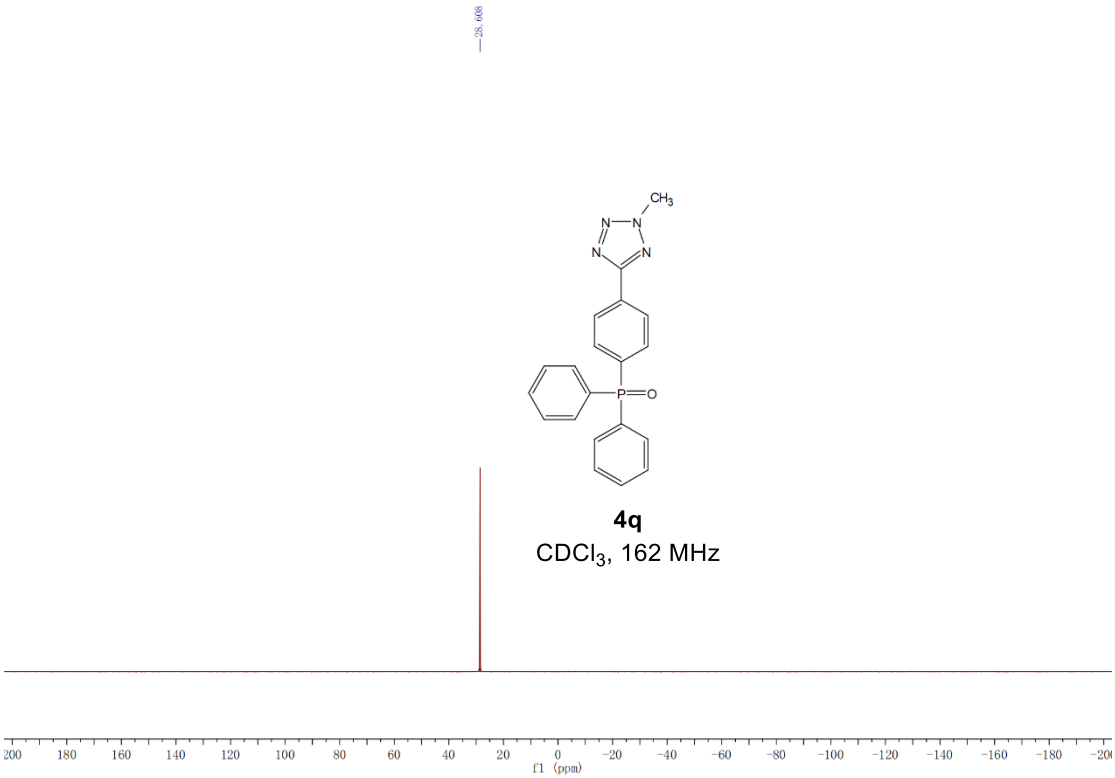

161.371
161.357
157.440
140.931
140.895
134.854
133.483
133.074
132.369
132.255
132.110
131.978
131.914
131.662
129.118
128.558
128.397
127.898
127.646
77.424
77.000
76.577
15.514
CH3
N
N
P=O
4p
CDCl3, 75 MHz
f1 (ppm)


28.936
CH3
N
N
P=O
4p
CDCl3, 121 MHz
f1 (ppm)

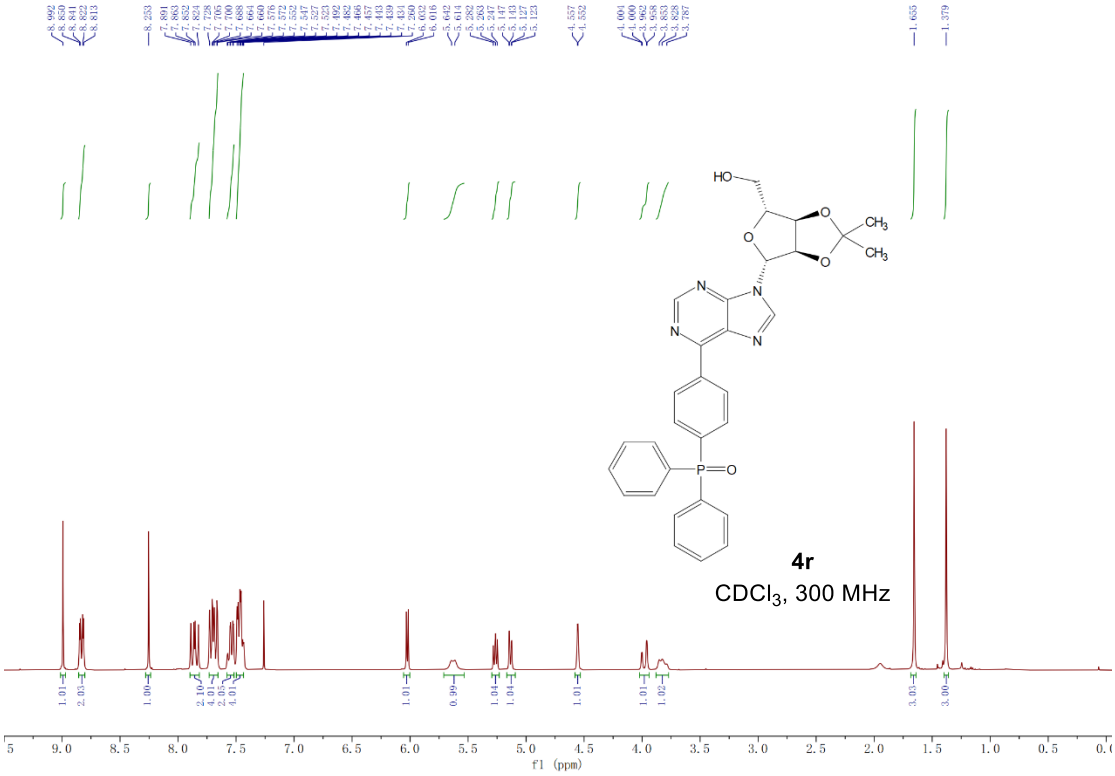
(4-(2-Methyl-2H-tetrazol-5-yl)phenyl)diphenylphosphine oxide (**4q**)

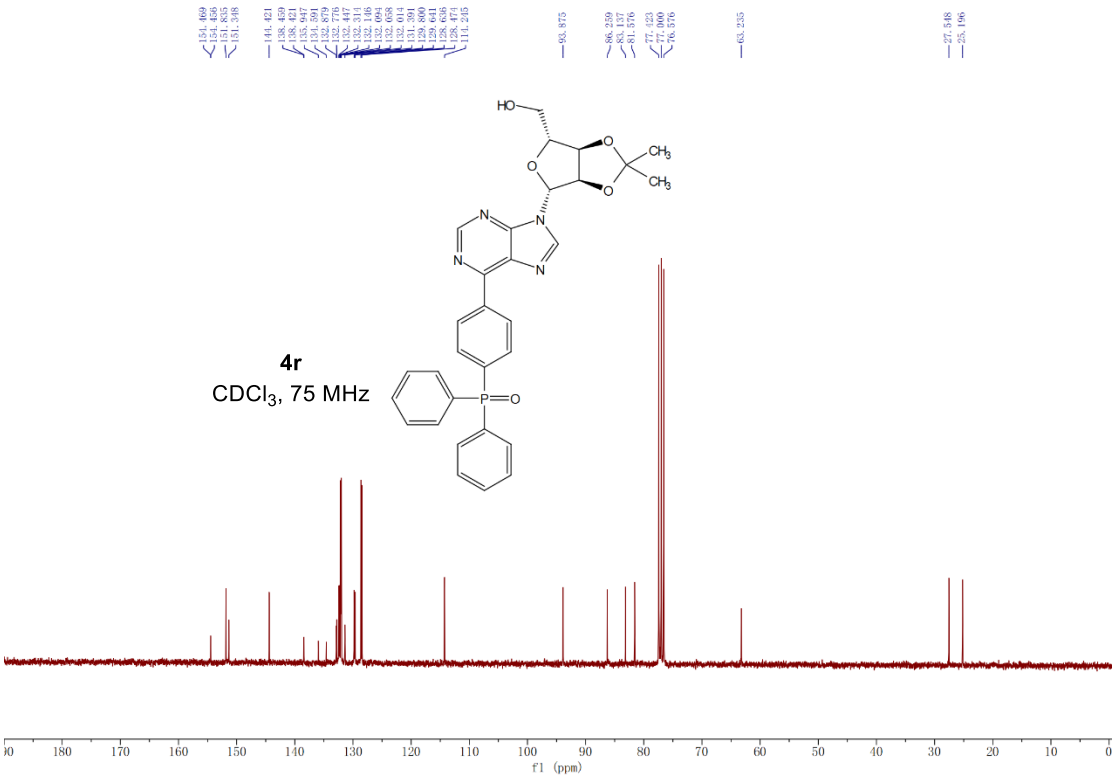


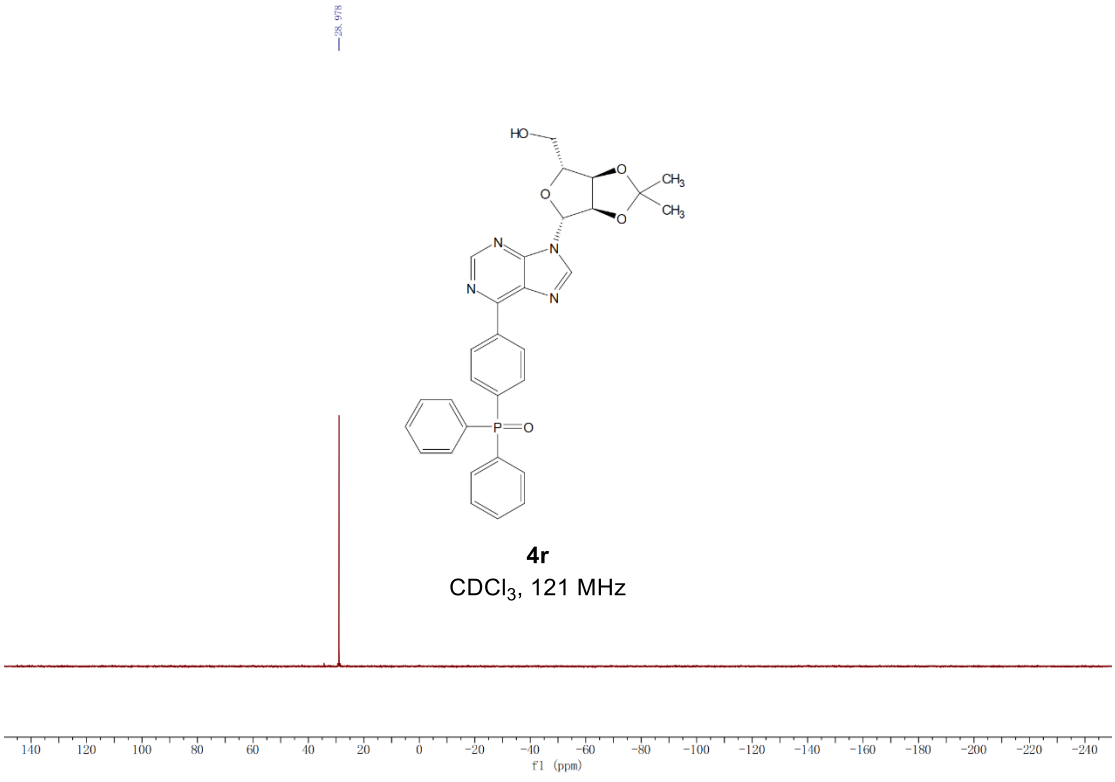




(4-(9-((3aR,4R,6R,6aR)-6-(Hydroxymethyl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)-9H-purin-6-yl)phenyl)diphenylphosphine oxide (**4r**)




154.469
154.435
151.855
151.348
144.421
138.459
138.421
135.947
131.591
132.679
132.575
132.447
132.311
132.146
132.064
132.058
132.014
131.391
130.960
129.641
128.636
128.471
111.245
93.975
86.259
83.137
81.976
77.423
77.000
76.576
63.235
27.548
25.196
HO
O
O
O
CH3
CH3
N
N
N
N
P=O
4r
CDCl3, 75 MHz
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


28.978
HO
O
O
O
CH3
CH3
N
N
N
N
P=O
4r
CDCl3, 121 MHz
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)