Simple Organic Molecules as Catalysts for Enantioselective Synthesis of Amines and Alcohols

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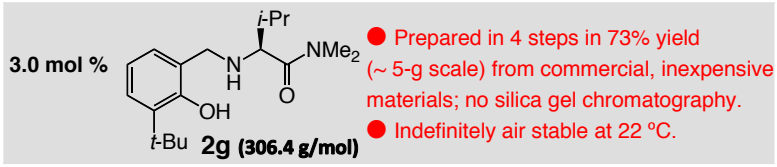
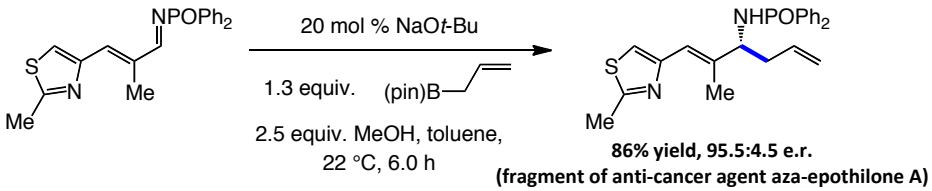
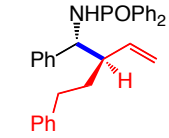
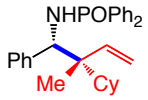


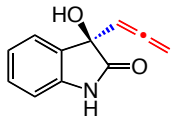




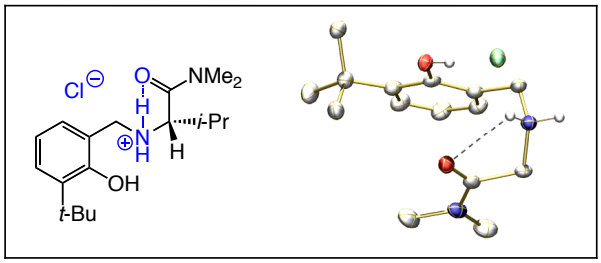
84% yield, 84:16 d.r., >98% α, 95:5 e.r.



70% yield, 89:11 d.r., >98% α, 95:5 e.r.



90% yield, >99:1 e.r. (gram-scale, 0.25 mol %)



Supplementary Information is in Four Parts: ***Page***

SUPPLEMENTARY INFORMATION; PART A

Table of Contents ***Page***

Diastereoselective Approaches to Synthesis of Homoallylic Amines & Derivatives

Significant advances have been made towards synthesis of diastereomerically enriched homoallylic amine derivatives through the use of an enantiomerically pure substrate or reagent. Some of the key disclosures in this area are provided below.

i. For examples that involve the use of a enantiomerically pure allylboron, see:

(a) Ramachandran, P. V. & Burghardt, T. E. Recent developments in the chiral synthesis of homoallylic amines via organoboranes. *Pure Appl. Chem.* **78**, 1397–1406 (2006).

(b) Ramandhar, T. R. & Batey, R. A. Allylation of imines and their derivatives with organoboron reagents: Stereocontrolled synthesis of homoallylic amines. *Synthesis* **9**, 1321–1346 (2011).

ii. For examples that involve the use of an enantiomerically pure allylsilane, see:

(c) Panek, J. S. & Jain, N. F. Direct amino-crotylsilylation of achiral acetals and aldehydes: Asymmetric synthesis of homoallylic amines and functionalized pyrrolidines. *J. Org. Chem.* **59**, 2674–2675 (1994).

(d) Leighton, J. L. Powerful and versatile silicon Lewis acids for asymmetric chemical synthesis. *Aldrichimica Acta* **43**, 3–14 (2010).

iii. For examples that involve the use of an enantiomerically pure alcohol, see:

(e) Takahashi, M., McLaughlin, M. & Micalizio, G. C. Complex allylation by the direct cross-coupling of imines with unactivated allylic alcohols. *Angew. Chem. Int. Ed.* **48**, 3648–3652 (2009).

(f) Lysenko, I. L., Lee, H. G. & Cha, J. K. Stereoselective cross-coupling between allylic alcohols and aldimines. *Org. Lett.* **11**, 3132–3134 (2009).

(g) Chen, M. Z. et al. Preparation of stereodefined homoallylic amines from the reductive cross-coupling of allylic alcohols with imines. *J. Org. Chem.* **75**, 8048–8059 (2010).

(h) Yang, D. & Micalizio, G. C. Convergent and stereodivergent synthesis of complex 1-aza-7-oxabicyclo[2.2.1]heptenes. *J. Am. Chem. Soc.* **133**, 9216–9219 (2011).

iv. For examples of reactions mediated by a chiral Lewis base, see:

(i) Kobayashi, S., Sugiura, M. & Ogawa, C. Neutral coordinate-organocatalysts in organic synthesis: Allylation of acylhydrazones with allyltrichlorosilanes. *Adv. Synth. Catal.* **346**, 1023–1034 (2004).

v. For examples of diasteroselective additions of an allyl group to enantiomerically pure imines bearing an Ellman-type auxillary, see:

(j) Cogan, D. A., Liu, G. & Ellman, J. Asymmetric synthesis of chiral amines by highly diastereoselective 1,2-additions of organometallic reagents to *N-tert*-butanesulfinyl imines *Tetrahedron* **55**, 8883–8904 (1999).

(k) Sun, X.-W., Xu, M.-H. & Lin, G.-Q. Room-temperature highly diastereoselective Zn-mediated allylation of chiral *N-tert*-butanesulfinyl imines: Remarkable reaction condition controlled stereoselectivity reversal. *Org. Lett.* **8**, 4979–4982 (2006).

(l) González-Gómez, J. C., Medjahdi, M.; Foubelo, F. & Yus, M. Stereoselective α-aminoallylation of aldehydes with chiral *tert*-butanesulfamides and allyl bromides. *J. Org. Chem.* **75**, 6308–6311 (2010).

(m) Liu, M., Shen, A., Sun, X.-W., Deng, F.; Xu, M.-H. & Lin, G.-Q. Dramatic lithium chloride effect on the reaction stereocontrol in Zn-mediated asymmetric cinnamylation: Highly practical synthesis of β-aryl homoallylic amines. *Chem. Commun.* **46**, 8460–8462 (2010).

vi. For examples of diasteroselective addition of an allyl group to enantiomerically pure imines derived from various α-amino acids, see:

(n) Yanada, R., Kaieda, A. & Takemoto, Y. Diasteroselective Barbier-type and palladium-mediated allylation of optically active aldimine with allylindium reagents. *J. Org. Chem.* **66**, 7516–7518 (2001).

(o) Sugimote, Y., Imamura, H., Sakoh, H., Yamada, K. & Morishima, H. Diastereoselective allylation of a chiral imine with allylzinc reagents: Diastereoselective synthesis of a novel broad spectrum carbapenem. *Synlett* **11**, 1747–1750 (2001).

(p) Cook, G. R., Maity, B. C. & Kargbo, R. Highly diastereoselective indium-mediated allylation of chiral hydrazones. *Org. Lett.* **6**, 1741–1743 (2004).

(q) Friestad, G. K., Korapala, C. S. & Ding, H. Dual activation in asymmetric allylsilane addition to chiral *N*-acylhydrazones: Method development, mechanistic studies, and elaboration of homoallylic amine adducts. *J. Org. Chem.* **71**, 281–289 (2006).

(r) Vilaivan, T., Winotapan, C., Banphavichit, V., Shinada, T. & Ohfune, Y. Indium-mediated asymmetric Barbier-type allylation of aldimies in alcoholic solvents: Synthesis of optically active homoallylic amines. *J. Org. Chem.* **70**, 3464–3471 (2005).

vii. For other categories of diasteroselective addition of an allyl group to enantiomerically pure imines, see:

(s) Laschat, S. & Kunz, H. Carbohydrates as chiral templates: Diastereoselective synthesis of *N*-glycosyl-*N*-homoallylamines and β-amino acids from imines. *J. Org. Chem.* **56**, 5883–5889 (1991).

(t) Kulkarni, N. A., Yao, C-f. & Chen, K. On the scope of diastereoselective allylation of various chiral glyoxylic oxime ethers with allyltributylstannane in the presence of a Lewis acid and triallylaluminum. *Tetrahedron* **63**, 7816–7822 (2007).

(u) Kattuboina, A., Kaur, P., Nguyen, T. & Li, G. Chiral *N*-phosphoyl imine chemistry: Asymmetric 1,2-additions of allylmagnesium bromides. *Tetrahedron Lett.* **49**, 3722–3724 (2008).

(v) Suh, Y-g. *et al.* Expedient synthesis of chiral homoallylamines via *N*,*O*-acetal TMS ethers and its application. *Org. Lett.* **13**, 5920–5923 (2011).

■ **General.** Infrared (IR) spectra were recorded on a Bruker alpha spectrophotometer, λ_{max} in cm^{-1}. Bands are characterized as broad (br), strong (s), medium (m), and weak (w). ^{1}H NMR spectra were recorded on a Varian Unity INOVA 400 (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm, CD_3OD: δ 3.34 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, br = broad, m = multiplet), and coupling constants (Hz). ^{13}C NMR spectra were recorded on a Varian Unity INOVA 400 (100 MHz) or a Varian Unity INOVA 500 (125 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16 ppm). Data are reported as follows: chemical shift, multiplicity (singlet unless otherwise noted), and coupling constants (Hz). ^{2}H NMR spectra were recorded on a Varian Unity INOVA 500 (76 MHz) tuned to the lock channel. High-resolution mass spectrometry was performed on a JEOL AccuTOF-DART (positive mode) at the Mass Spectrometry Facility, Boston College. Enantiomer ratios (er) values were determined by HPLC analysis using either a Shimadzu LC-2010AHT or SCL-10AVP chromatograph (Chiral Technologies Chiralcel OD (4.6 x 250 mm), Chiral Technologies Chiralcel OD-H (4.6 x 250 mm), Chiral Technologies Chiralcel OJ-H (4.6 x 250 mm), Chiral Technologies Chiralpak AD-H (4.6 x 250 mm), Chiral Technologies Chiralcel AZ-H (4.6 x 250 mm) columns), or GLPC (gas-liquid partition chromatography) with an Agilent chromatograph (Alltech Associated Chiraldex CD-BDM column (30 m x 0.25 mm) or a Hewlett Packard 5890 Series II chromatograph (Alltech Associated Betadex 120 column (30 m x 0.25 m). Specific rotations were measured on a Rudolph Research Analytical Autopol IV Polarimeter. Melting points were determined using a Thomas Hoover Uni-melt capillary melting point apparatus.

■ **Solvents:** Unless otherwise noted, solvents were purged with Ar and purified under a positive pressure of dry Ar by a modified Innovative Technologies purification system. Toluene (Fisher, ACS Grade) was passed successively through activated copper and alumina columns. Dichloromethane (Fisher, ACS Grade) and diethyl ether (Aldrich, Chromasolv®) were passed successively through two activated alumina columns. Tetrahydrofuran was purified by distillation from sodium benzophenone ketyl immediately prior to use. Dimethyl Sulfoxide (anhydrous, 99.9+%) was purchased from Alfa Aesar and used as received. $CDCl_3$ was purchased from Cambridge Isotope Laboratories and stored over activated 4Å molecular sieves prior to use. CD_3OD was purchased from Cambridge Isotope Laboratories and used as received. $CD_3C_6D_5$ (d_8–toluene) was purchased from Cambridge Isotope Laboratories and distilled from sodium metal onto activated 4Å molecular sieves prior to use. All work-up and purification procedures were carried out in air with reagent grade solvents (purchased from Fisher).

■ **Reagents:**

Allenylboronic Acid Pinacol Ester (19) was obtained from Frontier Scientific and used as received.

Allylboronates: Allylboronic acid pinacol ester (**1a**) was purchased from Aldrich or obtained as a gift from Frontier Scientific, Inc and distilled prior to use. 1,1-Di-deuterioallylboronic acid pinacol ester (***d*$_2$-1a**) was synthesized and purified in accordance with a procedure in the literature.[1] (2-Methylallyl)boronic acid pinacol ester (**1b**) was synthesized and purified in accordance with a procedure in the literature.[2] (2-Phenylallyl)boronic acid pinacol ester (**1c)** was synthesized and purified in accordance with a procedure in the literature.[3] Enantiomerically enriched α-substituted allylboronates ***S*-9**, ***R*-9**, and **12** were synthesized and purified in accordance with a procedure in with the literature.[4]

Benzyl Chloride was purchased from Aldrich and distilled from $CaCl_2$ prior to use.

Boc-Val-OH was purchased from Advanced ChemTech and used as received.

***tert*-Butanol** was purchased from Aldrich and distilled from sodium metal before use.

***n*-Butylamine** was purchased from Aldrich and used as received.

***tert*-Butyldimethylsilyl Chloride** was purchased from Strem and used as received.

3-*tert*-Butyl-2-hydroxybenzaldehyde was purchased from Aldrich and used as received.

1,8-Diazabicycloundec-7-ene (DBU) was purchased from Aldrich and distilled from CaH_2 prior to use.

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(1) Sieber, J. D.; Morken, J. P. *J. Am. Chem. Soc.* **2008**, *130*, 4978–4983.

(2) Zhang, P.; Roundtree, I. A.; Morken, J. P. *Org. Lett.* **2012**, *14*, 1416–1419.

(3) Corberan, R.; Mszar, N. W.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2011**, *50*, 7079–7082.

(4) Guzman-Martinez, A.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2010**, *132*, 10634–10637.

Diethylzinc was purchased from Aldrich and used as received.

Dimethylamine (40 wt % in H_2O) was purchased from Aldrich and used as received.

1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide Hydrochloride (EDC•HCl) was purchased from Advanced ChemTech and used as received.

Hydrochloric Acid (4.0 M in 1,4-dioxane) was purchased from Aldrich and used as received.

Hydrochloric Acid (12 M, 36.5-38.0 wt %) was purchased from Alfa Aesar and used as received.

1-Hydroxy-benzotriazole Hydrate (HOBt•H_2O) was purchased from Advanced ChemTech and used as received.

Isatins. Isatin and 5-methylisatin were purchased from Aldrich and used as received. 5-methoxyisatin was purchased from Oakwood and used as received. 4,6-Dibromoisatin was purchased from D-L Chiral Chemicals and was dissolved in methanol and copious purple solid impurities were removed by filtration.

L-*tert*-Leucine was purchased from Chem-Impex and Boc protected prior to use.

Magnesium Sulfate was purchased from Fisher and flame-dried under vacuum prior to use.

Magnesium Bromide Diethyl Etherate ($MgBr_2$•Et_2O) was purchased from Aldrich and used as received.

Methanol was purchased from Acros (99.8% anhydrous) and distilled at 1 atm from sodium metal prior to use or used as received.

Potassium Carbonate was purchased from Fisher and dried at 80 ºC under vacuum for 12 h prior to use.

Pyrrolidine was purchased from Aldrich and used as received.

Sodium Borohydride was purchased from Aldrich and used as received.

Sodium *tert*-Butoxide was purchased from Strem and used as received.

Sodium Hydride (60 wt% in oil) was purchased from Strem and used as received.

Sodium Periodate was purchased from Acros and used as received.

Titanium Tetrachloride ($TiCl_4$) was purchased from Aldrich and used as received.

Triethylamine was purchased from Aldrich and distilled from CaH_2 prior to use.

2-(Trimethylsilyl)ethoxymethyl Chloride, technical grade (SEM-Cl) was purchased from Aldrich and used as received.

***p*-Toluenesulfonic Acid Monohydrate** was purchased from Aldrich and used as received.

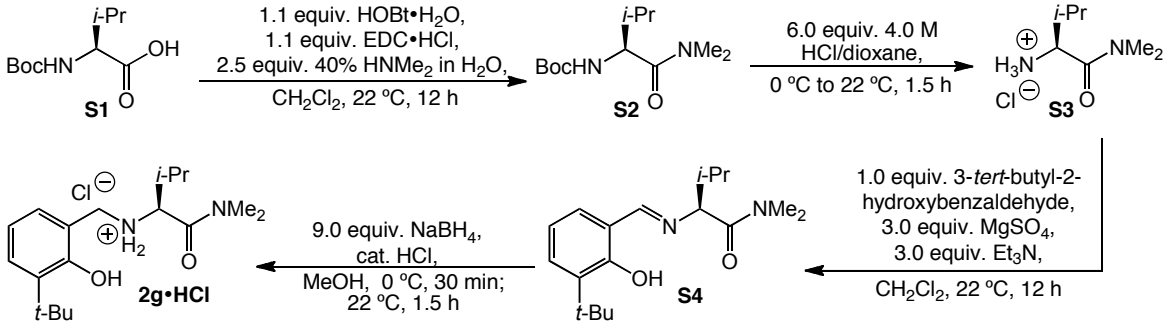
L-Valine Ethyl Ester Hydrochloride was purchased from Aldrich and used as received.

Zinc *tert*-Butoxide was prepared by reaction of *tert*-butanol with diethylzinc. A flame-dried round bottom flask is purged with nitrogen, sealed with a septum and electrical tape,

and charged with toluene (100 mL) and *tert*-butanol (1.8 mL, 19 mmol) by syringe. The solution is cooled to –78 ºC and diethylzinc (**Caution Pyrophoric!** 1.5 mL, 15 mmol) is added dropwise by syringe over 10 minutes. The reaction is allowed to warm to 22 ºC and to stir for 18 h. The toluene is removed by distillation under nitrogen at 1 atm. and the resulting solid is dried under vacuum for 12 h. The solid is removed from the flask in a nitrogen-filled glovebox to afford 1.5 g (7.1 mmol, 46% yield) of a white powder.

■ Synthesis, Purification, and Analytical Data for Amino Acid-Based Aminophenols 2a–2h

Scheme S1: Representative Experimental Procedure for Synthesis of Aminophenol 2g (Figure 2a)



EDC•HCl (4.22 g, 22.0 mmol), reagent grade CH_2Cl_2 (80 mL), HOBt•H_2O (3.36 g, 22.0 mmol), and Boc-Val-OH (4.34 g, 20.0 mmol) are added successively at 22 °C under air to a 250 mL round bottom flask equipped with a stir bar. The light yellow solution is allowed to stir for five minutes and dimethylamine (40 wt % in H_2O, 5.3 mL, 50 mmol) is added drop-wise over one minute. The flask with the resulting light yellow solution is sealed with a rubber septum and allowed to stir for 12 h at 22 °C. An aqueous solution of citric acid (10 wt %, 80 mL) is then added and the mixture is allowed to stir for 0.5 h during which time a white precipitate is formed. The precipitate is removed by filtration and the resulting two layers are separated. The organic layer is washed sequentially with an aqueous solution of citric acid (10 wt %, 80 mL), a saturated aqueous solution of $NaHCO_3$ (80 mL), and brine (80 mL) and is dried over Na_2SO_4 to give (*S*)-*tert*-butyl (1-(dimethylamino)-3-methyl-1-oxobutan-2-yl)carbamate (**S2**) as pale yellow oil, which is employed without purification in the subsequent deprotection.

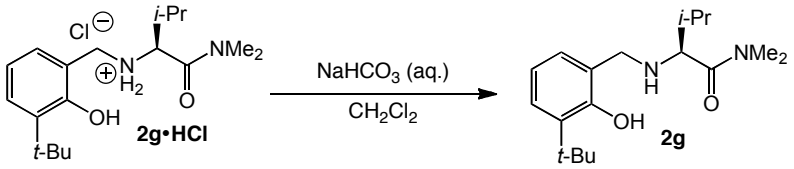
In a 100 mL round bottom flask, (*S*)-*tert*-butyl (1-(dimethylamino)-3-methyl-1-oxobutan-2-yl)carbamate **S2** (4.65 g, 19.3 mmol, 1.00 equiv.) is allowed to stir with a 4.0 M solution of hydrochloric acid in dioxane (28.9 mL, 116 mmol, 6.00 equiv.) for 1.5 h at 22 °C under air, after which the solution is purged with nitrogen for 30 min (removal of HCl gas) and the solvent is removed under reduced pressure to yield (*S*)-2-amino-*N*,*N*,3-trimethylbutanamide as HCl salt **S3**, which is used without purification in the subsequent condensation.

To the same flask (purged with nitrogen) is added 3-(*tert*-butyl)-2-hydroxybenzaldehyde

(3.43 g, 19.3 mmol, 1.00 equiv.) and $MgSO_4$ (6.93 g, 57.8 mmol, 3.00 equiv.), followed by the addition of dichloromethane (70 mL) and triethylamine (8.11 mL, 57.8 mmol, 3.00 equiv.) through a syringe. The mixture is allowed to stir overnight at 22 °C under nitrogen during which time the solution becomes bright yellow. The mixture is filtered through a small plug of silica gel to remove both $MgSO_4$ and triethylamine hydrochloride (which inhibits the following reduction) and silica plug is eluted with hexanes:ethyl acetate (2:1) until the solution becomes colorless. After evaporation of the volatiles, the remaining yellow oil is washed several times with hexanes (to remove residual triethylamine hydrochloride salt) and the combined filtrates are concentrated to afford (*S*,*E*)-2-((3-(*tert*-butyl)-2-hydroxybenzylidene)amino)-*N*,*N*,3-trimethyl-butanamide (**S4**) as yellow oil, which is utilized without purification in the follow-up reduction procedure.

To a 500 mL round bottom flask containing a solution of imine **S4** in 50 mL MeOH cooled to 0 ºC, $NaBH_4$ is added (5.83 g, 154 mmol, 8.00 equiv.) followed by a drop of 12 M aqueous hydrochloric acid. There is vigorous gas evolution upon addition of the acid and the yellow color of the solution disappears immediately. After the solution is allowed to stir for 30 min, the excess reducing agent is quenched through slow addition of a 2.0 M solution of aqueous HCl until the pH is less than one. The aqueous phase is then washed with dichloromethane (4 x 50 mL) and the combined organic layers are dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The white solid is purified by trituration from 10 mL dichloromethane and 80 mL hexanes to afford (*S*)-*N*-(3-(*tert*-butyl)-2-hydroxybenzyl)-1-(dimethylamino)-3-methyl-1-oxobutan-2-aminium chloride **2g•HCl** as a white solid (5.30 g, 15.5 mmol, 78% yield based on Boc-Val-NMe_2 **S1**). Crystals suitable for X-ray crystallography were grown by vapor diffusion from a dichloromethane/toluene solvent system. See Part D of the Supplementary Information for the X-ray crystal structure.

(*S*)-*N*-(3-(*tert*-Butyl)-2-hydroxybenzyl)-1-(dimethylamino)-3-methyl-1-oxobutan-2-aminium (2g•HCl; see above): M.p. = 182–183 °C. IR (neat): 2952 (br, s), 2821 (m), 2733 (m), 1664 (s), 1649 (s), 1548 (m), 1438 (s), 1396 (s), 1373 (m), 1360 (m), 1323 (m), 1285 (m), 1209 (s), 1176 (s), 1139 (m), 1097 (m), 874 (m), 792 (m), 756 (s), 484 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 10.62 (1H, br s), 8.24 (1H, br s), 7.61 (1H, br s), 7.30 (1H, app dd, *J* = 7.6, 1.6 Hz), 7.04 (1H, app dd, *J* = 7.6, 1.6 Hz), 6.85 (1H, t, *J* = 7.6 Hz), 4.44–4.38 (1H, m), 4.29–4.21 (2H, m), 2.95 (3H, s), 2.86 (3H, s), 2.50–2.44 (1H, m), 1.40 (9H, s), 1.13 (6H, app d, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 155.3, 141.3, 130.1, 129.1, 121.0, 119.9, 61.0, 47.9, 37.6, 36.2, 35.2, 30.3, 30.0, 18.7, 18.5.



(*S*)-2-((3-(*tert*-Butyl)-2-hydroxybenzyl)amino)-*N*,*N*,3-trimethylbutanamide (2g, Table 1): The salt **2g•HCl** (5.30 g, 15.5 mmol) is dissolved in 100 mL dichloromethane and deprotonated with 200 mL of a saturated aqueous solution of $NaHCO_3$. The layers are separated and the aqueous phase is washed twice with 50 mL dichloromethane. The combined organic phases are dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure to afford **2g** as white solid (4.45 g, 14.5 mmol, 73% yield based on Boc-Val-NMe_2 **S1**). Crystals suitable for X-ray crystallography were grown by slow evaporation of ethyl acetate. See Part D of the Supplementary Information for the X-ray crystal structure. M.p. = 97–99 ºC. IR (neat): 3310 (w), 2943 (w, br), 2872 (w, br), 1638 (s), 1589 (w), 1485 (m), 1459 (m), 1241 (m), 1183 (m), 929 (m), 870 (w), 855 (w), 841(w), 753 (s), 648 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 11.03 (1H, br s), 7.19 (1H, app dd, J = 7.0, 1.2 Hz), 6.80–6.75 (1H, m), 6.70 (1H, t, J = 7.6 Hz), 4.10 and 3.46 (2H, ABq, J_{AB} = 13.6 Hz), 3.28 (1H, br s), 3.04 (3H, s), 2.89 (3H, s), 2.65 (1H, br s), 1.90–1.84 (1H, m), 1.42 (9H, s), 0.97 (3H, d, J = 6.8 Hz), 0.94 (3H, d, J = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 157.1, 137.1, 126.9, 126.2, 122.9, 118.5, 61.2, 51.5, 37.1, 35.8, 34.8, 31.3, 29.6, 20.1, 18.0; HRMS Calcd for $C_{18}H_{31}N_2O_2$ $[M + H]^+$: 307.23855; Found: 307.23736. $[\alpha]^{20}_D = -37$ (c = 0.68, $CHCl_3$).

(*S*)-*N*-Butyl-2-((2-hydroxybenzyl)amino)-3-methylbutanamide (2a, Table 1): The title compound is prepared according to the representative synthesis of aminophenol **2g** except for the following changes: 1) For the amide formation (step 1), 2.5 equiv. of neat *n*-butylamine is used instead of dimethylamine. 2) For the imine formation (step 3) salicylaldehyde is utilized. 3) The product from the reduction is quenched with a saturated solution of aqueous $NaHCO_3$ (formation of the HCl salt is omitted) and the aminophenol is then purified by silica gel chromatography (100% dichloromethane to 98:2 dichloromethane:methanol) to afford **2a** as an off-white solid. M.p. = 50–52 ºC. IR (neat): 3318 (w), 3294 (w, br), 3255 (w), 2958 (w), 2930 (w, br), 2872 (w), 1628 (s), 1560 (m), 1469 (m), 1387 (w), 1253 (s), 1101 (w), 970 (w), 750 (s), 682 (w, br) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 10.58 (1H, br s), 7.18 (1H, app dt, J = 7.9, 1.4 Hz), 6.93 (1H, d, J = 7.6 Hz), 6.85 (1H, d, J = 8.1 Hz), 6.77 (1H, t, J = 7.1 Hz), 5.46 (1H, br s), 4.10 and 3.64 (2H, ABq, J_{AB} = 13.9 Hz), 3.34 (2H, app. dd, J = 13.0, 7.1 Hz), 2.66 (1H, d, J = 7.0 Hz), 2.41 (1H, br s), 1.94–1.85 (1H, m), 1.56–1.49 (2H, m), 1.42–1.33 (2H, m), 1.01 (3H, d, J = 6.8 Hz), 0.97–0.93 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.6, 158.1, 129.1, 128.8, 122.4, 119.3, 116.5, 67.5, 51.0, 39.4, 31.9, 31.7, 20.2, 19.8, 19.2, 13.9; HRMS Calcd for $C_{16}H_{27}N_2O_2$ $[M + H]^+$: 279.20725; Found: 279.20754. $[\alpha]^{20}_D = -33$ (c = 0.55, $CHCl_3$).

(*S*,*E*)-*N*-Butyl-2-((2-hydroxybenzylidene)amino)-3-methylbutanamide (2b, Table 1):

This material is synthesized in a manner analogous to aminophenol **2a** except the final reduction step is not performed. The analytical data are fully consistent with those reported previously.[5]

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(5) Wen, J.; Zhao, J.; Wang, X.; Dong, J.; You, T. *J. Mol. Cat. A: Chem*, **2006**, *245*, 242–247.

(*S*)-*N*-(1-(Butylamino)-3-methyl-1-oxobutan-2-yl)-2-hydroxybenzamide (2c, Table 1):
The title compound is prepared according to the representative synthesis of aminophenol **2a** except after the second step; H_2N-Val-NH*n*-Bu is treated with salicylic acid under the standard amide formation conditions outlined in the first step. The resulting off-white solid is purified by silica gel chromatography (5:1 hexanes:ethyl acetate) to afford **2c** as a white solid. M.p. = 123–125 ºC. IR (neat): 3279 (w), 3090 (w, br), 2930 (m), 1620 (s), 1605 (s), 1547 (s), 1530 (s), 1454 (s), 1371 (m, br), 1229 (m), 756 (s), 643 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 12.07 (1H, s), 7.51 (1H, d, J = 8.0 Hz), 7.40–7.36 (1H, m), 7.29 (1H, br s), 6.97 (1H, dd, J = 8.4, 0.9 Hz), 6.85–6.81 (1H, m), 6.00 (1H, br s), 4.36 (1H, t, J = 7.7 Hz), 3.39–3.30 (1H, m), 3.27–3.19 (1H, m), 2.25–2.17 (1H, m), 1.54–1.47 (2H, m), 1.39–1.30 (2H, m), 1.03 (3H, d, J = 3.3 Hz), 1.01 (3H, d, J = 3.2 Hz), 0.91 (3H, t, J = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.8, 169.8, 161.4, 134.5, 126.3, 119.0, 118.5, 114.4, 58.9, 39.6, 31.7, 31.6, 20.2, 19.3, 18.7, 13.8; HRMS Calcd for $C_{16}H_{25}N_2O_3$ $[M + H]^+$: 293.18652; Found: 293.18532. $[\alpha]^{20}_D$ = –34 (c = 0.63, $CHCl_3$).

(*S*)-*N*-Butyl-2-((3-(*tert*-butyl)-2-hydroxybenzyl)amino)-3-methylbutanamide (2d, Table 1): The title compound is prepared according to the representative synthesis of aminophenol **2g** except for the following changes: 1) For the first amide formation, 2.5 equiv. of neat *n*-butylamine is used instead of dimethylamine. 2) The reduction is quenched with a saturated solution of aqueous $NaHCO_3$ (formation of the HCl salt is omitted) and the desired product is purified by silica gel chromatography (100% dichloromethane to 98:2 dichloromethane:methanol) to afford **2d** as a white solid. M.p. = 97–99 ºC. IR (neat): 3268 (w, br), 3084 (w, br), 2957 (m), 2871 (w), 1644 (s), 1561 (m), 1435 (s), 1259 (s), 835 (m), 784 (m), 750 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 10.83 (1H, br s), 7.21 (1H, app dd, J = 7.8, 1.6 Hz), 6.80 (1H, dd, J = 7.3, 1.6 Hz), 6.71 (1H, t, J = 7.6 Hz), 5.52 (1H, br s), 4.13 and 3.59 (2H, ABq, J_{AB} = 13.8 Hz), 3.37–3.29 (2H, m), 2.59 (1H, d, J = 7.3 Hz), 1.90–1.81 (1H, m), 1.58–1.46 (2H, m), 1.43-1.33 (11H, m), 1.00 (3H, d, J = 6.8 Hz), 0.95 (3H, t, J = 7.3 Hz), 0.91 (3H, d, J = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.9, 157.1, 137.1, 127.0, 126.3, 122.6, 118.5, 67.0, 51.2, 39.3, 34.8, 31.9, 31.7, 29.6, 20.2, 20.0, 19.1, 13.8; HRMS Calcd for $C_{20}H_{35}N_2O_2$ $[M + H]^+$: 335.26985; Found: 335.27112. $[\alpha]^{20}_D$ = –68 (c = 0.63, $CHCl_3$).

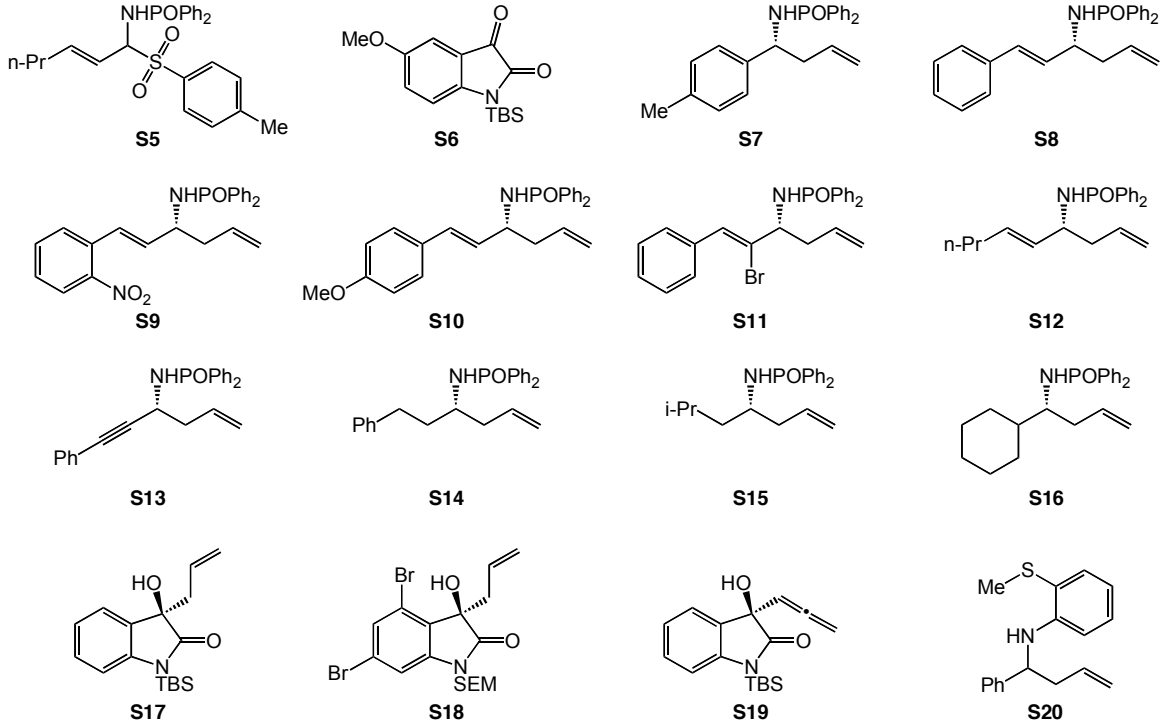
(*S*)-Ethyl 2-((3-(*tert*-butyl)-2-hydroxybenzyl)amino)-3-methylbutanoate (2e, Table 1): The title compound is prepared according to the representative synthesis of aminophenol **2g** except for the following changes: 1) Initial amide formation carried out with L-Valine methyl ester hydrochloride instead of Boc-Val-OH. 2) The reduction is quenched with a saturated solution of aqueous $NaHCO_3$ (formation of the HCl salt is omitted) and the desired product is purified by silica gel chromatography (100% hexanes to 30:1 hexanes:diethyl ether) to afford **2e** as a yellow oil. IR (neat): 2960 (m, br), 1728 (s), 1459 (s), 1237 (m), 1186 (s), 1140 (s), 1023 (m), 747 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 10.57 (1H, br s), 7.21 (1H, app dd, J = 7.8, 1.7 Hz), 6.84–6.82 (1H, m), 6.72 (1H, t, J =

7.6 Hz), 4.28–4.21 (2H, m), 4.08 and 3.66 (2H, ABq, J_{AB} = 13.3 Hz), 3.08 (1H, d, J = 4.9 Hz), 2.27 (1H, br s), 2.04–1.96 (1H, m), 1.41 (9H, s), 1.31 (3H, t, J = 7.1 Hz), 0.99 (6H, app dd, J = 10.5, 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.0, 156.9, 137.1, 127.1, 126.4, 122.8, 118.6, 65.6, 61.0, 51.9, 34.8, 31.5, 29.7, 19.7, 18.3, 14.5; HRMS Calcd for $C_{18}H_{30}NO_3$ $[M + H]^+$: 308.22257; Found: 308.22291. $[\alpha]^{20}_D$ = –42 (c = 0.73, $CHCl_3$).

(*S*)-2-((3-(*tert*-Butyl)-2-hydroxybenzyl)amino)-3-methyl-1-(pyrrolidin-1-yl)butan-1-one (2f, Table 1): The title compound is prepared according to the representative synthesis of aminophenol **2g** except for the following changes: 1) For the first step, 2.5 equiv. of neat pyrrolidine is used instead of dimethylamine. 2) For the reduction of the imine in the last step of the synthesis, 20.0 equiv. $NaBH_4$ is used. 3) The reduction is quenched with a saturated solution of aqueous $NaHCO_3$ (formation of the HCl salt is omitted) and the desired product is purified by silica gel chromatography (hexanes to 5:1 hexanes:ethyl acetate to 3:1 hexanes:ethyl acetate) to afford **2f** as a clear, colorless oil. IR (neat): 3279 (w, br), 2956 (w, br), 2873 (w), 1632 (s), 1424 (s), 1356 (w), 1239 (m), 1184 (w), 1141 (w), 1085 (w), 880 (m), 748 (s), 529 (w); ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.06 (1H, br s), 7.19 (1H, app dd, J = 7.0, 1.2 Hz), 6.77 (1H, app dd, J = 7.3, 1.5 Hz), 6.69 (1H, t, J = 7.5 Hz), 4.13 (1H, app d, J = 13.6 Hz), 3.66–3.60 (1H, m), 3.53–3.45 (2H, m), 3.28–3.14 (2H, m), 3.05 (1H, d, J = 6.7 Hz), 2.60 (1H, br s), 1.91–1.81 (5H, m), 1.42 (9H, s), 1.00 (3H, d, J = 6.7 Hz), 0.93 (3H, d, J = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.1, 157.2, 137.1, 126.8, 126.2, 122.9, 118.4, 63.4, 51.3, 46.5, 45.8, 34.8, 31.4, 29.6, 26.2, 24.3, 20.1, 18.5; HRMS Calcd for $C_{20}H_{33}N_2O_2$ $[M + H]^+$: 333.25420; Found: 333.25561. $[\alpha]^{20}_D$ = –58 (c = 0.58, $CHCl_3$).

(*S*)-2-((3-(*tert*-Butyl)-2-hydroxybenzyl)amino)-*N*,*N*,3,3-tetramethylbutanamide (2h, Table 1): The title compound is prepared according to the representative synthesis of aminophenol **2g** except for the following changes: 1) Initial amide formation carried out with Boc-Tle-OH instead of Boc-Val-OH. 2) The product from the reduction process is quenched with a saturated solution of aqueous $NaHCO_3$ (formation of the HCl salt is omitted) and the desired product is purified by silica gel chromatography (9:1 hexanes:ethyl acetate to 6:1 hexanes:ethyl acetate to 4:1 hexanes:ethyl acetate) to afford **2h** as a white solid. M.p. = 96–98 ºC. IR (neat): 2948 (w, br), 1639 (s), 1460 (m), 1433 (m), 1352 (m), 1240 (m), 1135 (m), 878 (m), 782 (m), 751 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.87 (1H, br s), 7.19 (1H, d, J = 7.3 Hz), 6.77 (1H, d, J = 7.3 Hz), 6.70 (1H, t, J = 7.5), 4.09 and 3.40 (2H, ABq, J_{AB} = 13.6 Hz), 3.31 (1H, d, J = 11.3 Hz), 3.03 (3H, s), 2.89 (3H, s), 2.71 (1H, br s), 1.40 (9H, s), 0.96 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.3, 157.0, 137.2, 126.9, 126.3, 122.9, 118.5, 62.4, 51.3, 38.0, 35.8, 34.8, 34.7, 29.6, 27.0; HRMS Calcd for $C_{19}H_{33}N_2O_2$ $[M + H]^+$: 321.25420; Found: 321.25442. $[\alpha]^{20}_D$ = –33 (c = 0.93, $CHCl_3$).

Chart S1: Supplementary Information Numbering for Aldimine Precursors,Isatins, Homoallylamides, 3-Allyl-3-hydroxy Oxindoles, 3-Allenyl-3-hydroxy Oxindoles, and Homoallylamines



■ **Preparation, Purification, and Analytical Data for Aldimine Substrates**: Aryl-, heteroaryl-, alkenyl-, and alkynyl-substituted *N*-diphenylphosphinoyl imines were synthesized through a $TiCl_4$-promoted reaction between *P*,*P*-diphenylphosphinic amide[6] and the corresponding aldehyde.[7] Alkyl-substituted aldimines as well as aldimines **3e**, **3g**, **3h** and **6** were synthesized through the intermediacy of the corresponding sulfinyl adducts according to previously disclosed methods.[7b,8] Occasionally, for optimal results, aryl-, heteroaryl-, alkenyl-, and alkynyl-substituted aldimines should be purified by silica gel chromatography (5% triethylamine in the slurry packed bed of silica) shortly before to their use.

General Procedure for Preparation of Aryl-, Heteroaryl-, Alkenyl-, and Alkynyl Aldimines (3j, Table 2): Aldimine **3j** was prepared following a modified reported procedure.[7a] A flame-dried 100 mL round-bottom flask, purged with nitrogen, is charged

(6) *P*,*P*-Diphenylphosphinic amide was routinely synthesized on deca-gram scale according to a previously reported procedure. See: Desrosiers, J-N.; Côté, A.; Boezio, A. A.; Charette, A. B. *Org. Syn.* **2006**, *83*, 8–9.

(7) (a) Jennings, W. B.; Lovely, C. J. *Tetrahedron* **1991**, *47*, 5561–5568. (b) Yamada, K-i.; Harwood, S. J.; Gröger, H.; Shibasaki, M. *Angew. Chem., Int. Ed.* **1999**, *38*, 3504–3506.

(8) (a) Côté, A.; Boezio, A. A.; Charette, A. B. *Proc. Natl. Acad. Sci.* **2004**, *101*, 5405–5410. (b) Yamaguchi, A.; Matsunaga, S.; Shibasaki, M. *Tetrahedron Lett.* **2006**, *47*, 3985–3989.

with 4-(dibutylamino) benzaldehyde [9] (5.51 g, 23.6 mmol, 1.25 equiv.), *P*,*P*-diphenylphosphinic amide (4.10 g, 18.9 mmol, 1.00 equiv.), triethylamine (10.6 mL, 75.6 mmol, 4.00 equiv.), and dichloromethane (60 mL). The resulting mixture is allowed to cool to −78 °C, followed by the drop-wise addition of neat $TiCl_4$ (1.14 mL, 10.4 mmol, 0.55 equiv.). The solution is allowed to stir for 12 h at 22 °C and is then filtered through a plug of Celite. The resulting yellow solid is purified by silica gel column chromatography (ethyl acetate:hexanes 2:1 followed by 100% ethyl acetate as eluent) and recrystallized from dichloromethane/hexanes to afford **3j** as pale yellow solid (6.40 g, 14.8 mmol, 78% yield).

***(E)*-*N*-(4-(dibutylamino)benzylidene)-*P*,*P*-diphenylphosphinic amide (3j, Table 2):** M.p. = 113–115 °C. IR (neat): 2951 (w), 2928 (w), 2869 (w), 1579 (m), 1525 (m), 1435 (m), 1364 (m), 1203 (m), 1173 (m), 1104 (m), 831 (s), 807 (m), 725 (m), 695 (s), 580 (m), 545 (s), 522 (s), 510 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.08 (1H, d, *J* = 32.0 Hz), 7.95–7.89 (4H, m), 7.85 (2H, d, *J* = 8.8 Hz), 7.48–7.38 (6H, m), 6.65 (2H, d, *J* = 9.2 Hz), 3.34 (4H, dd, *J* = 7.6, 7.2 Hz), 1.63–1.56 (4H, m), 1.37 (4H, app sextet, *J* = 7.6 Hz), 0.97 (6H, t, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.1 (d, *J* = 6.9 Hz), 152.3, 134.4 (d, *J* = 126.0 Hz), 132.7 (br peak as the result of hindered rotation around the (Ar)–(C=NR) bond), 131.7 (d, *J* = 9.1 Hz), 131.4 (d, *J* = 2.7 Hz), 128.4 (d, *J* = 12.3 Hz), 123.5 (d, *J* = 26.2 Hz), 111.0, 51.0, 29.4, 20.4, 14.1; HRMS Calcd for $C_{27}H_{34}N_2OP$ $[M + H]^+$: 433.24087; Found: 433.23945.

(*E*)-*N*-((*E*)-3-(2-Nitrophenyl)allylidene)-*P*,*P*-diphenylphosphinic amide (5b, Table 3): White solid. M.p. = 148–149 °C. IR (neat): 3076 (w), 3041 (w), 2856 (w), 1625 (m), 1608 (m), 1591 (m), 1520 (m), 1437 (w), 1344 (m), 1205 (s), 1157 (w), 1124 (m), 1108 (m), 966 (w), 874 (m), 845 (m), 798 (s), 784 (m), 752 (w), 741 (w), 725 (s), 693 (s), 676 (m), 577 (w), 547 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.09 (1H, dd, *J* = 31.6, 8.8 Hz), 8.06 (1H, d, *J* = 8.4 Hz), 7.94–7.86 (5H, m), 7.70 (1H, t, *J* = 8.0 Hz), 7.67 (1H, t, *J* = 7.6 Hz), 7.58–7.42 (7H, m), 7.02 (1H, ddd, *J* = 15.6, 8.8, 1.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1 (d, *J* = 7.9 Hz), 148.1, 145.0, 133.8, 133.0 (d, *J* = 28.6 Hz), 132.5 (d, *J* = 126.0 Hz), 132.1 (d, *J* = 2.8 Hz), 131.7 (d, *J* = 9.3 Hz), 130.8, 130.7 (d, *J* = 1.4 Hz), 129.0, 128.7 (d, *J* = 12.6 Hz), 125.3; HRMS Calcd for $C_{21}H_{18}N_2O_3P$ $[M + H]^+$: 377.10550; Found: 377.10545.

(*E*)-*N*-((*E*)-3-(4-Methoxyphenyl)allylidene)-*P*,*P*-diphenylphosphinic amide (5c, Table 3): Pale yellow solid. M.p. = 150–151 °C. IR (neat): 3064 (w), 3053 (w), 3014 (w), 2939 (w), 2844 (w), 1619 (m), 1586 (s), 1568 (s), 1513 (m), 1436 (m), 1311 (m), 1258 (s), 1203 (s), 1180 (m), 1160 (m), 1123 (m), 1106 (m), 1023 (m), 875 (m), 818 (s), 753 (m), 723 (m), 696 (s), 595 (m), 546 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.01 (1H, dd, *J* = 31.6, 8.8 Hz), 7.91–7.86 (4H, m), 7.53–7.42 (8H, m), 7.33 (1H, d, *J* = 15.6 Hz), 7.00 (1H, ddd, *J*

(9) Tian, L.; Hu, Z.; Shi, P.; Zhou, H.; Wu, J.; Tian, Y.; Zhou, Y.; Tao, X.; Jiang, M. *J. Lumin.* **2007**, *127*, 423–430

= 15.6, 9.2, 2.0 Hz), 6.93 (2H, d, *J* = 8.4 Hz), 3.85 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.1 (d, *J* = 7.7 Hz), 162.0, 150.7, 133.3 (d, *J* = 126.0 Hz), 131.8 (d, *J* = 2.8 Hz), 131.7 (d, *J* = 9.1 Hz), 130.2, 128.6 (d, *J* = 12.5 Hz), 127.6 (d, *J* = 1.2 Hz), 126.7 (d, *J* = 28.5 Hz), 114.6, 55.6; HRMS Calcd for $C_{22}H_{21}NO_2P$ $[M + H]^+$: 362.13099; Found: 362.12964.

(*E*)-*N*-((*Z*)-2-Bromo-3-phenylallylidene)-*P*,*P*-diphenylphosphinic amide (5d, Table 3): White solid. M.p. = 144–145 °C. IR (neat): 3074 (w), 3061 (w), 3025 (w), 3012 (w), 2958 (w), 1620 (m), 1593 (s), 1569 (m), 1438 (m), 1199 (s), 1160 (w), 1134 (m), 1122 (s), 1106 (m), 1070 (w), 877 (s), 808 (m), 752 (m), 726 (s), 702 (s), 684 (s), 659 (m), 587 (m), 550 (s), 517 (m), 501 (s), 468 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (1H, d, *J* = 29.2 Hz), 7.99–7.93 (6H, m), 7.78 (1H, s), 7.53–7.43 (9H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.3 (d, *J* = 5.2 Hz), 148.2, 133.8, 132.9 (d, *J* = 127.0 Hz), 132.0 (d, *J* = 2.8 Hz), 131.7 (d, *J* = 9.3 Hz), 131.1, 130.9, 128.7, 128.7 (d, *J* = 11.5 Hz), 124.1 (d, *J* = 31.6 Hz); HRMS Calcd for $C_{21}H_{18}BrNOP$ $[M + H]^+$: 410.03094; Found: 410.02999.

(*E*)-*P*,*P*-Diphenyl-*N*-(1-tosylhex-2-en-1-yl)phosphinic amide (S5, not shown in manuscript, see Chart S1): The title compound is synthesized following a previously reported procedure[7] from *P*,*P*-diphenylphosphinic amide (2.17 g, 10.0 mmol, 1.00 equiv.), (*E*)-hex-2-enal (2.31 mL, 20.0 mmol, 2.00 equiv.), and *p*-toluenesulfinic acid[10] (2.34 g, 15.0 mmol, 1.50 equiv.) to obtain **S5** as white solid (3.22 g, 7.10 mmol, 71% yield). M.p. = 138–139 °C. IR (neat): 3177 (w, br), 2959 (w), 2933 (w), 2870 (w), 1661 (m), 1596 (w), 1437 (m), 1300 (m), 1281 (m), 1214 (m), 1185 (s), 1170 (m), 1138 (m), 1125 (s), 1106 (m), 1083 (m), 955 (m), 894 (m), 752 (m), 726 (s), 693 (s), 662 (m), 583 (s), 568 (m), 536 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79–7.71 (4H, m), 7.59 (2H, d, *J* = 8.4 Hz), 7.59–7.54 (2H, m), 7.50–7.43 (4H, m), 7.23 (2H, d, *J* = 8.0 Hz), 5.90 (1H, ddd, *J* = 13.6, 11.6, 9.6 Hz), 5.31 (1H, t, *J* = 10.0 Hz), 4.73 (1H, dd, *J* = 14.0, 10.4 Hz), 3.28 (1H, app td, *J* = 10.8, 3.6 Hz), 2.42 (3H, s), 1.97–1.88 (1H, m), 1.52–1.32 (2H, m), 1.20–1.10 (1H, m), 0.82 (3H, t, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 134.7, 132.8, 132.6 (d, *J* = 2.9 Hz), 132.5 (d, *J* = 2.9 Hz), 132.2 (d, *J* = 10.1 Hz), 131.9 (d, *J* = 10.1 Hz), 131.4 (d, *J* = 128.0 Hz), 131.1 (d, *J* = 128.0 Hz), 129.6, 129.2, 128.9 (d, *J* = 12.9 Hz), 128.9 (d, *J* = 13.0 Hz), 101.9 (d, *J* = 9.9 Hz), 67.6, 29.7, 21.8, 20.0, 13.7.

(*E*)-*N*-((*E*)-Hex-2-en-1-ylidene)-*P*,*P*-diphenylphosphinic amide (6, Table 3): Following a modification to a previously reported procedure,[7b] **6** is synthesized through vigorous stirring of a suspension of sulfinic adduct **S5** (see above, 150 mg, 0.330 mmol) in 5 mL of diethyl ether and 5 mL of an aqueous saturated solution of Na_2CO_3 until the white solid dissolves completely (~8 h). The layers are separated and the aqueous phase is washed with diethyl ether. The combined organic phases are dried with anhydrous sodium sulfate and the filtrate is concentrated to dryness. The residue is dissolved again in dichloromethane, filtered, and the solvent is evaporated to afford **6** as colorless viscous oil (97.7 mg, 0.328 mmol, 99% yield). IR (neat): 3056 (w), 2959 (w), 2930 (w), 2871 (w), 1637 (m), 1596 (s),

(10) Sisko, J.; Mellinger, M.; Sheldrake, P. W.; Baine, N. H. *Org. Syn.* **2000**, *77*, 198–205.

1203 (s), 1122 (m), 1106 (m), 826 (s), 724 (s), 693 (s), 571 (m), 544 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.86 (1H, dd, *J* = 32.4, 8.8 Hz), 7.89–7.83 (4H, m), 7.50–7.41 (6H, m), 6.73 (1H, dt, *J* = 15.6, 6.8 Hz), 6.50–6.42 (1H, m), 2.30 (2H, app quartet, *J* = 7.2 Hz), 1.53 (2H, app sextet, *J* = 7.2 Hz), 0.95 (3H, t, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 175.5 (d, *J* = 8.0 Hz), 156.7, 133.1 (d, *J* = 126.0 Hz), 132.3 (d, *J* = 26.8 Hz), 131.8 (d, *J* = 2.8 Hz), 131.6 (d, *J* = 9.1 Hz), 128.5 (d, *J* = 12.4 Hz), 35.2, 21.4, 13.8; HRMS Calcd for $C_{18}H_{21}NOP$ $[M + H]^+$: 298.13608; Found: 298.13599.

■ Preparation, Purification, and Analytical Data for Isatin Substrates

General Procedure for Preparation of N-tert-Butyldimethylsilyl Isatins: In a 250 mL flame dried round bottom flask equipped with a stir bar, *tert*-butyldimethylsilyl chloride (4.5 g, 30 mmol) is dissolved in 150 mL dichloromethane. To this solution, in a single portion, isatin (2.2 g, 15 mmol) and 4-dimethylaminopyridine (0.18 g, 1.5 mmol) are added. The flask is sealed with a rubber septum and purged with nitrogen. Triethylamine (6.3 mL, 45 mmol) is added in one portion through a syringe and mixture is allowed to stir for 24 h at 22 ºC. The volatiles are removed *in vacuo* and the resultant dark orange solid is purified by silica gel chromatography (hexanes to 1:1 hexanes:dichloromethane to dichloromethane) to afford an orange solid, which is recrystallized from hot EtOH (details below) to afford **14a** (2.6 g, 9.9 mmol, 67% yield) as an orange crystalline solid. Please note that for long-term storage, *N-tert*-butyldimethylsilyl protected isatins should be kept under an inert atmosphere at –15 ºC. **1-(*tert*-Butyldimethylsilyl)indoline-2,3-dione** (**14a, Figure 5**): M.p. = 123–124 °C. IR (neat): 2929 (w), 2853 (w), 1731 (s), 1603 (m), 1589 (m), 1463 (m), 1325 (m), 1252 (m), 1170 (m), 1139 (m), 927 (m), 835 (s), 796 (m), 752 (s), 686 (m), 466 (m), 424 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.63–7.61 (1H, m), 7.53–7.49 (1H, m), 7.10–7.03 (2H, m), 1.02 (9H, s), 0.56 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.2, 164.9, 155.4, 138.3, 125.6, 123.4, 120.0, 115.1, 26.4, 19.7, –3.3; HRMS Calcd for $C_{14}H_{20}NO_2Si$ $[M + H]^+$: 262.12633; Found: 262.12608.

1-(*tert*-Butyldimethylsilyl)-5-methoxyindoline-2,3-dione (S6, not shown in the manuscript, see Chart S1): Crimson crystalline solid. M.p. = 169–171 °C. IR (neat): 2929 (w, br), 2859 (w), 1731 (s), 1625 (w), 1589 (w), 1492 (m), 1310 (m), 1270 (m), 1142 (m), 942 (w), 847 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.12–7.07 (2H, m), 6.96 (1H, d, *J* = 9.0 Hz), 3.79 (3H, s), 1.01 (9H, s), 0.54 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.7, 165.3, 156.0, 149.5, 125.6, 120.4, 116.0, 108.8, 56.0, 26.5, 19.8, –3.3; HRMS Calcd for $C_{15}H_{22}NO_3Si$ $[M + H]^+$: 292.13689; Found: 292.13766.

4,6-Dibromo-1-((2-(trimethylsilyl)ethoxy)methyl)indoline-2,3-dione (**14b, not shown in the manuscript, see Chart S1**): Amide protection performed in accordance to a previously disclosed procedure.[11] Yellow crystalline solid, M.p. = 142–143 °C. IR (neat): 3077 (w), 2896 (w), 1742 (m), 1595 (s), 1562 (m), 1419 (w), 1244 (m), 1073 (s), 1024 (m),

(11) Trost, B. M.; Frederiksen, M. U. *Angew. Chem., Int. Ed.* **2005**, *44*, 308–310.

839 (s), 733 (m), 456 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.51 (1H, d, J = 1.6 Hz), 7.28 (1H, d, J = 1.2 Hz), 5.16 (2H, s), 3.85 (2H, m), 0.94 (2H, m), –0.01 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 179.5, 157.2, 152.2, 133.5, 131.5, 122.1, 115.3, 114.3, 70.0, 67.1, 17.9, –1.3; HRMS Calcd for $C_{14}H_{21}Br_2N_2O_3Si$ $[M + NH_4]^+$: 450.96882; Found: 450.96873.

Synthesis of N-Bn Isatins: Synthesized in accordance to a published procedure[12] with the following modification: After isolation of the unpurified *N*-protected isatin, a small portion (~10 mg) of the solid is passed through a small plug of silica gel using dichloromethane as the elutant. If a dark (usually maroon) residue remains on the silica gel after the *N*-protected isatin is eluted, then the entire unpurified *N*-Bn isatin is dissolved in dichloromethane and passed through a short plug of silica gel using dichloromethane as an elutant. After concentration *in vacuo*, the isatin is purified as described below.

Purification of N-Bn, N-SEM, and N-TBS isatins: With hot EtOH as the solvent, ~95 % of the resulting solid is dissolved and filtered while hot through a fritted glass funnel (this initial filtration is critical to obtain *N*-protected isatins of sufficient purity). The filtered solids are discarded. The filtrate is allowed to cool to room temperature during which time the desired product crystallizes from solution. The desired product is collected by filtration through a fritted glass funnel. Concentrating the mother liquor in vacuo and recrystallization of the resultant solids from hot EtOH yields additional product. The products are then dried azeotropically with anhydrous benzene prior to use.

■ **Procedure for *Gram-Scale* Catalytic Enantioselective Allyl Addition to Aldimine 3a to Afford Homoallylamide 4a (Figure 4a)**:

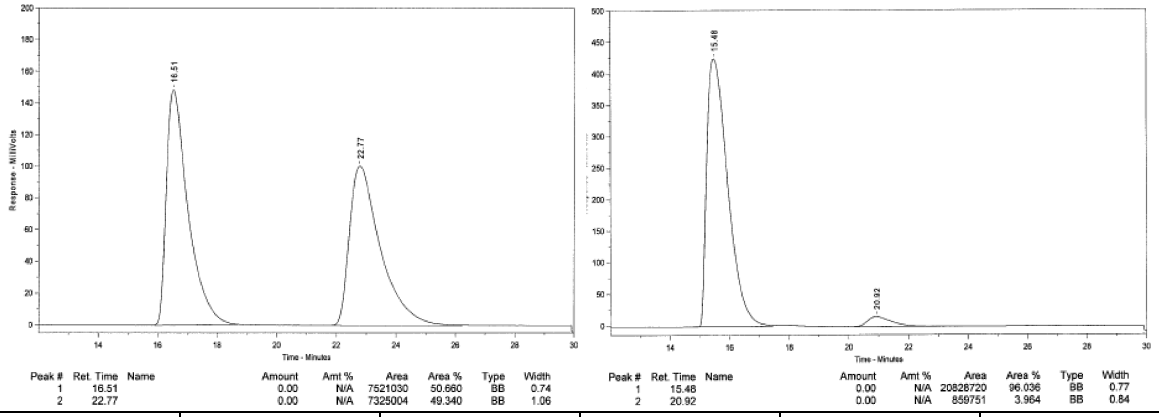
Preparation of the catalyst suspension: Aminophenol **2g** (15.0 mg, 0.0490 mmol) is weighed out in air into a 4 mL vial to which is added 263 μL of a solution of sodium hydroxide (1.95 mg, 0.0490 mmol) in reagent-grade methanol [111 mg NaOH pellet (Fisher) is dissolved in 15 ml methanol]). After removal of the solvent *in vacuo*, the resultant white oil is azeotropically dried with reagent grade toluene. The obtained white solid is allowed to dry at 0.5 Torr for 30 min and the vial is sealed with a cap containing a teflon septum. Toluene (1.0 mL) is added to yield a suspension after sonication (2 min).

A round bottom flask (50 mL, equipped with a magnetic stirring bar) is charged with imine **3a** (1.00 g, 3.28 mmol) and dried at 0.5 Torr for 30 min, purged with nitrogen and sealed with a rubber septum. Toluene (30 mL) is added, followed by allylboronic acid pinacol ester **1a** (800 μl, 4.26 mmol) from a septum-sealed bottle (Frontier Scientific, Inc., as received) and methanol (200 μL, 4.92 mmol) from a septum-sealed bottle (Acros, grade: 99.9% ExtraDry, as received). A suspension of the catalyst containing aminophenol **2g** (10.1 mg, 33 μmol, 0.0100 equiv.) and sodium hydroxide (1.31 mg, 33 μmol, 0.0100 equiv.) in 0.67 mL toluene is added with a syringe to the mixture (see below). After two h,

(12) Karimi, A. R.; Sedaghatpour, F. *Synthesis* **2010**, *10*, 1731–1735.

the solvent is evaporated and the residue is taken up in 30 mL hexanes. The suspension is allowed to sonicate for two min, filtered and washed with hexanes (4 x 3 mL). The desired product, dried under vacuum, is obtained in 97.5:2.5 er (1.04 g, 3.01 mmol, 92% yield). Elemental analysis for $C_{22}H_{22}NOP$: Calcd: C, 76.06; H, 6.38; N, 4.03. Found: C, 75.77; H, 6.43; N 3.98.

(*R*)-P,P-Diphenyl-*N*-(1-phenylbut-3-en-1-yl)phosphinic amide (4a, Table 2): The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89–7.84 (2H, m), 7.79–7.74 (2H, m), 7.51–7.47 (1H, m), 7.45–7.41 (3H, m), 7.34–7.18 (7H, m), 5.61 (1H, dddd, J = 17.2, 10.0, 7.2, 7.2 Hz), 5.11–5.03 (2H, m), 4.47 (1H, dddd, J = 10.4, 10.4, 6.4, 6.4 Hz), 3.35 (1H, br dd, J = 9.6, 6.0 Hz), 2.74–2.60 (2H, m); HRMS Calcd for $C_{22}H_{23}NOP$ $[M + H]^+$: 348.15173; Found: 348.15251; $[\alpha]^{20}_D$ = +52 (c = 0.40, $CHCl_3$) for a 96:4 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4a**: 16 min (major) and 21 min (minor).



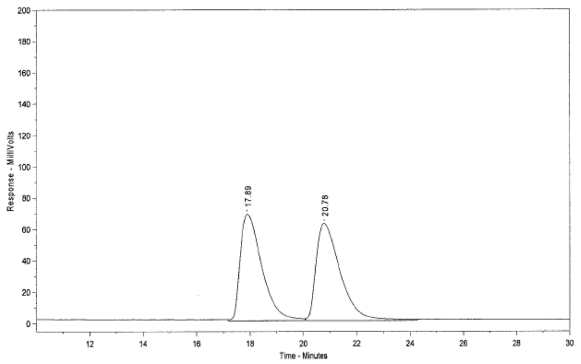
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.5 min	50.660	1	15.5 min	96.036
2	22.8 min	49.340	2	20.9 min	3.964

■ **Representative Procedure for *Small Scale* Catalytic Enantioselective Allyl Additions to Aryl-, Heteroaryl-, Alkenyl-, and Alkynyl *N*-Diphenylphosphinoyl Imines (Table 3)**: In a nitrogen-filled glovebox (not needed for gram scale; only used when reactions are performed at mg scale to achieve highly reproducible data), aminophenol **2g** (6.9 mg, 0.023 mmol) is added to an oven-dried two dram vial equipped with a stir bar followed by 1.5 mL of a stock solution of NaO*t*-Bu in toluene (9.6 mg, 0.10 mmol/8.0 mL) and the solution is allowed to stir at 22 ºC for ~10 minutes. A separate vial equipped with a stir bar is charged sequentially with aldimine **3b** (32.3 mg, 0.100 mmol), 800. µL of toluene, MeOH (10. µL, 0.25 mmol), and allylboronic acid pinacol ester **1a** (28 µL, 0.15 mmol) under nitrogen. To this mixture is added 200. µL of the **2g**/NaO*t*-Bu

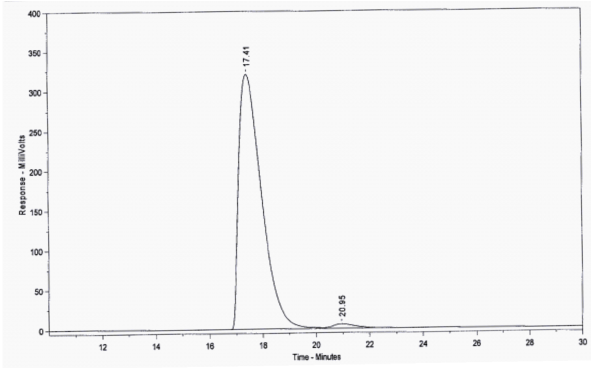
(13) Vieira, E. M.; Snapper, M. L.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2011**, *133*, 3332–3335.

solution and a cap is attached to the vial and sealed (electrical tape). The clear and colorless solution is allowed to stir at 22 ºC for four hours during which time the solution becomes cloudy and white. The cap is removed and 3 mL of a solution of saturated aqueous $NaIO_4$ is added and the biphasic mixture is allowed to stir for 20 minutes. The aqueous layer is washed with ethyl acetate (4 x 4 mL), dried over Na_2SO_4, and concentrated *in vacuo* to yield a pale yellow solid. The homoallylamide product is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 10 mL hexanes, 10 mL 3:1 hexanes:ethyl acetate, 10 mL 1:1 hexanes:ethyl acetate, 10 mL 1:3 hexanes:ethyl acetate, and 15 mL ethyl acetate) to afford **4b** (35.2 mg, 0.0960 mmol, 96% yield) as a white solid.

(*R*)-*N*-(1-(2-Fluorophenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (4b, Table 2): The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87–7.82 (2H, m), 7.78–7.72 (2H, m), 7.51–7.47 (1H, m), 7.44–7.39 (3H, m), 7.34–7.29 (2H, m), 7.23–7.18 (1H, m), 7.15 (1H, ddd, *J* = 7.6, 7.6, 1.6 Hz), 7.05 (1H, ddd, *J* = 7.6, 7.6, 1.2 Hz), 6.97 (1H, ddd, *J* = 10.8, 8.0, 0.8 Hz), 5.61 (1H, dddd, *J* = 17.2, 10.0, 7.2, 7.2 Hz), 5.09–5.01 (2H, m), 4.47 (1H, dddd, *J* = 10.4, 10.4, 6.4, 6.4 Hz), 3.56 (1H, br dd, *J* =10.4, 6.8 Hz), 2.78–2.60 (2H, m); HRMS Calcd for $C_{22}H_{21}FNOP$ [M + H]$^+$: 366.14230; Found: 366.14250. $[\alpha]^{20}_D$ = +34 (*c* =0.39, $CHCl_3$) for a 98.5:1.5 er sample. The enantiomeric purity was determined by HPLC analysis in comparison to authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm) t_R of **4b**: 17 min (major) and 21 min (minor).



Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	17.89		0.00	N/A	3830492	49.348	BB	0.85
2	20.78		0.00	N/A	3931760	50.652	BB	0.94

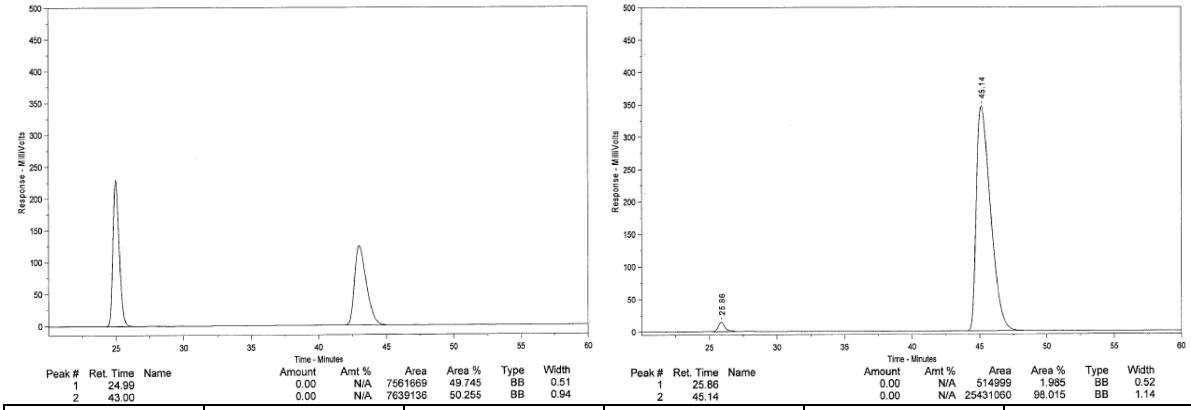


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	17.41		0.00	N/A	19007440	98.321	BV	0.92
2	20.95		0.00	N/A	324616	1.679	VB	0.88

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	17.9	49.348	1	17.4	98.321
2	20.8	50.652	2	21.0	1.679

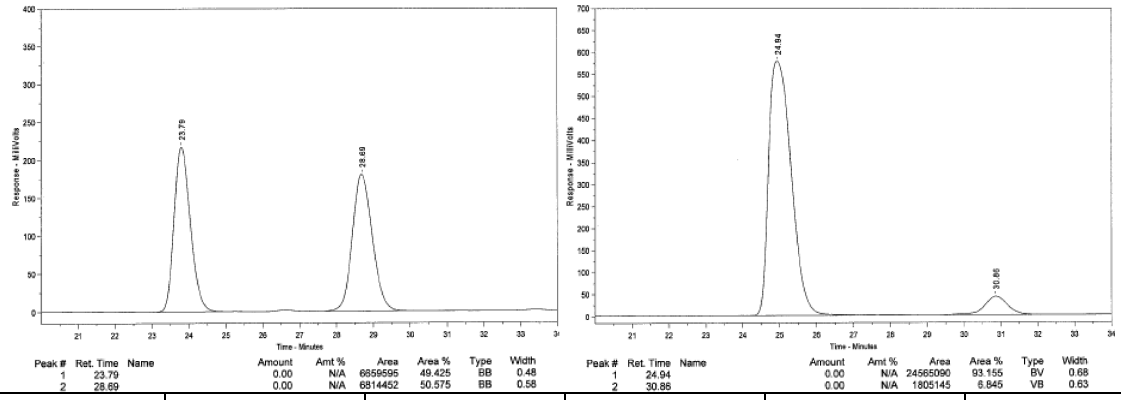
(*R*)-*N*-(1-(2-Bromophenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (**4c, Table 2**): The title compound is purified in a manner identical to **4b** affording **4c** (38.0 mg, 0.0891 mmol, 89% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87–7.82 (2H, m), 7.75–7.70 (2H, m), 7.51–7.47 (1H, m), 7.44–7.39 (4H, m), 7.35–7.27 (4H, m), 7.07 (1H, ddd, *J* = 8.8, 8.0, 2.0 Hz), 5.64 (1H, dddd, *J* = 17.4, 10.4, 7.2, 7.2 Hz), 5.14–5.10 (2H, m), 4.71 (1H, dddd, *J*

= 10.4, 10.4, 6.0, 6.0 Hz), 3.56 (1H, br dd, *J* = 9.6, 6.0 Hz), 2.64 (2H, app t, *J* = 6.4 Hz); HRMS Calcd for $C_{22}H_{22}BrNOP$ $[M + H]^+$: 426.06224; Found: 426.06229. $[\alpha]^{20}_D$ = +2.30 (*c* =1.00, $CHCl_3$) for a 98.0:2.0 er sample. The enantiomeric purity was determined by HPLC analysis in comparison to authentic racemic material (Chiracel AD-H, 87:13 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm) t_R of **4c:** 26 min (minor) and 45 min (major).



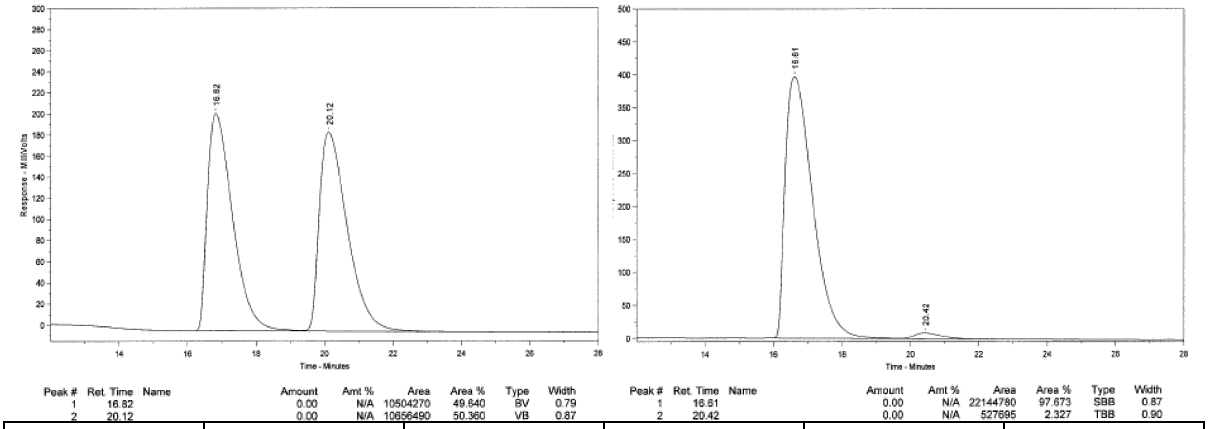
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	25.0	49.745	1	25.9	1.985
2	43.0	50.255	2	45.1	98.015

(*R*)-*P*,*P*-Diphenyl-*N*-(1-(*o*-tolyl)but-3-en-1-yl)phosphinic amide (**4d, Table 2**): The title compound is synthesized and purified analogously to **4b** (six h reaction time) affording **4d** (34.3 mg, 0.0949 mmol, 95% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88–7.83 (2H, m), 7.72–7.67 (2H, m), 7.50–7.46 (1H, m), 7.44–7.38 (3H, m), 7.33 (1H, d, *J* = 7.7 Hz), 7.29–7.21 (3H, m), 7.12 (1H, ddd, *J* = 8.4, 7.6, 1.6 Hz), 7.00 (1H, d, *J* = 7.5 Hz), 5.61 (1H, dddd, *J* = 17.2, 10.0, 7.2, 7.2 Hz), 5.11–5.03 (2H, m), 4.54 (1H, dddd, *J* = 10.0, 10.0, 6.4, 6.4 Hz), 3.43 (1H, br dd, *J* = 9.6, 6.4 Hz), 2.65–2.52 (2H, m), 1.91 (3H, s); HRMS Calcd for $C_{23}H_{25}NOP$ $[M + H]^+$: 362.16738; Found: 362.16744. $[\alpha]^{20}_D$ = +7.20 (*c* =1.00, $CHCl_3$) for a 94:6 er sample. The enantiomeric purity was determined by HPLC analysis in comparison to authentic racemic material (Chiracel AD-H, 87:13 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm) t_R of **4d**: 25 min (major) and 31 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	23.8	49.425	1	24.9	93.155
2	28.7	50.575	2	30.9	6.845

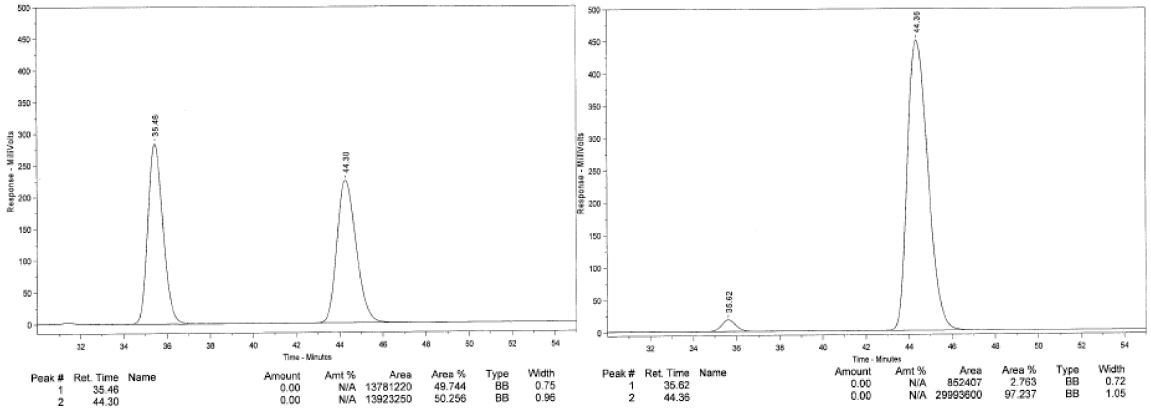
(*R*)-*N*-(1-(3-Bromophenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (**4e, Table 2**): The title compound is purified identically to **4b** affording **4e** (39.5 mg, 0.0927 mmol, 93% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87–7.82 (2H, m), 7.77–7.71 (2H, m), 7.53–7.47 (1H, m), 7.45–7.40 (3H, m), 7.35–7.30 (4H, m), 7.13–7.11 (2H, m), 5.58 (1H, dddd, J = 17.2, 10.0, 7.2, 7.2 Hz), 5.13–5.07 (2H, m), 4.31 (1H, dddd, J = 10.0, 10.0, 6.4, 6.4 Hz), 3.42 (1H, br dd, J = 9.4, 6.0 Hz), 2.67–2.58 (2H, m); HRMS Calcd for $C_{22}H_{22}BrNOP$ $[M + H]^+$: 426.06224; Found: 426.06326. $[\alpha]^{20}_D$ = +59 (c = 0.57, $CHCl_3$) for a 97.5:2.5 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4e**: 17 min (major) and 20 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.8	49.640	1	16.6	97.673
2	20.1	50.360	2	20.4	2.327

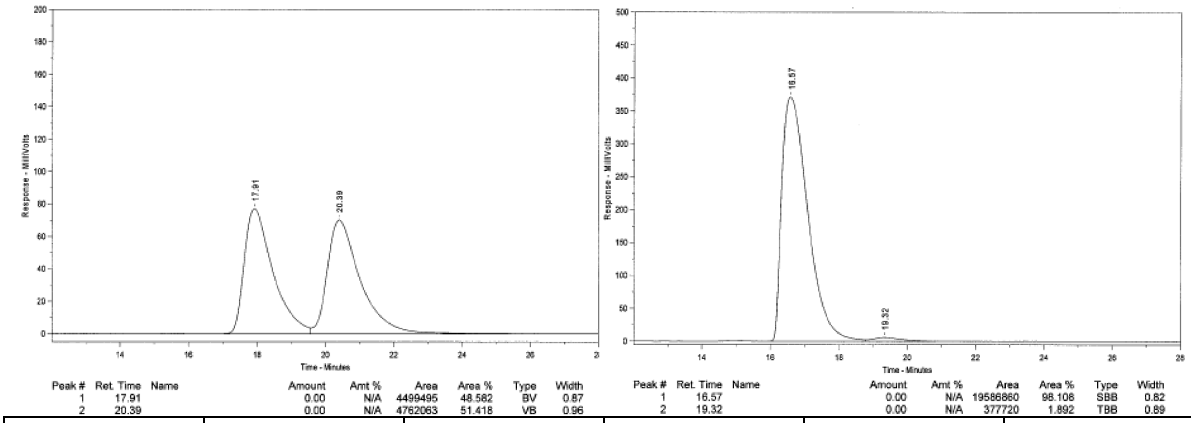
(*R*)-*N*-(1-(4-Bromophenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (**4f, Table 2**): The title compound is purified identically to **4b** affording **4f** (39.2 mg, 0.0920 mmol, 92% yield) as a white solid. The analytical data are fully consistent with those reported

previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87–7.82 (2H, m) 7.78–7.72 (2H, m), 7.51–7.47 (1H, m), 7.45–7.37 (5H, m), 7.35–7.30 (2H, m), 7.08–7.05 (2H, m), 5.57 (1H, dddd, *J* = 16.8, 10.0, 7.2, 7.2 Hz), 5.13–5.06 (2H, m), 4.31 (1H, dddd, *J* = 10.0, 10.0, 6.4, 6.4 Hz), 3.30 (1H, br dd, *J* = 9.6, 5.6 Hz), 2.69–2.55 (2H, m); HRMS Calcd for $C_{22}H_{22}BrNOP$ $[M + H]^+$: 426.0622; HRMS Calcd for $C_{22}H_{22}BrNOP$ $[M + H]^+$: 426.06224; Found: 426.06197. $[\alpha]^{20}_D$ = +73 (*c* = 1.0, $CHCl_3$) for a 97:3 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 97:3 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4f**: 36 min (minor) and 44 min (major).



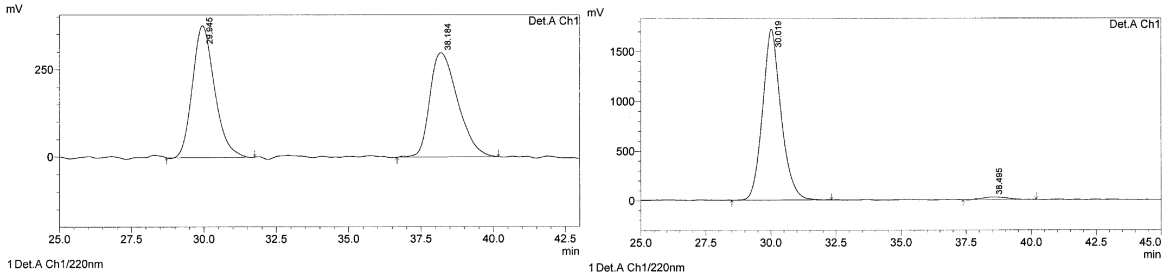
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	35.5	49.744	1	35.6	2.763
2	44.3	50.256	2	44.4	97.237

(*R*)-*P*,*P*-Diphenyl-*N*-(1-(4-(trifluoromethyl)phenyl)but-3-en-1-yl)phosphinic amide (**4g, Table 2**): The title compound is purified identically to **4b** affording **4g** (38.8 mg, 0.0934 mmol, 93% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88–7.83 (2H, m) 7.75–7.70 (2H, m), 7.52–7.48 (3H, m), 7.45–7.40 (3H, m), 7.32–7.28 (4H, m), 5.58 (1H, dddd, *J* = 17.2, 10.0, 7.2, 7.2 Hz), 5.14–5.08 (2H, m), 4.41 (1H, dddd, *J* = 9.6, 9.6, 6.4, 6.4 Hz), 3.49 (1H, br dd, *J* = 8.8, 6.2 Hz), 2.71–2.58 (2H, m); HRMS Calcd for $C_{23}H_{22}F_3NOP$ $[M + H]^+$: 416.13911; Found: 416.13996. $[\alpha]^{20}_D$ = +57 (*c* = 0.45, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4g**: 17 min (major) and 19 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	17.9	48.582	1	16.6	98.108
2	20.4	51.418	2	19.3	1.892

(*R*)-Methyl-4-(1-((diphenylphosphoryl)amino)but-3-en-1-yl)benzoate (4h, Table 2): The title compound is synthesized and purified analogously to **4b** except for the following changes: 1) 2.5 mol % aminophenol **2g** (instead of 3 mol % **2g**) 2) 1.5 equiv. MeOH (instead of 2.5 equiv.). Homoallylamide **4h** (74.4 mg, 0.183 mmol, 92% yield) is obtained as a white solid. M.p. = 128 °C. IR (neat): 3144 (w, br), 3055 (w), 3006 (w), 2948 (w), 2872 (w), 1720 (s), 1610 (w), 1435 (m), 1277 (s), 1193 (s), 1181 (s), 1106 (s), 1067 (m), 926 (m), 907 (m), 721 (s), 694 (s), 561 (m), 527 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.93 (2H, d, *J* = 8.4 Hz), 7.86–7.80 (2H, m), 7.74–7.68 (2H, m), 7.47–7.37 (4H, m), 7.30–7.25 (2H, m), 7.25 (2H, d, *J* = 8.0 Hz), 5.55 (1H, dddd, *J* = 17.2, 10.0, 7.6, 6.8 Hz), 5.09–5.03 (2H, m), 4.38 (1H, app tt, *J* = 10.1, 6.2 Hz), 3.88 (3H, s), 3.52 (1H, br dd, *J* = 9.9, 5.9 Hz), 2.70–2.56 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 148.4 (d, *J* = 5.0 Hz), 133.2, 132.9 (d, *J* = 127.0 Hz), 132.5 (d, *J* = 9.7 Hz), 132.0 (d, *J* = 2.7 Hz), 131.9 (d, *J* = 130.0 Hz), 131.9 (d, *J* = 3.9 Hz, one peak is overlapping with the other d at 131.9), 131.9 (d, *J* = 9.5 Hz), 129.8, 129.0, 128.6 (d, *J* = 12.5 Hz), 128.4 (d, *J* = 12.6 Hz), 126.6, 119.4, 54.3, 52.2, 43.6 (d, *J* = 4.2 Hz); HRMS Calcd for $C_{24}H_{25}NO_3P$ $[M + H]^+$: 406.15720; Found: 406.15720. $[\alpha]^{20}_D$ = +75.5 (*c* = 2.40, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD–H, 80:20 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **4h**: 30 min (major) and 38 min (minor).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.945	20067493	376847	50.019	55.792
2	38.184	20052576	298603	49.981	44.208
Total		40120069	675450	100.000	100.000

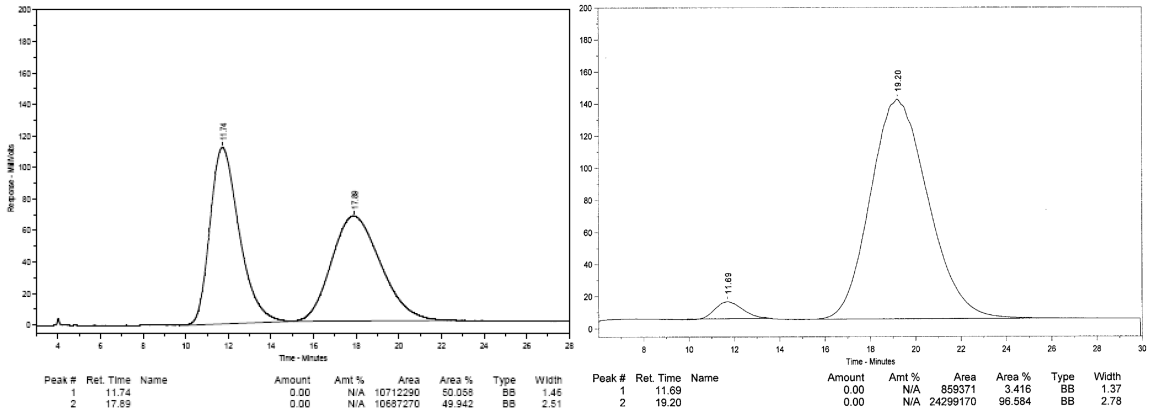
PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.019	84765285	1719371	98.190	98.562
2	38.495	1562574	25084	1.810	1.438
Total		86327859	1744455	100.000	100.000

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	29.9	50.019	1	30.0	98.190
2	38.2	49.981	2	38.5	1.810

(*R*)-*N*-(1-(4-Methoxyphenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (4i, Table 2): The title compound is synthesized and purified analogously to **4b** except for the following changes: 1) 2.5 mol % aminophenol **2g** (instead of 3 mol % **2g**) 2) 1.5 equiv. MeOH (instead of 2.5 equiv.). Homoallylamide **4i** (74.1 mg, 0.196 mmol, 98% yield) is afforded as a white solid. The analytical data are fully consistent with those reported previously.[13] M.p. = 116–117 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88–7.83 (2H, m), 7.80–7.75 (2H, m), 7.49–7.38 (3H, m), 7.35–7.30 (2H, m), 7.14–7.10 (2H, m), 6.83–6.79 (2H, m), 5.56 (1H, dddd, *J* = 17.2, 10.4, 6.8, 6.8 Hz), 5.10–5.02 (2H, m), 4.30 (1H, dddd, *J* = 9.6, 9.6, 6.4, 6.4 Hz), 3.79 (3H, s), 3.28 (1H, br dd, *J* = 9.6, 6.0 Hz), 2.72–2.57 (2H, m); HRMS Calcd for $C_{23}H_{25}NO_2P$ $[M + H]^+$: 378.16229; Found: 378.16236. $[\alpha]^{20}_D$ = +54.7 (*c* = 1.99, $CHCl_3$) for a 96.5:3.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OJ–H, 92:8 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **4i**: 12 min (minor) and 19 min (major).

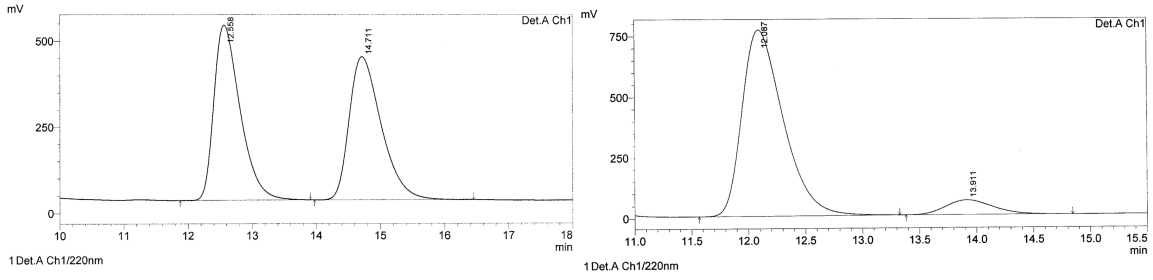


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	11.74		0.00	N/A	10712290	50.058	BB	1.46
2	17.89		0.00	N/A	10687270	49.942	BB	2.51

Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	11.69		0.00	N/A	859371	3.416	BB	1.37
2	19.20		0.00	N/A	24299170	96.584	BB	2.78

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	11.7	50.058	1	11.7	3.416
2	17.9	49.942	2	19.2	96.584

(*R*)-*N*-(1-(4-(Dibutylamino)phenyl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (4j, Table 2): The title compound is synthesized analogously to **4b** except for the following changes: 1) 2.5 mol % aminophenol **2g** (instead of 3 mol % **2g**) 2) 1.5 equiv. MeOH (instead of 2.5 equiv.). 3) Reaction time is six h. 4) After $NaIO_4$ workup (see representative procedure above), the unpurified mixture is treated for 12 h while allowing it to stir with ~ 1 g basic aluminum oxide in 4 mL dichloromethane:diethyl ether (1:1) to hydrolyze unreacted **3j**, after which the aluminum oxide is filtered off and washed with dichloromethane and ethyl acetate (20 mL). The product is purified as described for **4b**, affording **4j** (44.2 mg, 0.0931 mmol, 93% yield) as a white solid. M.p. = 83–84 °C. IR (neat): 3154 (w, br), 3071 (w), 2955 (m), 2930 (m), 2870 (m), 1614 (m), 1519 (m), 1455 (m), 1436 (m), 1368 (w), 1283 (w), 1181 (s), 1107 (s), 1066 (m), 925 (m), 900 (m), 752 (w), 722 (s), 693 (s), 553 (s), 521 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.89–7.79 (4H, m), 7.49–7.32 (6H, m), 7.03 (2H, d, J = 8.8 Hz), 6.54 (2H, d, J = 8.8 Hz), 5.63 (1H, app ddt, J = 17.2, 10.0, 7.2 Hz), 5.10-4.99 (2H, m), 4.26–4.19 (1H, m), 3.23 (4H, app dd, J = 7.8, 7.2 Hz), 3.26–3.21 (1H, m, overlapping with the dd at 3.23), 2.75–2.58 (2H, m), 1.59–1.52 (4H, m), 1.40–1.30 (4H, app sextet, J = 7.6 Hz), 0.96 (6H, t, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 134.6, 133.6 (d, J = 127.0 Hz), 132.6 (d, J = 9.5 Hz), 132.4 (d, J = 130.0 Hz), 131.9 (d, J = 9.3 Hz), 131.7 (d, J = 2.7 Hz), 131.6 (d, J = 2.7 Hz), 129.2 (d, J = 6.3 Hz), 128.4 (d, J = 12.3 Hz), 128.3 (d, J = 12.4 Hz), 127.6, 118.1, 111.5, 54.3, 50.9, 43.5 (d, J = 3.7 Hz), 29.5, 20.4, 14.1; HRMS Calcd for $C_{30}H_{40}N_2OP$ $[M + H]^+$: 475.28782; Found: 475.28783. $[\alpha]^{20}_D$ = +61.6 (c = 1.33, $CHCl_3$) for a 92:8 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD–H, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4j**: 12 min (major) and 14 min (minor).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.558	14499159	507916	50.161	54.997
2	14.711	14406117	415611	49.839	45.003
Total		28905276	923527	100.000	100.000

PeakTable

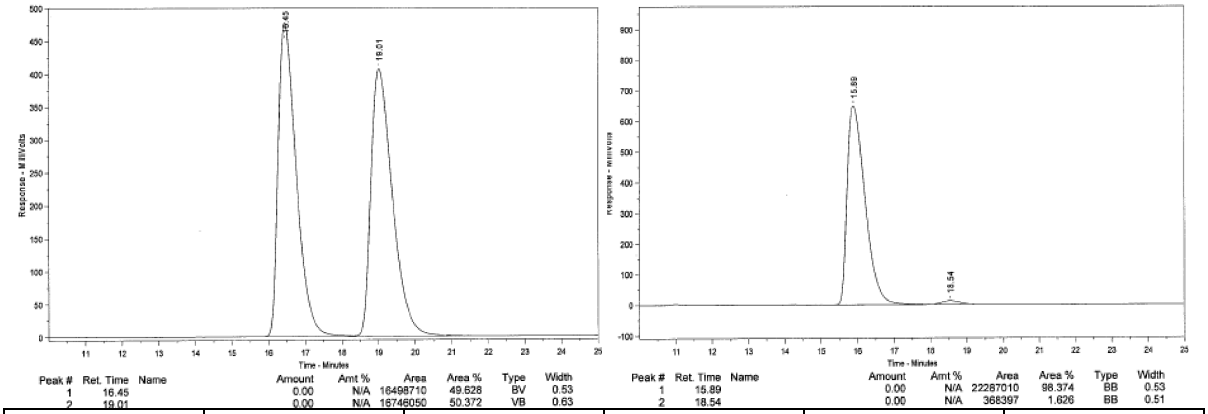
Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.087	19265334	767060	91.817	92.781
2	13.911	1716879	59680	8.183	7.219
Total		20982212	826740	100.000	100.000

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	12.6	50.161	1	12.1	91.817
2	14.7	49.839	2	13.9	8.183

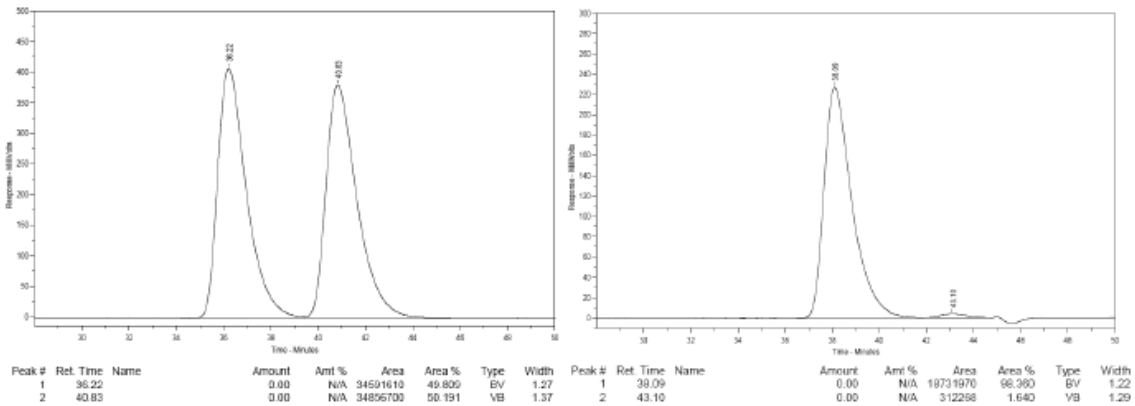
(*R*)-*N*-(1-(Furan-2-yl)but-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (4k, Table 2): The title compound is synthesized and purified analogously to **4b** (only with a six h reaction time) affording **4k** (32.2 mg, 0.0955 mmol, 96% yield) as a light tan solid. The analytical data are fully consistent with those reported previously.[13] ^1H NMR (400 MHz, $CDCl_3$): δ

7.89–7.82 (4H, m), 7.50–7.37 (6H, m), 7.32–7.31 (1H, m), 6.25–6.24 (1H, m), 6.12–6.11 (1H, m), 5.63 (1H, dddd, J = 17.6, 10.0, 7.6, 7.6 Hz), 5.14–5.05 (2H, m), 4.37 (1H, dddd, J = 10.0, 10.0, 6.4, 6.4 Hz), 3.34 (1H, br dd, J = 10.4, 7.2 Hz), 2.79–2.61 (2H, m); HRMS Calcd for $C_{20}H_{21}NO_2P$ $[M + H]^+$: 338.13099; Found: 338.13157. $[\alpha]^{20}_D$ = +53.3 (c = 1.00, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4k**: 16 min (major) and 19 min (minor).



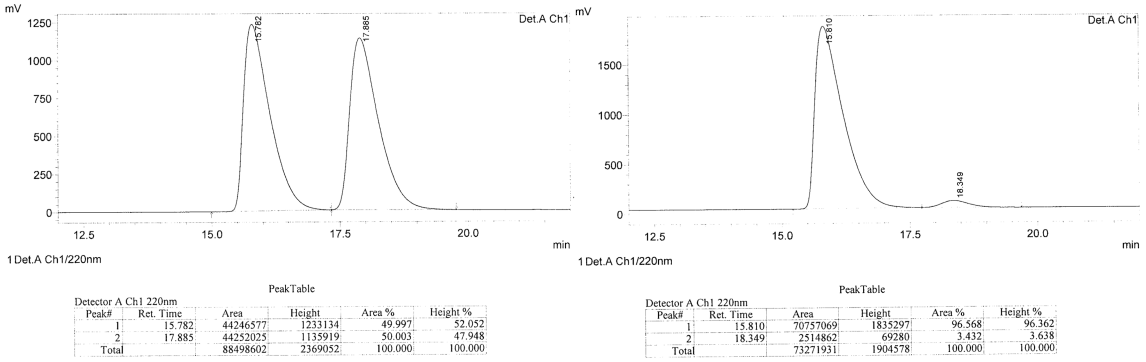
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.5	49.828	1	15.9	98.374
2	19.0	50.372	2	18.5	1.626

(*R*)-*P*,*P*-diphenyl-*N*-(1-(pyridin-3-yl)but-3-en-1-yl)phosphinic amide (**4l, Table 2**): The title compound is synthesized analogously to **4b** and purified analogously to **4o** (see below). M.p. = 133-134 °C. IR (neat): 3169 (w, br), 1438 (m), 1184 (s), 1123 (m), 1109 (m), 1071 (m), 921 (w), 754 (w), 725 (m), 698 (m), 533 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.39 (2H, br dd, J = 4.8, 1.6 Hz), 8.36 (1H, br d, J = 2.4 Hz), 7.82–7.77 (2H, m), 7.70–7.65 (2H, m), 7.419–7.42 (2H, m), 7.40–7.34 (3H, m), 7.28–7.23 (2H, m), 7.15–7.11 (1H, m), 5.53 (1H, dddd, J = 16.8, 10.4, 7.2, 7.2 Hz), 5.08–5.03 (2H, m), 4.35 (1H, dddd, J = 9.6, 9.6, 6.4, 6.4 Hz), 3.33 (1H, br dd, J = 8.0, 5.6 Hz), 2.65–2.55 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.6 (d, J = 15.6 Hz), 138.5 (d, J = 4.5 Hz), 134.4, 132.9, 132.7 (d, J = 127 Hz, peak overlaps with doublet at 132.06), 132.5 (d, J = 9.7 Hz), 132.2 (d, J = 2.2 Hz), 132.1 (d, J = 2.9 Hz), 131.9 (d, J = 8.9 Hz), 131.8 (d, J = 127 Hz, peak overlaps with doublet at 132.5), 128.7 (d, J = 12.6 Hz), 128.5 (d, J = 12.7 Hz), 123.4, 119.9, 52.5, 43.4 (d, J = 4.5 Hz); HRMS Calcd for $C_{21}H_{22}N_2OP$ $[M + H]^+$: 349.14697; Found: 349.14651. $[\alpha]^{25}_D$ = +45.2 (c = 1.00, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiralpak AD-H, 86:14 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **4l**: 38 min (major) and 43 min (minor).



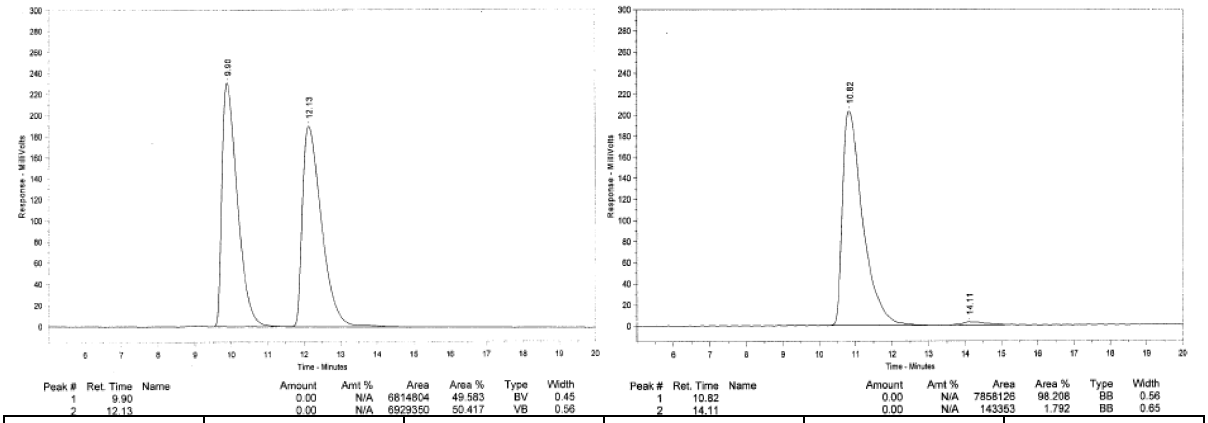
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	36.2 min	49.809	1	39.1 min	98.360
2	40.8 min	50.191	2	43.1 min	1.640

(*R*)-*P*,*P*-Diphenyl-*N*-(1-(p-4-methylphenyl)but-3-en-1-yl)phosphinic amide (S7, not shown in manuscript, see Chart S1): This compound is not listed in Table 2 of the publication, but has been used for determination of the absolute stereochemistry through X-ray analysis. It was synthesized and purified analogously to **4b** except for the following changes: 1) 2.5 mol % aminophenol **2g** (instead of 3 mol % **2g**) 2) 1.5 equiv. MeOH (instead of 2.5 equiv.). Homoallylamide **S7** (70.8 mg, 0.196 mmol, 98% yield) is obtained as a white solid. Crystals suitable for X-ray crystallography were obtained by slow evaporation of dichloromethane (See Part D of the Supplementary Information for the X-ray crystal structure). M.p. = 130–131 °C. IR (neat): 3178 (w, br), 3076 (w), 3052 (w), 3007 (w), 2977 (w), 2919 (w), 2882 (w), 1454 (m), 1435 (m), 1181 (s), 1123 (m), 1108 (m), 1078 (s), 917 (m), 899 (m), 748 (m), 723 (s), 694 (s), 561 (m), 535 (s), 497 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.88–7.75 (4H, m), 7.49–7.29 (6H, m), 7.09 (4H, app s), 5.58 (1H, app ddt, J = 17.2 10.0, 7.2 Hz), 5.10–5.00 (2H, m), 4.33–4.26 (1H, m), 3.40 (1H, br dd, J = 10.0, 6.4 Hz), 2.74–2.58 (2H, m), 2.31 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1 (d, J = 5.7 Hz), 136.6, 133.9, 133.3 (d, J = 127.0 Hz, 1 peak hidden under 133.9), 132.6 (d, J = 9.6 Hz), 132.2 (d, J = 130.0 Hz), 131.9 (d, J = 9.6 Hz), 131.8 (d, J = 3 Hz, 1 peak hidden under 131.9), 131.7 (d, J = 2.7 Hz), 129.1, 128.5 (d, J = 12.5 Hz), 128.3 (d, J = 12.6 Hz), 126.4, 118.6, 54.5, 43.7 (d, J = 3.8 Hz), 21.1; HRMS Calcd for $C_{23}H_{25}NOP$ $[M + H]^+$: 362.16738; Found: 362.16709. $[\alpha]^{20}_D$ = +50.8 (c = 2.11, $CHCl_3$) for a 96.5:3.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD–H, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **S7**: 16 min (major) and 18 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	15.8	49.997	1	15.8	96.568
2	17.9	50.003	2	18.3	3.432

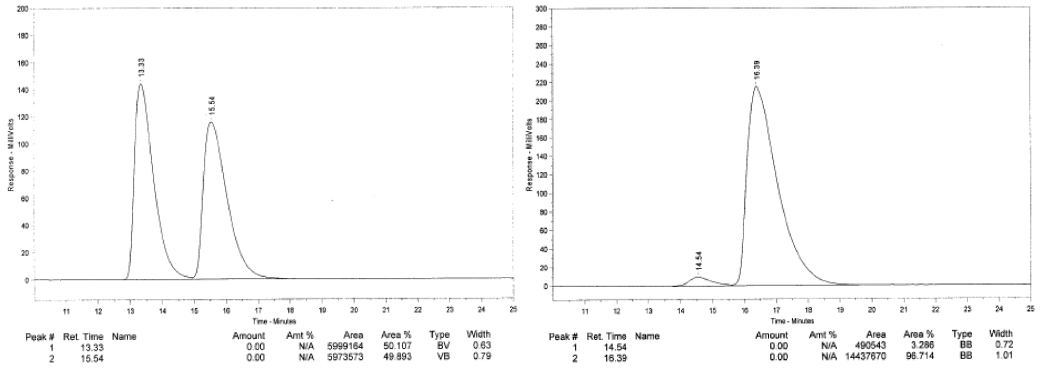
(*R*)-*N*-(3-Methyl-1-phenylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (**4m, Table 2**): The title compound is synthesized and purified analogously to **4b** [except allylboronic acid pinacol ester **1b** (32 μL, 0.15 mmol) is used as the nucleophile instead of **1a**], affording **4m** (34.4 mg, 0.0952 mmol, 95% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86–7.80 (2H, m), 7.76–7.70 (2H, m), 7.50–7.46 (1H, m), 7.44–7.38 (3H, m), 7.29–7.17 (7H, m), 4.78 (1H, s), 4.69 (1H, s), 4.40 (1H, dddd, *J* = 16.4, 16.4, 8.4, 8.4 Hz), 3.32 (1H, br dd, *J* = 8.0, 6.0 Hz), 2.62 (1H, dd, *J* = 13.6, 7.2 Hz), 2.53 (1H, dd, *J* = 14.0, 7.2 Hz), 1.58 (3H, s); HRMS Calcd for $C_{23}H_{25}NOP$ $[M + H]^+$: 362.16738; Found: 362.16649. $[\alpha]^{20}_D$ = +39 (*c* = 1.2, $CHCl_3$) for a 97.5:2.5 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 92:8 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **4m**: 11 min (major) and 14 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	9.90	49.583	1	10.8	98.206
2	12.1	50.417	2	14.1	1.792

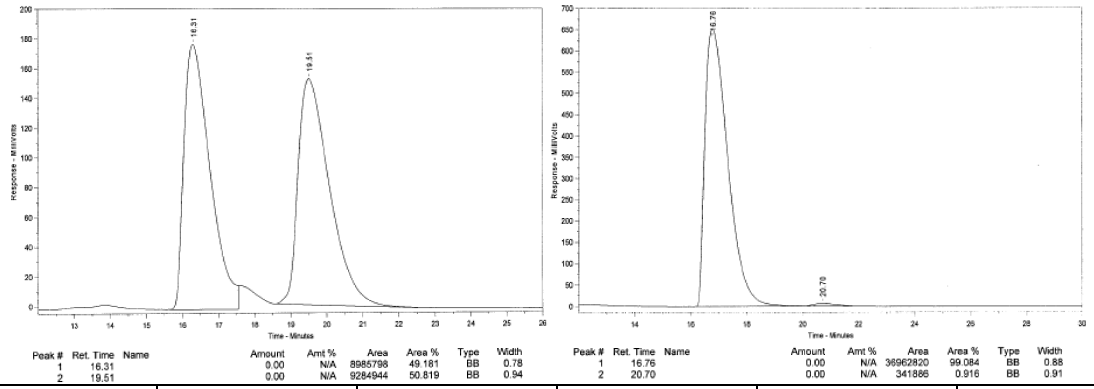
(*R*)-*N*-(1,3-Diphenylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (**4n, Table 2**): The title compound is synthesized and purified analogously to **4b** [except allylboronic acid pinacol ester **1c** (37 μL, 0.15 mmol) is used as the nucleophile instead of **1a** and the

reaction time is 6 h] affording **4n** (42.1 mg, 0.0994 mmol, >98% yield) as a white foam. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76–7.70 (4H, m), 7.47–7.40 (2H, m), 7.37–7.30 (4H, m), 7.27–7.16 (8H, m), 7.07–7.00 (2H, m), 5.21 (1H, d, J = 1.2 Hz), 4.87 (1H, d, J = 1.2 Hz), 4.27 (1H, dddd, J = 8.4, 8.4, 6.4, 6.4 Hz), 3.29 (1H, br dd, J = 8.8, 5.6 Hz), 3.25 (1H, dd, J = 14.0, 6.0 Hz), 2.99 (1H, dd, J = 14.0, 8.0 Hz); HRMS Calcd for $C_{28}H_{27}NOP$ $[M + H]^+$: 424.18303; Found: 424.18255. $[\alpha]^{20}_D$ = +26 (c = 1.7, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 92:8 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **4n**: 15 min (minor) and 16 min (major).



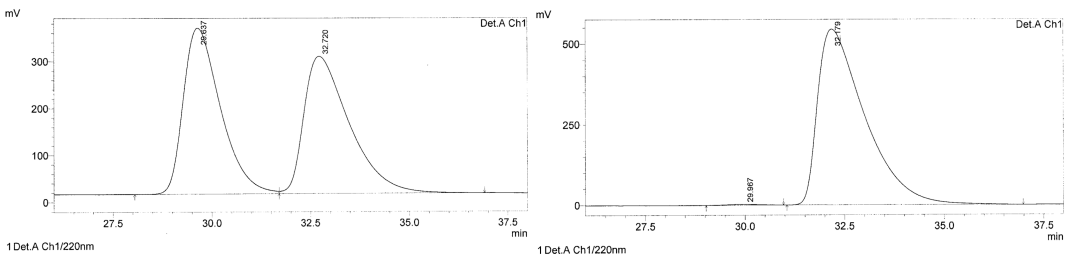
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	13.3	50.107	1	14.5	3.286
2	15.5	49.893	2	16.4	96.714

(*R*,*E*)-*P*,*P*-Diphenyl-*N*-(1-phenylhexa-1,5-dien-3-yl)phosphinic amide (**S8, not shown in manuscript, see Chart S1**): The title compound is purified in the manner identical to that used for **4b** to afford **S8** (31.3 mg, 0.0838 mmol, 84% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96–7.87 (4H, m), 7.51–7.39 (6H, m), 7.31–7.26 (4H, m), 7.24–7.21 (1H, m), 6.46–6.42 (1H, m), 6.15 (1H, ddd, J = 15.9, 6.3, 2.4 Hz), 5.78 (1H, dddd, J = 14.4, 7.6, 6.8, 6.8 Hz), 5.20–5.12 (2H, m), 4.01–3.92 (1H, m), 3.09 (1H, br dd, J = 9.6, 6.0 Hz), 2.59–2.45 (2H, m); HRMS Calcd for $C_{24}H_{25}NOP$ $[M + H]^+$: 374.16738; Found: 374.16756. $[\alpha]^{20}_D$ = +89 (c = 0.65, $CHCl_3$) for a 99:1 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **S8**: 17 min (major) and 21 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.3	49.181	1	16.8	99.084
2	19.5	50.819	2	20.7	0.916

(*R*,*E*)-*N*-(1-(2-Nitrophenyl)hexa-1,5-dien-3-yl)-*P*,*P*-diphenylphosphinic amide (S9, not shown in the manuscript, see Chart S1): The title compound is purified identically to **4b** affording **S9** (39.6 mg, 0.095 mmol, 95% yield) as a white solid. M.p. = 135 °C. IR (neat): 3149 (m, br), 3067 (w), 2857 (w), 1641 (w), 1605 (w), 1571 (w), 1520 (s), 1436 (m), 1350 (m), 1178 (s), 1123 (m), 1106 (m), 1067 (m), 952 (m), 918 (m), 745 (m), 724 (s), 691 (s), 541 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.00–7.88 (5H, m), 7.55–7.35 (9H, m), 7.01 (1H, dd, *J* = 16.0, 1.6 Hz), 6.17 (1H, dd, *J* = 15.6, 5.6 Hz), 5.80 (1H, dddd, *J* = 16.8, 10.0, 7.6, 6.4 Hz), 5.22–5.14 (2H, m), 4.02–3.96 (1H, m), 3.16 (1H, br dd, *J* = 9.6, 5.6 Hz), 2.62–2.49 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 137.0 (d, *J* = 6.0 Hz), 133.3, 133.3, 132.9, 132.9 (d, *J* = 128.0 Hz), 132.5 (d, *J* = 9.4 Hz), 132.4 (d, *J* = 130.0 Hz), 132.0 (2 d peaks exactly overlapping, *J* = 3 Hz), 132.0 (d, *J* = 9.3 Hz), 129.2, 128.7 (2 d peaks exactly overlapping, *J* = 12.6 Hz), 128.2, 125.9, 124.6, 119.5, 52.5, 42.0 (d, *J* = 4.2 Hz); HRMS Calcd for $C_{24}H_{24}N_2O_3P$ $[M + H]^+$: 419.15245; Found: 419.15207. $[\alpha]^{20}_D$ = +94.4 (*c* = 1.00, $CHCl_3$) for a 99.5:0.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD–H, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **S9** 30 min (minor) and 32 min (major).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.637	23154936	353487	49.698	54.717
2	32.720	23436642	292542	50.302	45.283
Total		46591578	646029	100.000	100.000

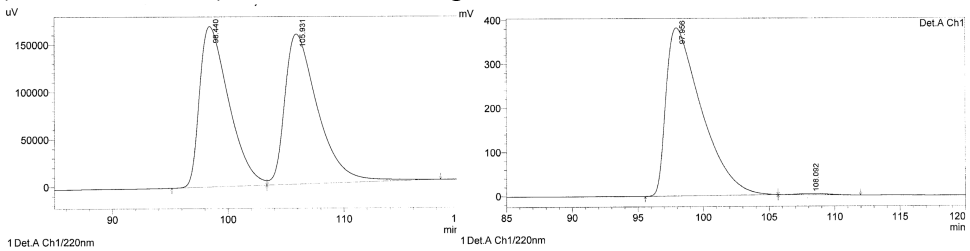
PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.967	145427	2568	0.321	0.469
2	32.179	45126070	545396	99.679	99.531
Total		45271497	547963	100.000	100.000

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	29.6	49.698	1	30.0	0.321
2	32.7	50.302	2	32.2	99.679

(*R*,*E*)-*N*-(1-(4-Methoxyphenyl)hexa-1,5-dien-3-yl)-*P*,*P*-diphenylphosphinic amide (S10, not shown in the manuscript, see Chart S1): The title compound is purified in the manner identical to that used for **4b** to generate **S10** (39.4 mg, 0.098 mmol, 98% yield) as a white solid. M.p. = 134 °C. IR (neat): 3180 (w, br), 3059 (w), 2929 (w), 2837 (w), 1607 (w), 1509 (m), 1433 (m), 1248 (m), 1185 (s), 1124 (m), 1108 (m), 1069 (m), 1031 (m), 976 (m), 912 (w), 811 (m), 745 (m), 725 (s), 693 (s), 541 (s), 516 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.96–7.86 (4H, m), 7.51–7.37 (6H, m), 7.22 (2H, d, *J* = 8.8 Hz), 6.82 (2H, d, *J* = 8.4 Hz), 6.37 (1H, d, *J* = 15.6 Hz), 6.01 (1H, dd, *J* = 16.0, 6.4 Hz), 5.79 (1H, dddd, *J* = 17.2, 10.4, 7.6, 7.2 Hz), 5.19–5.10 (2H, m), 3.94 (1H, m), 3.80 (3H, s), 3.08 (1H, br dd, *J* = 9.6, 6.0 Hz), 2.58–2.43 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 133.9, 133.3 (d, *J* = 127.0 Hz), 132.7 (d, *J* = 130.0 Hz), 132.6 (d, *J* = 9.4 Hz), 132.0 (d, *J* = 9.5 Hz), 131.9 (d, *J* = 2.8 Hz), 131.8 (d, *J* = 2.8 Hz), 129.9, 129.6, 129.3 (d, *J* = 5.7 Hz), 128.6 (d, *J* = 12.4 Hz), 128.5 (d, *J* = 12.6 Hz), 127.7, 119.0, 114.0, 55.4, 52.9, 42.4 (d, *J* = 4.5 Hz); HRMS Calcd for $C_{25}H_{27}NO_2P$ $[M + H]^+$: 404.17794; Found: 404.17730. $[\alpha]^{20}_D$ = +128.2 (*c* = 1.00, $CHCl_3$) for a 99:1 er sample.



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	98.440	29803902	169432	48.621	51.643
2	105.931	31494841	158651	51.379	48.357
Total		61298742	328083	100.000	100.000

PeakTable

Detector A Ch1 220nm

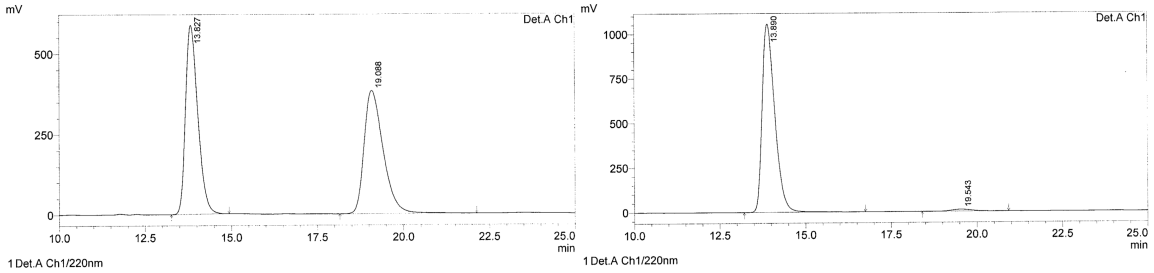
Peak#	Ret. Time	Area	Height	Area %	Height %
1	97.956	71854288	382013	99.431	99.315
2	108.092	411019	2636	0.569	0.685
Total		72265307	384649	100.000	100.000

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	98.4	48.621	1	98.0	99.431
2	105.9	51.379	2	108.1	0.569

The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD–H, 95:5 hexanes:*i*-PrOH, 0.2 mL/min, 220 nm): t_R of **S10**: 98 min (major) and 108 min (minor).

(*R*,*Z*)-*N*-(2-Bromo-1-phenylhexa-1,5-dien-3-yl)-*P*,*P*-diphenylphosphinic amide (S11, not shown in manuscript, see Chart S1): The title compound is purified identically to **4b** affording **S11** (43.4 mg, 0.096 mmol, 96% yield) as a white solid. M.p. = 123 °C. IR (neat): 3133 (m, br), 3077 (w), 3056 (w), 2910 (w), 2861 (w), 1643 (w), 1591 (w), 1458 (w), 1434 (m), 1182 (s), 1123 (m), 1105 (m), 1088 (m), 984 (m), 952 (m), 916 (m), 865 (m), 746 (m), 723 (s), 691 (s), 594 (m), 568 (m), 536 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.95–7.85 (4H, m), 7.54–7.28 (11H, m), 6.56 (1H, s), 5.74 (1H, app ddt, *J* =

17.2, 10.0, 7.2 Hz), 5.19–5.08 (2H, m), 4.04–3.95 (1H, m), 3.40 (1H, br dd, J = 9.6, 8.4 Hz), 2.68–2.51 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.1, 133.3, 133.0 (d, J = 127.0 Hz), 132.8 (d, J = 9.8 Hz), 132.2 (d, J = 2.7 Hz), 132.1 (d, J = 2.9 Hz), 131.9 (d, J = 130.0 Hz), 131.8 (d, J = 9.6 Hz), 129.7 (d, J = 5.4 Hz), 129.4, 129.1, 128.7 (d, J = 12.5 Hz), 128.5 (d, J = 12.8 Hz), 128.2, 128.1, 118.6, 58.8, 41.3 (d, J = 4.3 Hz); HRMS Calcd for $C_{24}H_{24}BrNOP$ $[M + H]^+$: 452.07789; Found: 452.07908. $[\alpha]^{20}_D$ = +7.5 (c = 1.00, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD–H, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **S11**: 14 min (major) and 19 min (minor).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.827	14545482	587197	49.618	60.510
2	19.088	14769733	383220	50.382	39.490
Total		29315216	970417	100.000	100.000

PeakTable

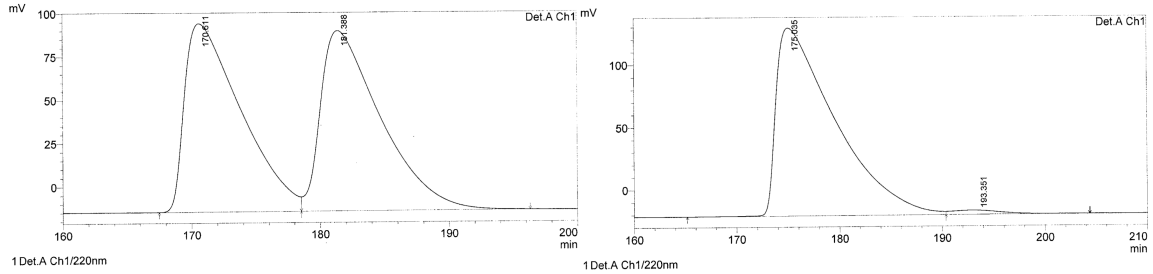
Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.890	27103659	1055854	98.297	98.951
2	19.543	469584	11196	1.703	1.049
Total		27573242	1067049	100.000	100.000

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	13.8	49.618	1	13.9	98.297
2	19.1	50.382	2	19.5	1.703

(*R*,*E*)-*N*-(Nona-1,5-dien-4-yl)-*P*,*P*-diphenylphosphinic amide (S12, not shown in the manuscript, see Chart S1): The title compound is prepared and purified analogously to **4b** from freshly prepared **6** (except 2.5 mol % aminophenol **2g** used in the reaction instead of 3.0 mol %) affording **S12** (32.7 mg, 0.096 mmol, 96% yield) as a white solid. Crystals suitable for x-ray crystallography were obtained by vapor diffusion from a dichloromethane/hexane solvent system at 22 ºC See Part D of the Supplementary Information for the X-ray crystal structure. M.p. = 87 °C. IR (neat): 3121 (m, br), 3057 (w), 2953 (w), 2928 (w), 2868 (w), 1639 (w), 1590 (w), 1458 (m), 1436 (m), 1198 (m), 1182 (m), 1107 (m), 1065 (m), 966 (m), 909 (m), 753 (w), 719 (s), 691 (s), 565 (m), 524 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94–7.83 (4H, m), 7.50–7.38 (6H, m), 5.74 (1H, dddd, J = 17.2, 10.4, 8.0, 6.8 Hz), 5.50 (1H, app dtd, J = 15.2, 6.4, 0.8 Hz), 5.39 (1H, app ddt, J = 15.6, 6.0, 1.0 Hz), 5.15–5.07 (2H, m), 3.78–3.68 (1H, m), 2.93 (1H, br dd, J = 9.6, 6.0 Hz), 2.47–2.31 (2H, m), 1.94 (2H, quartet, J = 6.8 Hz), 1.33 (2H, app sextet, J = 7.2 Hz), 0.86 (3H, t, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.1, 133.4 (d, J = 127.0 Hz), 132.9 (d, J = 130.0 Hz), 132.6 (d, J = 9.4 Hz), 132.0 (d, J = 9.5 Hz), 131.8 (2 d exactly overlapping, J = 2.5 Hz), 131.7 (d, J = 5.7 Hz), 131.5, 128.5 (d, J = 12.5 Hz), 128.5 (d, J = 12.5 Hz), 118.4, 52.6, 42.7 (d, J = 4.5 Hz), 34.4, 22.4, 13.8; HRMS Calcd for $C_{21}H_{27}NOP$ $[M + H]^+$: 340.18303; Found: 340.18359. $[\alpha]^{20}_D$ = +7.40 (c = 1.00, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC

analysis in comparison with authentic racemic material (Chiracel OD–H, 98.5:1.5 hexanes:*i*-PrOH, 0.15 mL/min, 220 nm): t_R of **S12**: 175 min (major) and 193 min (minor).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	170.611	33080046	108668	49.503	51.091
2	181.388	33744364	104028	50.497	48.909
Total		66824410	212697	100.000	100.000

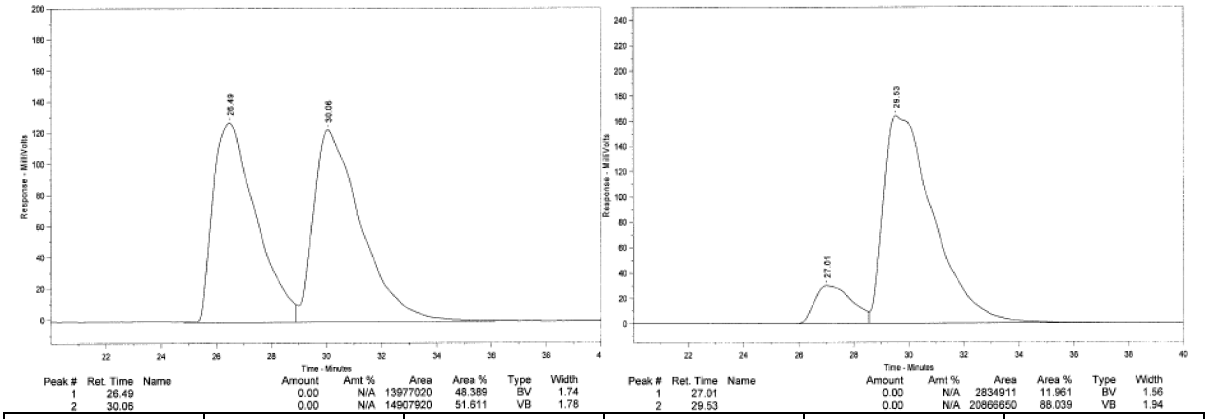
PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	175.035	60112701	150311	98.210	97.855
2	193.351	1095862	3295	1.790	2.145
Total		61208563	153606	100.000	100.000

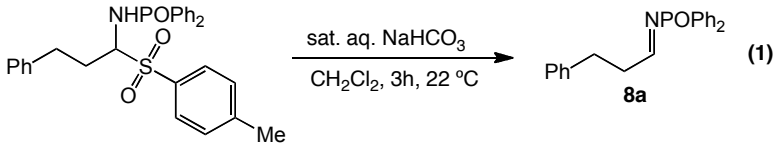
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	170.6	49.503	1	175.0	98.210
2	181.4	50.497	2	193.4	1.790

(*R*)-*P*,*P*-Diphenyl-*N*-(1-phenylhex-5-en-1-yn-3-yl)phosphinic amide (S13, not shown in the manuscript, see Chart S1): The title compound is purified identically to **4b** affording **S13** (33.9 mg, 0.0913 mmol, 91% yield) as a yellow solid. M.p. = 105–107 ºC. IR (neat): 3132 (m, br), 3076 (w), 3055 (w), 2913 (w), 2857 (w), 1641 (w), 1591 (w), 1488 (m), 1312 (m), 1181 (s), 1125 (s), 1107 (s), 1070 (m), 945 (m), 747 (s), 725 (s), 690 (s), 530 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.04–7.99 (2H, m), 7.89–7.84 (2H, m), 7.52–7.40 (6H, m), 7.35–7.32 (2H, m), 7.32–7.24 (3H, m) 5.97 (1H, dddd, J = 17.0, 10.0, 7.6, 6.9 Hz), 5.29–5.19 (2H, m), 4.31–4.23 (1H, m), 3.37 (1H, dd, J = 10.1, 8.3 Hz), 2.70–2.53 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.2, 133.0 (d, J = 127.6 Hz), 132.9 (d, J = 9.8 Hz), 132.1 (d, J = 2.7 Hz), 132.0 (d, J = 130.4 Hz), 131.8 (d, J = 9.8 Hz, only the peak at 131.9 is visible, the other is overlapping), 131.8, 128.8 (d, J = 12.6 Hz), 128.8 (d, J = 12.9 Hz), 128.4 (d, J = 5.5 Hz, only the peak at 128.4 is visible, the other is overlapping), 122.9, 119.7, 89.7 (d, J = 8.0 Hz), 84.1, 43.4, 42.9 (d, J = 3.5 Hz); HRMS Calcd for $C_{24}H_{23}NOP$ $[M + H]^+$: 372.15173; Found: 372.15177. $[\alpha]^{20}_D$ = -100 (c = 0.85, $CHCl_3$) for a 88:12 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 97:3 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **S13**: 27 min (minor) and 30 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	26.5	48.389	1	27.0	11.961
2	30.1	51.611	2	29.5	88.039

Representative Procedure for Enantioselective Allyl Additions to Alkyl-Substituted *N*-Diphenylphosphinoyl Imines:[7,8]



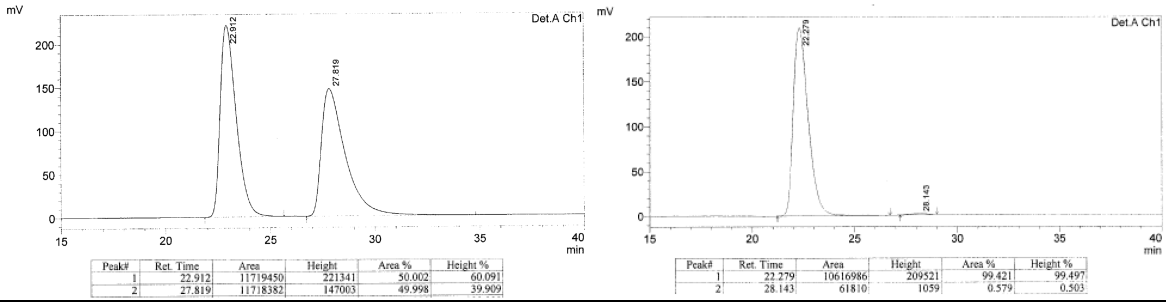
Preparation of the alkyl-substituted aldimine: A six-dram vial equipped with an 11 x 4 mm stir bar is charged with sulfinyl adduct (eq. 1, 0.4 mmol) to which is added CH_2Cl_2 (8.0 mL) and a saturated aqueous solution of $NaHCO_3$ (8.0 mL) consecutively. The biphasic mixture is allowed to stir vigorously enough for the solution to be homogeneous for 3 h at 22 °C. The organic layer is separated and the aqueous phase is washed with CH_2Cl_2 (3 x 5 mL). The combined organic layers are dried over $MgSO_4$. The volatiles are removed under reduced pressure and the unpurified imine is azeotropically dried under vacuum with anhydrous benzene to afford aldimine **8a** as light yellow oil (>98% conversion and yield are assumed). The vessel containing **8a** is sealed with a rubber septum and anhydrous toluene (2 mL) is added to prepare a stock solution of 0.1 mmol **8a**/500. µL toluene.

Preparation of catalyst solution (small scale): In a nitrogen-filled glovebox (not needed for gram scale; only used when reactions are performed at mg scale to achieve highly reproducible data), aminophenol **2g** (6.9 mg, 0.023 mmol) is added to an oven-dried two-dram vial equipped with a stir bar followed by 1.5 mL of a stock solution of NaO*t*-Bu in toluene (9.6 mg, 0.10 mmol/8.0 mL). The vial is sealed with a cap (phenolic open top cap with a red PFTE/white silicone septa) and electrical tape and allowed to stir under nitrogen at 22 ºC for ~10 minutes.

An oven-dried two-dram vial equipped with a stir bar and sealed with a cap (phenolic open top cap with a red PFTE/white silicone septa) and electrical tape is charged with toluene (100. µL), methanol (10. µL, 0.25 mmol), and allylboronic acid pinacol ester (28 µL, 0.15

mmol). To this mixture is added 500. μL of the stock solution of aldimine **8a** (described above), followed by 400. μL of the catalyst solution (described above) of [**2g** (1.82 mg, 6.00 μmol) and NaO*t*-Bu (0.48 mg, 5.0 μmol)]. The clear and colorless solution is allowed to stir at 22 ºC for four h during which time no visible change occurs. The cap is removed and 3 mL of saturated aqueous $NaIO_4$ is added and the biphasic mixture is allowed to stir for 20 minutes. The aqueous layer is washed with ethyl acetate (4 x 4 mL), and the combined organic layers are dried over Na_2SO_4 and concentrated *in vacuo*. The resulting yellow oil was purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 10 mL hexanes, 10 mL 3:1 hexanes:ethyl acetate, 10 mL 2:1 hexanes:ethyl acetate, 10 mL 1:1 hexanes:ethyl acetate, and 10 mL ethyl acetate) to afford **S14** (19.2 mg, 0.0511 mmol, 51% yield) as a white solid.

(*S*)-*P*,*P*-Diphenyl-*N*-(1-phenylhex-5-en-3-yl)phosphinic amide (**S14, not shown in the manuscript, see Chart S1**): The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91–7.84 (4H, m), 7.49–7.39 (6H, m), 7.24–7.19 (2H, m), 7.15–7.10 (3H, m), 5.78 (1H, dddd, *J* = 17.2, 10.4, 7.6, 7.6 Hz), 5.14–5.09 (2H, m), 3.25–3.16 (1H, m), 2.82 (1H, br dd, *J* = 10.8, 6.4 Hz), 2.73–2.57 (2H, m), 2.39–2.35 (2H, m), 1.86–1.80 (2H, m); HRMS Calcd for $C_{24}H_{27}NOP$ $[M + H]^+$: 376.18303; Found: 376.18135. $[\alpha]^{20}_D$ = –2.6 (*c* = 0.43, $CHCl_3$) for a >99:1 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 95:5 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **S14**: 22 min (major) and 28 min (minor).



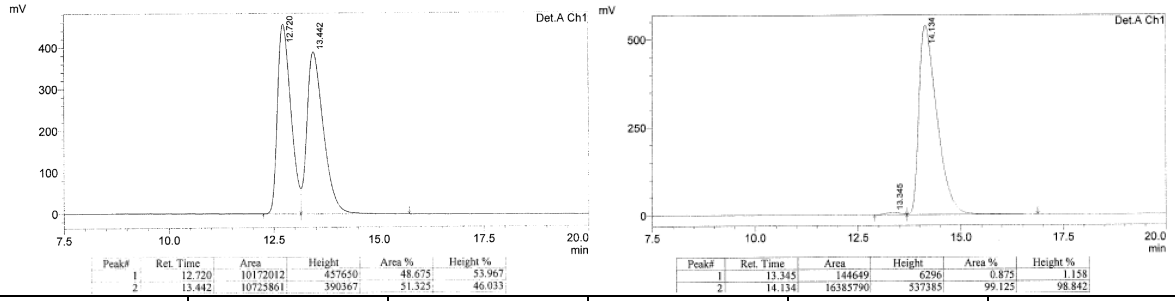
Peak	Ret. Time	Area	Height	Area %	Height %
1	22.912	1171945	221341	50.002	60.091
2	27.819	1171838	147003	49.998	39.909

Peak	Ret. Time	Area	Height	Area %	Height %
1	22.279	10616986	209521	99.421	99.497
2	28.143	61810	1059	0.579	0.503

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	22.9	50.002	1	22.3	99.421
2	27.8	49.998	2	28.1	0.579

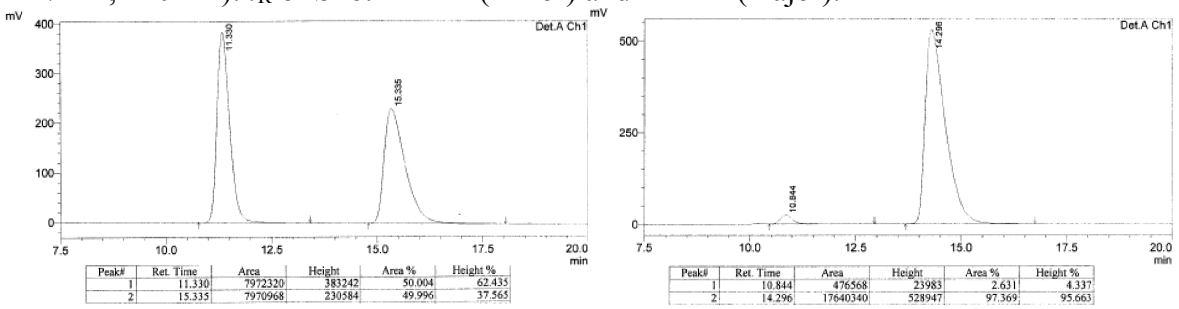
(*S*)-*N*-(6-Methylhept-1-en-4-yl)-*P*,*P*-diphenylphosphinic amide (**S15, not shown in manuscript, see Chart S1**): The title compound is purified identically to **S14**, affording **S15** (17.7 mg, 0.0540 mmol, 54% yield) as a white solid. The analytical data are fully consistent with those reported previously.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93–7.87 (4H, m), 7.51–7.41 (6H, m), 5.79 (1H, dddd, *J* = 17.6, 10.4, 7.6, 7.6 Hz), 5.14–5.10 (2H, m), 3.25–3.14 (1H, m), 2.75 (1H, br dd, *J* = 10.8, 6.0 Hz), 2.39–2.28 (2H, m), 1.84–1.70 (1H, m), 1.42–1.29 (2H, m), 0.80 (3H, d, *J* = 6.6 Hz), 0.76 (3H, d, *J* = 6.5 Hz); HRMS Calcd

for $C_{20}H_{27}NOP$ $[M + H]^+$: 328.18303; Found: 328.18398. $[\alpha]^{20}_D$ = –38 (*c* = 0.73, $CHCl_3$) for a 98.5:1.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 95:5 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **S15**: 13 min (minor) and 14 min (major).



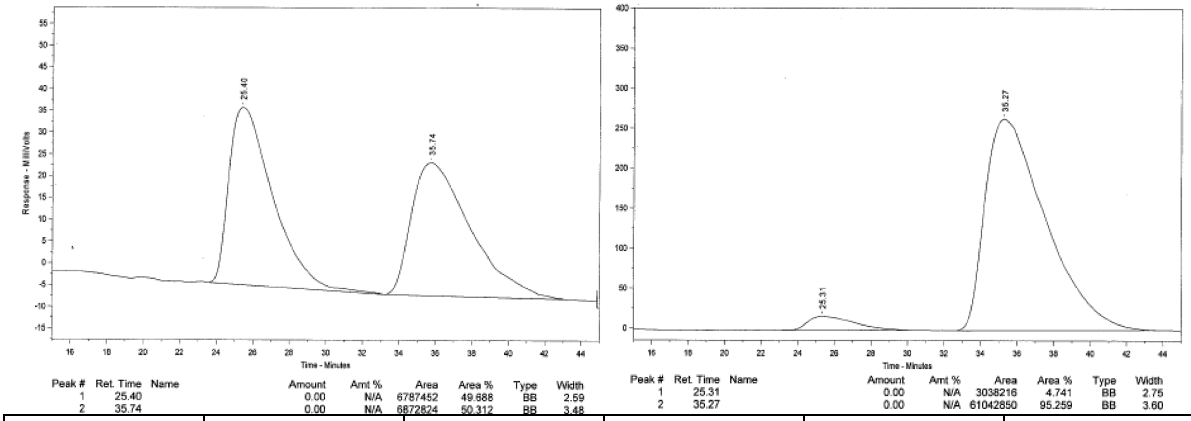
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	12.7	48.675	1	13.3	0.875
2	13.4	51.325	2	14.1	99.125

(*R*)-*N*-(1-Cyclohexylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (S16, not shown in the manuscript, see Chart S1): The title compound is synthesized and purified identically to **S14** (except 8.5 mol % of NaO*t*-Bu is used in the reaction instead of 5 mol %) affording **S16** (27.2 mg, 0.0769 mmol, 77% yield) as a white solid. M.p. = 120–122 °C. IR (neat): 3207 (w, br), 3075 (w), 3057 (w), 2921 (m), 2850 (m), 1639 (w), 1436 (s), 1187 (s), 1123 (s), 1108 (s), 1067 (m), 994 (w), 909 (m), 722 (s), 694 (s), 533 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.93–7.87 (4H, m), 7.50–7.42 (6H, m), 5.77 (1H, dddd, *J* = 17.3, 10.1, 7.3, 7.3 Hz), 5.12–5.06 (2H, m), 3.02–2.87 (1H, m), 2.77 (1H, br dd, *J* = 10.7, 6.1 Hz), 2.09 (2H, app t, *J* = 6.5 Hz), 1.82–1.61 (5H, m), 1.46–1.41 (1H, m), 1.24–1.15 (4H, m), 0.98-0.92 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.1, 133.3 (d, *J* = 128.7 Hz), 133.2 (d, *J* = 129.8 Hz, only peak at 132.8 is visible, the other is overlapping), 132.5 (d, *J* = 9.3 Hz), 132.3 (d, *J* = 9.3 Hz), 131.80 (d, *J* = 1.4 Hz), 131.78 (d, *J* = 1.4 Hz), 127.50 (d, *J* = 12.5 Hz), 127.48 (d, *J* = 12.5 Hz), 117.8, 55.9 (d, *J* = 2.2 Hz), 42.1 (d, *J* = 5.1 Hz), 38.5 (d, *J* = 4.2 Hz), 29.5, 28.8, 26.6, 26.5, 26.4; HRMS Calcd for $C_{22}H_{29}NOP$ $[M + H]^+$: 354.19868; Found: 354.19835. $[\alpha]^{20}_D$ = –21 (*c* = 0.78, $CHCl_3$) for a 97.5:2.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 95:5 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **S16**: 11 min (minor) and 14 min (major).

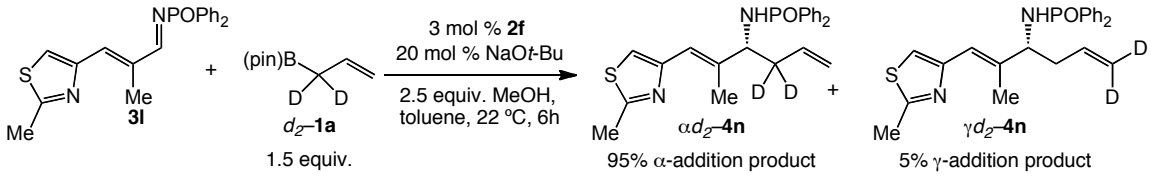


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	11.3	50.004	1	10.8	2.631
2	15.5	49.996	2	14.3	97.369

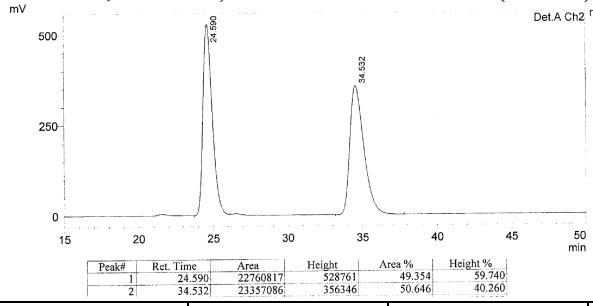
(*R*,*E*)-*N*-(2-Methyl-1-(2-methylthiazol-4-yl)hexa-1,5-dien-3-yl)-*P*,*P*-diphenylphosphinic amide (4o, Figure 4b): Please note that the data (reaction conditions/stoichiometries, yield, e.r.) in Figure **4b** of the manuscript refer to the reaction with **1a** as the nucleophile instead of *d*$_2$–**1a**. The title compound is synthesized analogously to **4o** except for the following changes: 1) The aminophenol catalyst **2f** is employed as a catalyst instead of **2g**. 2) 20 mol % of NaO*t*-Bu is used in the reaction instead of 3 mol %. 3) Reaction time is six h. The product is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 10 mL hexanes, 10 mL 1:1 hexanes:ethyl acetate, 15 mL diethyl ether, 6 mL ethyl acetate and 16 mL 5:1 ethyl acetate:MeOH) to afford **4o** (37.7 mg, 0.0923 mmol, 92% yield) as a pale yellow oil. IR (neat): 3357 (w, br), 3193 (w, br), 3076 (w), 3058 (w), 2966 (w), 2926 (w), 2871 (w), 1574 (w), 1437 (m), 1184 (s), 1121(m), 1108 (m), 952 (m), 910 (m), 723 (s), 694 (s), 525 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92–7.84 (4H, m), 7.40–7.37 (6H, m), 6.83 (1H, s), 6.30 (1H, s), 5.70 (1H, dddd, *J* = 17.1, 9.9, 7.2, 7.2 Hz), 5.14–5.06 (2H, m), 3.81 (1H, dddd, *J* = 9.4, 9.4, 6.6, 6.6 Hz), 3.16 (1H, dd, *J* = 9.5, 5.6 Hz), 2.69 (3H, s), 2.60–2.53 (1H, m), 2.50–2.43 (1H, m), 2.00 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.5, 152.9, 139.9 (d, *J* = 5.0 Hz), 133.9, 133.1 (d, *J* = 127.6 Hz), 132.6 (d, *J* = 9.5 Hz), 132.4 (d, *J* = 131.1 Hz), 131.9 (d, *J* = 9.5 Hz), 131.9 (d, *J* = 2.8 Hz), 131.8 (d, *J* = 2.8 Hz), 128.6 (d, *J* = 12.6 Hz), 128.5 (d, *J* = 12.7 Hz), 120.2, 118.6, 115.7, 58.0, 40.4 (d, *J* = 4.3 Hz), 19.3, 15.5; HRMS Calcd for $C_{24}H_{26}N_2OPS_1$ $[M + H]^+$: 409.15034; Found: 409.15018. $[\alpha]^{20}_D$ = +94 (*c* = 0.45, $CHCl_3$) for a 95:5 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD, 86:14 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4o**: 25 min (minor) and 35 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	25.4	49.688	1	25.3	4.741
2	35.7	50.312	2	35.3	95.259



(*R*,*E*)-*N*-(4,4-Dideuterio-2-methyl-1-(2-methylthiazol-4-yl)hexa-1,5-dien-3-yl)-*P*,*P*-diphenylphosphinic amide (*d*$_2$–4o, Figure 4b): The title compound is synthesized and purified analogously to **4o,** except 1,1-dideuterioallylboronic acid pinacol ester (***d*$_2$-1a**) is used as the nucleophile (contaminated with ~50% vinylboronic acid pinacol ester). The reaction proceeded to 85% conversion (based on 400 MHz ^{1}H NMR analysis and affords ***d*$_2$-4o** (24.5 mg, 0.0597 mmol, 60% yield) in 95:5 α:γ addition products (see above; determined by ^{2}H NMR) as yellow oil. The following analytical data is for α addition product α–***d*$_2$-4o**, unless otherwise noted. IR (neat): 3357 (w, br), 3193 (w, br), 3076 (w), 3058 (w), 2966 (w), 2926 (w), 2871 (w), 1574 (w), 1437 (m), 1184 (s), 1121(m) 1108 (m), 910 (m), 723 (s), 694 (s), 525 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95–7.85 (4H, m), 7.51–7.36 (6H, m), 6.84 (1H, s), 6.31 (1H, s), 5.70 (1H, dd, *J* = 17.1, 10.1 Hz), 5.15–5.07 (2H, m), 3.79 (1H, app t, *J* = 9.6 Hz), 3.16 (1H, dd, *J* = 9.8, 5.6 Hz), 2.70 (3H, s), 2.60–2.53 (1H, m), 2.50–2.43 (γ-addition product; 0.17 H, m), 2.00 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 152.9, 139.9 (d, *J* = 5.1 Hz), 133.8, 133.0 (d, *J* = 127.7 Hz), 132.6 (d, *J* = 9.5 Hz), 132.4 (d, *J* = 131.1 Hz), 132.0 (d, *J* = 9.5 Hz), 132.0 (d, *J* = 2.9 Hz), 131.9 (d, *J* = 2.6 Hz), 128.6 (d, *J* = 12.6 Hz), 128.5 (d, *J* = 12.7 Hz), 120.2, 118.7, 115.7, 57.9, 40.4–39.2 (m), 19.4, 15.5; ^{2}H NMR (76 MHz, 9:1 $CHCl_3$:$CDCl_3$): δ 5.22–5.08 (γ-addition product; 0.09H, m), 2.51 (α-addition product; 2H, d, *J* = 6.1 Hz); HRMS Calcd for $C_{24}H_{24}D_2N_2OPS$ $[M + H]^+$: 411.16290; Found: 411.16232. $[\alpha]^{20}_D$ = +47 (*c* = 0.73, $CHCl_3$) for a 95:5 er sample. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 86:14 hexanes:*i*-PrOH, 0.5 mL/min, 254 nm): t_R of ***d*$_2$-4o**: 25 min (minor) and 35 min (major).



Peak#	Ret. Time	Area	Height	Area %	Height %
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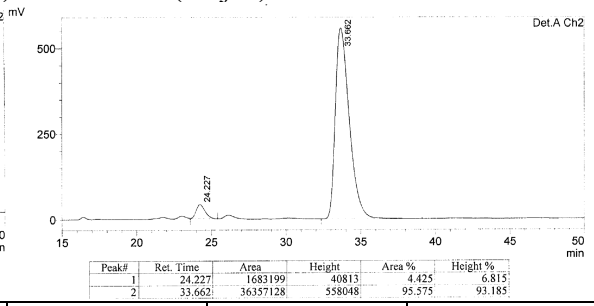
2	34.532	23357086	356346	50.646	40.260



Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.227	1683199	40813	4.425	6.815
2	33.662	36357128	558048	95.575	93.185

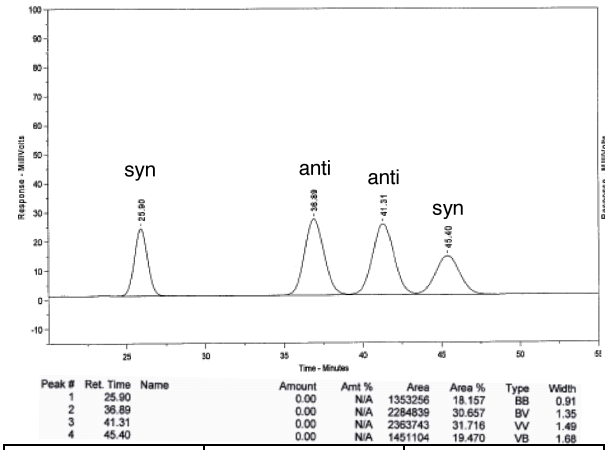
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	24.6	49.354	1	24.2	4.425
2	34.5	50.646	2	33.7	95.575

■ **Representative Procedure for Enantioselective Allyl Additions with Enantiomerically Enriched Allylboronates (Figure 4c)**: *Preparation of catalyst solution and allylboronate Solution*: Under an atmosphere of nitrogen, aminophenol **2g** (6.1 mg, 0.02 mmol) is added to an oven-dried two-dram vial equipped with a stir bar followed by 1.0 mL of a stock solution of NaO*t*-Bu in toluene (9.6 mg, 0.010 mmol/6.0 mL) and the solution is allowed to stir at 22 ºC for ~10 minutes. In a separate oven-dried two-dram vial, allylboronate ***S*-9** (70.8 mg, 0.260. mmol) and MeOH (17.5 μL, 0.690. mmol) are dissolved in 700. μL of toluene to make a stock solution of ***S*-9** and MeOH.

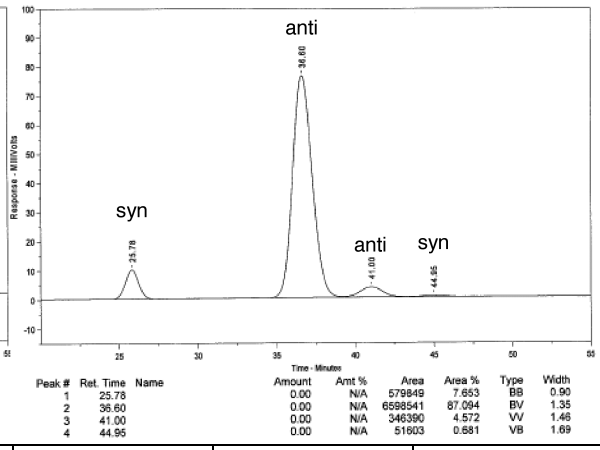
An oven-dried one-dram vial equipped with a stir bar is charged with phenyl-substituted aldimine **3a** (15.3 mg, 50.0 μmol), 150. μL of toluene, and 200. μL of the prenominate stock solution of ***S*-9** (20 mg, 74 μmol) and MeOH (4.0 mg, 13 μmol). To this mixture is added 150. μL of the catalyst solution (described above) of **2g** (0.92 mg, 3.0 μmol) and NaO*t*-Bu (0.24 mg, 2.5 μmol) and a cap is attached to the vial and sealed with electrical tape. The clear and colorless solution is allowed to stir at 22 ºC for 18 hours during which time it becomes cloudy and white. The cap is removed and 3 mL of a saturated aqueous solution of $NaIO_4$ is added and the biphasic mixture is allowed to stir for 20 minutes. The aqueous layer is washed with ethyl acetate (4 x 4 mL), dried over Na_2SO_4, and concentrated *in vacuo* to provide a yellow solid. The homoallylamide product was purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 10 mL hexanes, 10 mL 1:1 hexanes:diethyl ether, 30 mL 1:3 hexanes:diethyl ether, 35 mL diethyl ether, 30 mL 4:1 diethyl ether:ethyl acetate) to afford **10** (19.3 mg, 0.0427 mmol, 85% yield of a 85:15 ratio of diastereomers) as an off white solid, which is re-crystallized from CH_2Cl_2/hexanes (vapor diffusion, 22 ºC) to give 6.4 mg (0.014 mmol, 28% yield) of **10** as clear, colorless, needles suitable for X-ray crystallography in >20:1 dr and >99:1 er (See Part D of the Supplementary Information for the X-ray crystal structure). This diastereo- and enantiomerically enriched product was used to obtain the data given below (excluding the HPLC chromatographs). The HPLC chromatograph of the authentic racemic material was obtained from a 60:40 ratio of anti:syn diastereomers (enriched by silica gel chromatography). The excess of the anti diastereomer allowed assignment of which peak corresponds to which diastereomer. The identity and absolute stereochemistry of the major enantiomer of the major diastereomer is determined by X-Ray crystallography.

***N*-((1*R*,2*R*)-2-Phenethyl-1-phenylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (10, Figure 4c)**: M.p. = 156–158 °C. IR (neat): 3228 (w, br), 3059 (w), 3027 (w), 2916 (w), 2857 (w), 1437 (w), 1187 (m), 1125 (m), 1109 (m), 1069 (m), 917 (m), 745 (m), 723 (m), 692 (s), 534 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.82–7.77 (2H, m), 7.64–7.59 (2H, m), 7.50–7.46 (1H, m), 7.40–7.33 (3H, m), 7.21–7.12 (8H, m), 7.04–7.02 (4H, m), 5.73 (1H, ddd, *J* = 17.5, 10.1, 9.1 Hz), 5.28 (1H, d, *J* = 10.3 Hz), 5.11 (1H, d, *J* = 17.1 Hz), 4.17 (1H, app dd, *J* = 18.2, 8.0 Hz), 3.37 (1H, app t, *J* = 7.1 Hz), 2.62 (1H, ddd, *J* = 14.2, 9.4, 5.3 Hz), 2.50–2.43 (1H, m), 2.40–2.33 (1H, m), 1.76-1.68 (1H, m), 1.63–1.53 (1H, m);

^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6 (d, J = 3.1 Hz), 142.0, 138.8, 133.5 (d, J = 127.2 Hz), 132.7 (d, J = 9.7 Hz, only peak at 132.6 is visible, the other is overlapping), 132.1 (d, J = 130.7 Hz, only peak at 131.4 is visible, the other is overlapping), 131.9 (d, J = 2.6 Hz), 131.8 (d, J = 9.6 Hz), 131.6 (d, J = 2.8 Hz), 128.6 (d, J = 12.5 Hz), 128.6, 128.4, 128.2, 128.1 (d, J = 12.8 Hz), 127.4, 127.1, 125.8, 118.8, 58.1, 51.1 (d, J = 5.5 Hz), 33.3, 32.1; HRMS Calcd for $C_{30}H_{31}NOP$ $[M + H]^+$: 452.21433; Found: 452.21249. $[\alpha]^{20}_D$ = +12 (c = 0.43, $CHCl_3$) for a >20:1 dr, >99:1 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AZ-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **10** (anti diastereomer): 37 min (major) and 41 min (minor); t_R of **10** (syn diastereomer): 26 min (major) and 45 min (minor).

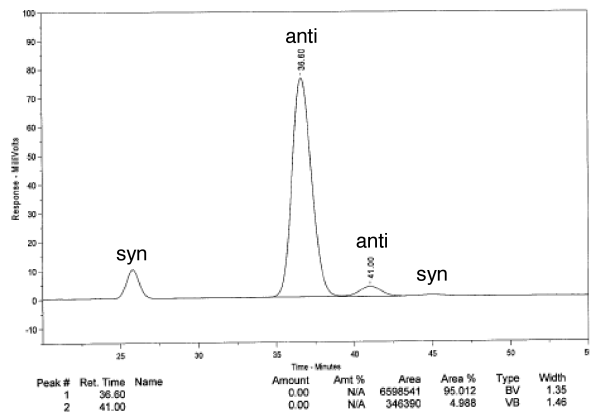


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.90		0.00	N/A	1353256	18.157	BB	0.91
2	36.89		0.00	N/A	2284839	30.657	BV	1.35
3	41.31		0.00	N/A	2363743	31.716	VV	1.49
4	45.40		0.00	N/A	1451104	19.470	VB	1.68

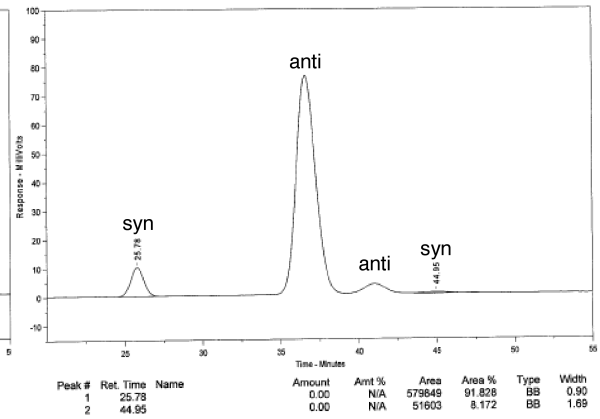


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.78		0.00	N/A	579849	7.653	BB	0.90
2	36.60		0.00	N/A	6598541	87.094	BV	1.35
3	41.00		0.00	N/A	346390	4.572	VV	1.46
4	44.95		0.00	N/A	51603	0.681	VB	1.69

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	25.9	18.157	1 (syn)	25.8	7.653
2 (anti)	36.9	30.657	2 (anti)	36.6	87.094
3 (anti)	41.3	31.716	3 (anti)	41.0	4.572
4 (syn)	45.4	19.470	4 (syn)	45.0	0.681



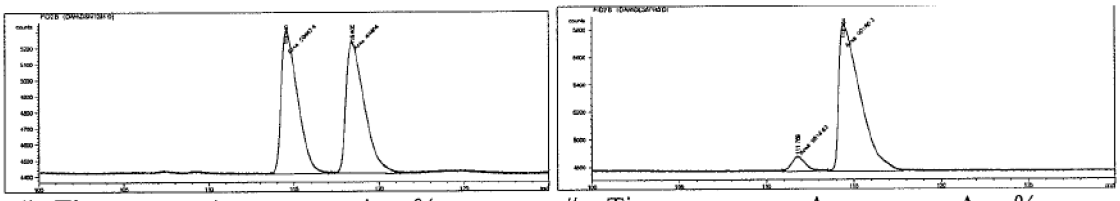
Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	36.60		0.00	N/A	6598541	95.012	BV	1.35
2	41.00		0.00	N/A	346390	4.988	VB	1.46



Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.78		0.00	N/A	579849	91.828	BB	0.90
2	44.95		0.00	N/A	51603	8.172	BB	1.69

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (anti)	36.6	95.012	1 (syn)	25.8	91.828
2 (anti)	41.0	4.988	2 (syn)	45.0	8.172

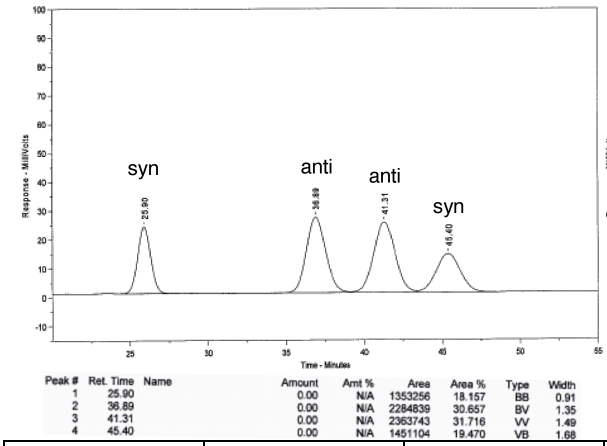
To measure the enantiomeric purity of ***S*-9**, allylboronate ***S*-9** was oxidized by hydrogen peroxide to the corresponding alcohol. The enantiomeric purity of allylboronate ***S*-9** was determined by GLPC analysis in comparison with authentic racemic material (Betadex 120 column, 110 ºC, 15 psi).



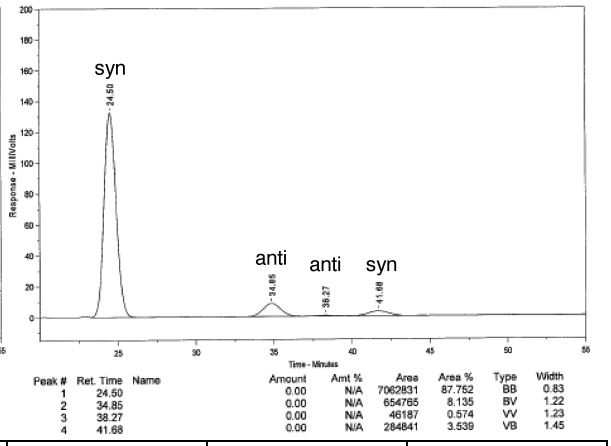
#	Time	Area	Area%	#	Time	Area	Area%
1	114.54	59663	49.690	1	111.769	5814.6	6.057
2	118.40	66041	50.310	2	114.434	90180.3	93.943

***N*-((1*R*,2*S*)-2-Phenethyl-1-phenylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (11, Figure 4c)**: The title compound is purified analogously to **10** affording **11** (22.5 mg, 0.0498 mmol, >98 % yield of a 85:15 ratio of diastereomers) as a white solid. Th e resulting solid was recrystallized from CH_2Cl_2/hexanes (vapor diffusion, 22 ºC) to give 7.4 mg (0.016 mmol, 32% yield) of **11** as clear, colorless needles suitable for x-ray crystallography in >20:1 dr and >99:1 er. This diastereo- and enantiomerically enriched product was used to obtain the data given below (excluding the HPLC chromatographs). The identity (and absolute stereochemistry of the major enantiomer) of the major diastereomer is determined by X-Ray crystallography (see Part D of the Supplementary Information). M.p. = 161–163 °C. IR (neat): 3215 (w, br), 3056 (w), 3027 (w), 2912 (w), 2855 (w), 1494 (m), 1184 (m), 1122 (m), 1106 (m), 1083 (m), 912 (m), 749 (m), 691 (s), 531 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.84–7.79 (2H, m), 7.67–7.62 (2H, m), 7.51–7.47 (1H, m), 7.42–7.36 (3H, m), 7.26–7.20 (7H, m), 7.15–7.12 (1H, m), 7.07–7.00 (4H, m), 5.49 (1H, ddd, *J* = 17.3, 10.0, 10.0 Hz), 5.30–5.26 (2H, m), 4.22 (1H, ddd, *J* = 11.1, 11.1, 4.7 Hz), 3.67 (1H, dd, *J* = 10.7, 6.4 Hz), 2.68–2.61 (1H, m), 2.58–2.42 (2H, m), 1.76 (1H, dddd, *J* = 13.5, 9.9, 6.3, 3.6 Hz), 1.29–1.19 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.3, 140.9 (d, *J* = 5.4 Hz), 137.6, 133.5 (d, *J* = 127.5 Hz, only peak at 134.1 is visible, the other is overlapping), 132.8 (d, *J* = 9.8 Hz, only peak at 132.7 is visible, the other is overlapping), 132.0 (d, *J* = 2.7 Hz), 131.9 (d, *J* = 131.7 Hz), 131.77 (d, *J* = 9.6 Hz), 131.78 (d, *J* = 2.8 Hz), 128.6 (d, *J* = 12.5 Hz), 128.5, 128.4, 128.3 (d, *J* = 12.8 Hz), 128.0, 127.8, 127.2, 125.9, 120.0, 58.0, 52.1 (d, *J* = 3.1 Hz), 34.2, 33.9; HRMS Calcd for $C_{30}H_{31}NOP$ $[M + H]^+$: 452.21433; Found: 452.21376. $[\alpha]^{20}_D$ = –16 (c = 0.20) for a >20:1 dr and >99:1 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material; see explanation of peak assignment in the analytical data for compound **10** (Chiracel AZ-H, 90:10 hexanes:*i*-PrOH,

0.8 mL/min, 220 nm): t_R of **11** (major diastereomer): 25 min (major) and 42 min (minor); t_R of **11** (minor diastereomer): 35 min (major) and 38 min (minor).

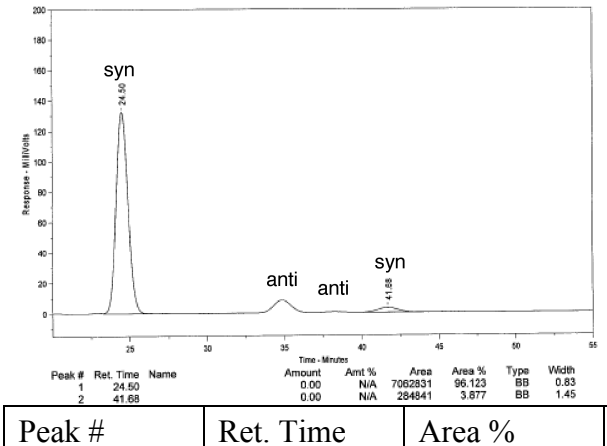


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.90		0.00	N/A	1353256	18.157	BB	0.91
2	36.89		0.00	N/A	2284839	30.657	BV	1.35
3	41.31		0.00	N/A	2363743	31.716	VV	1.49
4	45.40		0.00	N/A	1451104	19.470	VB	1.68

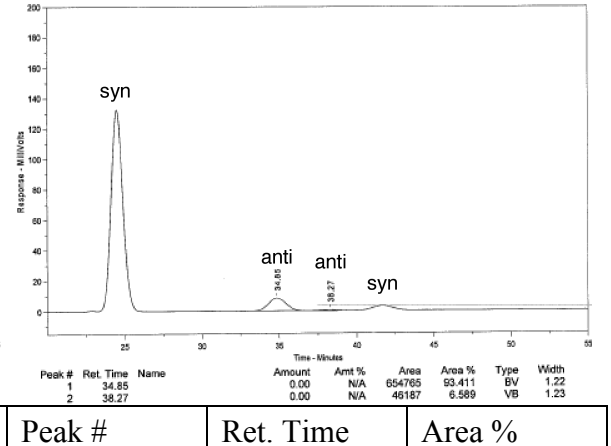


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	24.50		0.00	N/A	7062831	87.752	BB	0.83
2	34.85		0.00	N/A	654765	8.135	BV	1.22
3	38.27		0.00	N/A	46187	0.574	VV	1.23
4	41.68		0.00	N/A	284841	3.539	VB	1.45

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	25.9	18.157	1 (syn)	24.5	87.752
2 (anti)	36.9	30.657	2 (anti)	34.9	8.135
3 (anti)	41.3	31.716	3 (anti)	38.3	0.574
4 (syn)	45.4	19.470	4 (syn)	41.7	3.539



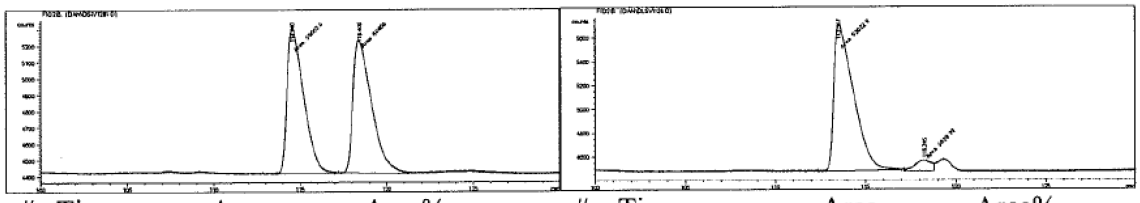
Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	24.50		0.00	N/A	7062831	96.123	BB	0.83
2	41.68		0.00	N/A	284841	3.877	BB	1.45



Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	34.85		0.00	N/A	654765	93.411	BV	1.22
2	38.27		0.00	N/A	46187	6.589	VB	1.23

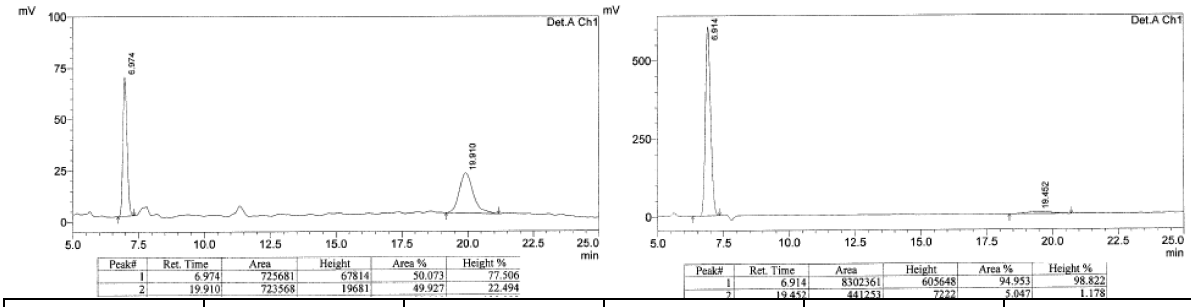
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	24.5	96.123	1 (anti)	34.9	93.411
2 (syn)	41.7	3.877	2 (anti)	38.3	6.589

To measure the enantiomeric purity of ***R*-9**, allylboronate ***R*-9** was oxidized by hydrogen peroxide to the corresponding alcohol. The enantiomeric purity of allylboronate ***R*-9** was determined by GLPC analysis in comparison with authentic racemic material (Betadex 120 column, 110 ºC, 15 psi).



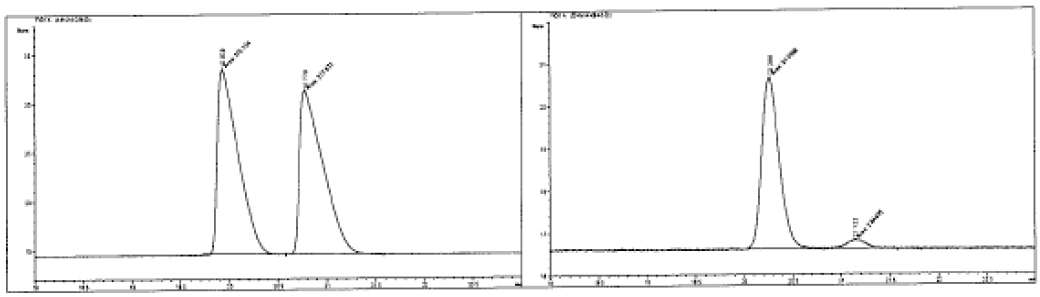
#	Time	Area	Area%	#	Time	Area	Area%
1	114.54	59663	49.690	1	113.517	93000	95.398
2	118.40	66041	50.310	2	118.245	4486.1	4.60

***N*-((1*S*,2*R*)-2-Cyclohexyl-2-methyl-1-phenylbut-3-en-1-yl)-*P*,*P*-diphenylphosphinic amide (13, Figure 4c)**: The title compound is synthesized in the manner identical to that used for the preparation of **10** (except when utilizing $Zn(O\textit{t}\text{-Bu})_2$ instead of $NaO\textit{t}\text{-Bu}$). The homoallylamide **13** is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 10 mL hexanes, 10 mL 1:1 hexanes:diethyl ether, 30 mL 1:3 hexanes:diethyl ether, 60 mL diethyl ether) to afford **13** (17.0 mg, 0.038 mmol, 76 % yield of isolated major diastereomer) as a white solid. Crystals suitable for X-ray crystallography were obtained by vapor diffusion from a diethyl ether/hexane solvent system at 22 ºC. The identity (and absolute stereochemistry of the major enantiomer) of the major diastereomer is determined by X-ray crystallography (see Part D of the Supplementary Information). M.p. = 137–139 °C. IR (neat): 3221 (w, br), 3058 (w), 2924 (s), 2851 (m), 1452 (m), 1184 (s), 1123 (s), 1108 (s), 1064 (m), 912 (m), 723 (s), 698 (s), 530 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79–7.74 (2H, m), 7.51–7.45 (3H, m), 7.41–7.38 (2H, m), 7.34–7.30 (1H, m), 7.23–7.20 (3H, m), 7.15 (2H, app ddd, J = 7.7, 7.7, 3.2 Hz), 7.00–6.98 (2H, m), 5.70 (1H, dd, J = 17.7, 11.0 Hz), 5.27 (1H, dd, J = 10.9, 1.4 Hz), 5.13 (1H, dd, J = 17.7, 1.4 Hz), 4.17 (1H, app t, J = 11.2 Hz), 3.56 (1H, app t, J = 9.8 Hz), 1.81 (1H, d, J = 12.9 Hz), 1.67 (1H, d, J = 10.8 Hz), 1.60–1.53 (2H, m), 1.36 (1H, d, J = 6.9 Hz), 1.22 (3H, s), 1.10–0.67 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.0, 141.9 (d, J = 3.3 Hz) 133.7 (d, J = 128.3 Hz), 132.8 (d, J = 9.9 Hz), 132.0 (d, J = 131.8 Hz), 131.83 (d, J = 3.1 Hz, only peak at 131.81 is visible, the other is overlapping), 131.79 (d, J = 9.4 Hz, only peak at 131.74 is visible, the other is overlapping), 131.5 (d, J = 2.8 Hz), 128.6 (d, J = 12.4 Hz), 128.4, 128.0 (d, J = 12.8 Hz), 127.7, 126.9, 115.9, 59.4, 48.5 (d, J = 3.8 Hz), 42.8, 29.1, 27.9, 27.1, 26.9, 26.6, 15.8; HRMS Calcd for $C_{29}H_{35}NOP$ $[M + H]^+$: 444.24563; Found: 444.24499. $[\alpha]^{20}_D$ = +8.9 (c = 0.87, $CHCl_3$) for a 95:5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 90:10 hexanes:*i*-PrOH, 1.0 mL/min, 220 nm): t_R of **13**: 7.0 min (major) and 20 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	7.0	50.073	1	6.9	94.953
2	19.9	49.927	2	19.5	5.047

To measure the enantiomeric purity of **12**, allylboronate **12** was oxidized by hydrogen peroxide to the corresponding alcohol. The enantiomeric purity of allylboronate **12** was determined by GLPC analysis in comparison with authentic racemic material (Chiral dex CD-BDM column, 140 ºC, 15 psi).



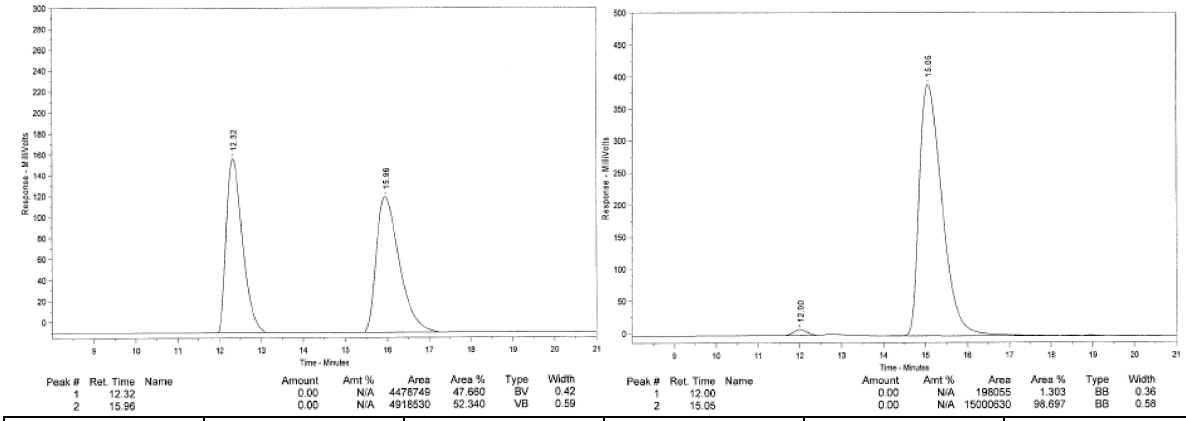
#	Time	Area	Area%	#	Time	Area	Area%
1	19.929	276.1	49.861	1	20.266	51.1	94.727
2	20.779	277.7	50.139	2	21.133	2.8	5.273

■ **Representative Procedure for *Small Scale* Catalytic Enantioselective Allyl Additions to Isatins (Figure 5a)**: Under an atmosphere of N_2, aminophenol **2g** (6.1 mg, 0.020 mmol) is added to an oven-dried two dram vial equipped with a stir bar followed by 2.0 mL of a stock solution of NaO*t*-Bu in toluene (7.7 mg, 0.080 mmol/8.0 mL). The vial is sealed with a cap (phenolic open top cap with a red PFTE/white silicone septa) and electrical tape, removed from the glovebox and allowed to stir under nitrogen at 22 ºC for ~10 minutes.

A separate vial equipped with a stir bar is charged with *N*-TBS-isatin **14a** (26.2 mg, 0.100 mmol)**,** sealed with a cap (phenolic open top cap with a red PFTE/white silicone septa) and electrical tape and purged with N_2. To this sealed vial under nitrogen is added toluene (0.95 mL), 50. uL of a catalyst solution [described above; **2g** (0.16 mg, 0.50 mmol) and NaO*t*-Bu (0.048 mg, 0.50 mmol)], MeOH (10 μL, 0.25 mmol) and allylboronic acid pinacol ester **1a** (28 μL, 0.15 mmol) by syringe in the stated order. The clear yellow solution is allowed to stir at 22 ºC for 1.5 h during which time it becomes colorless, which signifies complete consumption of the highly pigmented starting material **14a**.

Removal of the TBS group: The cap is removed and the mixture is concentrated *in vacuo*. The resultant pale yellow oil is then dissolved in a solution of *p*-toluenesulfonic acid monohydrate (22.8 mg, 0.120 mmol) in methanol (0.5 mL, Fisher ACS grade). The mixture is allowed to stir at 22 ºC for 3 h after which time 1 mL of a saturated solution of aqueous $NaHCO_3$ is added drop-wise over one minute. Ethyl acetate (1 mL) is subsequently added, the organic and the aqueous layers are separated, which are then washed with ethyl acetate (3 x 1 mL). The combined organic layers are dried over Na_2SO_4 and concentrated *in vacuo* to provide a white solid that is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in hexanes. The off-white solid residue is dry loaded on silica gel and eluted with 10 mL 4:1 hexanes:ethyl acetate, 20 mL 2:1 hexanes:ethyl acetate, 20 mL 1:1 hexanes:ethyl acetate) to afford **15a** (17.5 mg, 0.0925 mmol, 98% yield) as a white solid. Crystals suitable for X-ray crystallography (see Part D of the Supplementary Information) were grown by slow evaporation from methanol at 22 ºC.

(*R*)-3-Allyl-3-hydroxyindolin-2-one (**15a, Figure 5a**): The analytical data are fully consistent with those reported previously.[14] ^{1}H NMR (400 MHz, CD_3OD): δ 7.36 (1H, d, J = 7.2 Hz), 7.26 (1H, t, J = 8.5 Hz), 7.07 (1H, t, J = 7.4 Hz), 6.89 (1H, d, J = 7.7 Hz) 5.54 (1H, app dq, J = 16.7, 8.1 Hz), 5.05–4.98 (2H, m), 2.76–2.59 (2H, m); HRMS Calcd for $C_{11}H_{12}N_1O_2$ $[M + H]^+$: 190.08680; Found: 190.08650. $[\alpha]^{20}_D$ = +11 (c = 1.3, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **15a**: 12 min (minor) and 15 min (major).

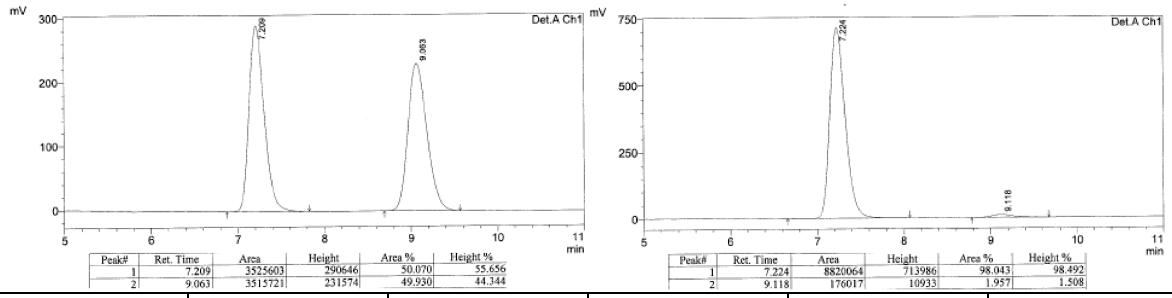


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	12.3	47.660	1	12.0	1.303
2	16.0	52.340	2	15.1	98.697

(*R*)-3-Allyl-1-(*tert*-butyldimethylsilyl)-3-hydroxyindolin-2-one (S17, not shown in manuscript, see Chart S1): To obtain the *N*-TBS protected hydroxyl-oxindole, after concentration *in vacuo*, the resultant pale yellow oil can be purified by silica gel

(14) Sano, D.; Nagata, K.; Itoh, T. *Org. Lett.* **2008**, *10*, 1593–1595.

chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in dichloromethane and eluted with 10 mL dichloromethane followed by 30 mL 20:1 dichloromethane:diethyl ether) to afford **S17** (30.4 mg, 0.100 mmol, >98% yield) as pale yellow oil. IR (neat): 3401 (w, br), 2953 (w), 2929 (w), 2858 (w), 1701 (s), 1613 (m), 1465 (s), 1255 (s), 1171 (s), 1105 (m), 945 (m), 824 (s), 732 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.36 (1H, dd, J = 7.4, 1.4 Hz), 7.22 (1H, td, J = 7.8, 1.5 Hz), 7.05 (1H, td, J = 7.5, 0.8 Hz), 6.99 (1H, d, J = 8.0 Hz), 5.54 (1H, dddd, J = 16.9, 10.1, 8.5, 6.2 Hz), 5.10–5.04 (2H, m), 2.96 (1H, s), 2.72–2.57 (2H, m), 0.99 (9H, s), 0.51 (3H, s), 0.50 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.3, 145.8, 131.6, 130.9, 129.4, 124.4, 122.7, 120.3, 113.2, 76.3, 43.9, 26.6, 19.8, –3.1, –3.3; HRMS Calcd for $C_{17}H_{26}NO_2Si$ $[M + H]^+$: 304.17328; Found: 304.17280. $[\alpha]^{20}_D$ = +24.2 (c = 1.5, $CHCl_3$) for a 94:6 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **S17**: 7 min (major) and 9 min (minor).



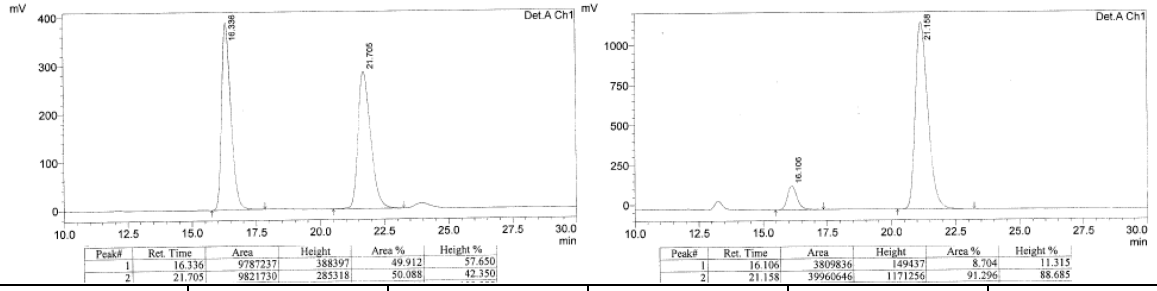
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.209	3525603	290646	50.070	55.656
2	9.063	3515721	231574	49.930	44.344

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.224	8820064	713986	98.043	98.492
2	9.118	176017	10933	1.957	1.508

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	7.2	50.070	1	7.2	98.043
2	9.1	49.930	2	9.1	1.957

(*R*)-3-Allyl-4,6-dibromo-3-hydroxyindolin-2-one (**15b, Figure 5a**): The enantioselective allyl addition to SEM-isatin **14b** is carried out following the representative procedure for aminophenol catalyzed enantioselective allyl additions to isatins. The procedure for removal of SEM group is as follows. After 2.0 h, the mixture of the enantioselective allyl addition turns from yellow to colorless (signifying complete consumption of highly pigmented **14b**), the cap is removed and the reaction mixture is concentrated *in vacuo*. The resultant pale yellow oil is transferred to a two-dram vial, sealed with a septum and purged with nitrogen. A separate oven dried one-dram vial equipped with a stir bar is charged with $MgBr_2 \bullet Et_2O$ (96.8 mg, 0.375 mmol), sealed with a cap (phenolic open top cap with a red PFTE/white silicone septa) and electrical tape, and removed from the glovebox. The unpurified 3-allyl-3-hydroxy oxindole **S18** is transferred through a syringe to the vial containing $MgBr_2 \bullet Et_2O$ using 3 x 300 uL of dichloromethane. The mixture is allowed to stir under nitrogen at 22 ºC for 60 h during which time it becomes a tan slurry. The cap is removed and the tan slurry is dissolved in methanol and passed through a short plug of Celite®; the plug is washed with methanol (15 mL) and the combined solution is concentrated *in vacuo* to afford a tan solid. The resulting solid is dissolved in 1 mL of

methanol and 2 mL of a solution of saturated aqueous $NaHCO_3$, and the cloudy light pink solution is allowed to stir open to the air at 22 ºC for five h. Ethyl acetate (2 mL) is added and the layers separate. The aqueous layer is extracted with 3 x 2 mL of ethyl acetate and the combined organic layers are dried over Na_2SO_4 and concentrated *in vacuo* to afford a light tan solid. The hydroxyoxindole product is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in dichloromethane and eluted with 15 mL dichloromethane followed by 10 mL 9:1 dichloromethane:diethyl ether, 10 mL 8:1 dichloromethane:diethyl ether, and 30 mL 4:1 dichloromethane:diethyl ether), affording **15b** (14.9 mg, 0.0429 mmol, 86% yield) as a white solid. The analytical data are fully consistent with those reported previously.[15] IR (neat): 3368 (m, br), 3169 (w, br), 2923 (w, br), 1703 (s), 1605 (s), 1572 (s), 1429 (m), 1364 (m), 1334 (m), 1300 (m), 1175 (m), 1086 (m), 1074 (m), 944 (m), 928 (m), 840 (s), 785 (m), 738 (m), 673 (s) cm^{-1}; ^1H NMR (400 MHz, CD_3OD): δ 7.38 (1H, s), 7.02 (1H, s), 5.39–5.28 (1H, m), 5.09–5.05 (1H, m), 4.97–4.94 (1H, m), 3.26–3.21 (1H, m), 2.72–2.67 (1H, m), 3.24–3.19 (1H, m), 2.92 (1H, br s), 2.84–2.79 (1H, m), 0.91 (2H, t, J = 8.0 Hz), –0.02 (9H, s); HRMS Calcd for $C_{11}H_{10}NO_2Br_2$ $[M + H]^+$: 347.90578; Found: 347.90587. $[\alpha]^{20}_D$ = –10 (c = 0.64, CH_3OH) for a 91.5:8.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 86:14 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **15b**: 16 min (minor) and 21 min (major).

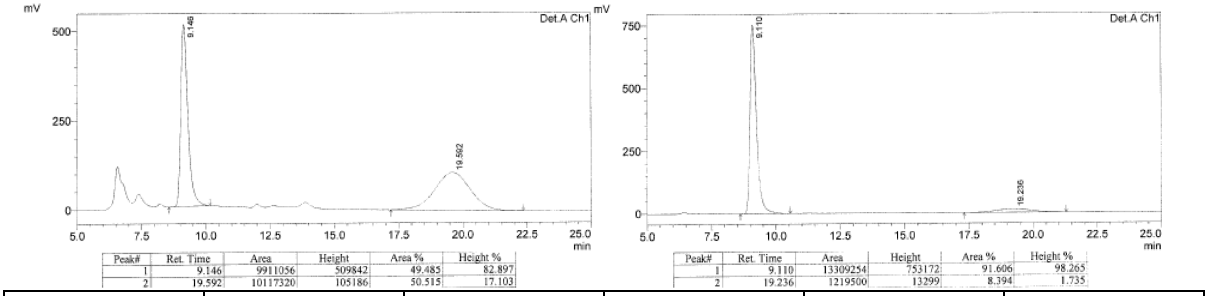


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.3	49.912	1	16.1	8.704
2	21.7	50.088	2	21.2	91.296

(*R*)-3-Allyl-4,6-dibromo-3-hydroxy-1-((2-(trimethylsilyl)ethoxy)methyl)indolin-2-one (S18, not shown in the manuscript, see Chart S1): If one wishes to obtain the *N*-SEM-protected hydroxyl-oxindole, then after concentration *in vacuo*, purify the resultant yellow oil by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in dichloromethane and eluted with 40 mL dichloromethane) to afford **S18** (23.0 mg, 0.0481 mmol, 96% yield) as a clear, colorless oil. IR (neat): 3400 (w, br), 3082 (w), 2953 (w), 2923 (w), 2895 (w), 1723 (m), 1597 (s), 1571 (m), 1249 (m), 1077 (s, br), 1010 (m), 922 (m), 857 (m), 831 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.41 (1H, s), 7.16 (1H,

(15) Cao, Z.-Y.; Zhang, Y.; Ji, C.-B.; Zhou, J. *Org. Lett.* **2011**, *13*, 6398–6401.

s), 5.34 (1H, dddd, J = 17.0, 17.0, 8.4, 8.4 Hz), 5.16–5.10 (2H, m), 5.00–4.97 (2H, m), 3.56–3.46 (2H, m), 3.24–3.19 (1H, m), 2.92 (1H, br s), 2.84–2.79 (1H, m), 0.91 (2H, t, J = 8.0 Hz), –0.02 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 176.6, 145.0, 129.9, 129.6, 126.2, 124.2, 121.0, 120.0, 112.9, 78.1, 70.0, 66.6, 40.1, 17.9, –1.3; HRMS Calcd for $C_{18}H_{24}NO_3NaSiBr_2$ $[M + Na]^+$: 497.97062; Found: 497.97090. $[\alpha]^{20}_D$ = +5.6 (c = 1.1, $CHCl_3$) for a 91.5:8.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OJ-H, 95:5 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **S18**: 9 min (major) and 20 min (minor).



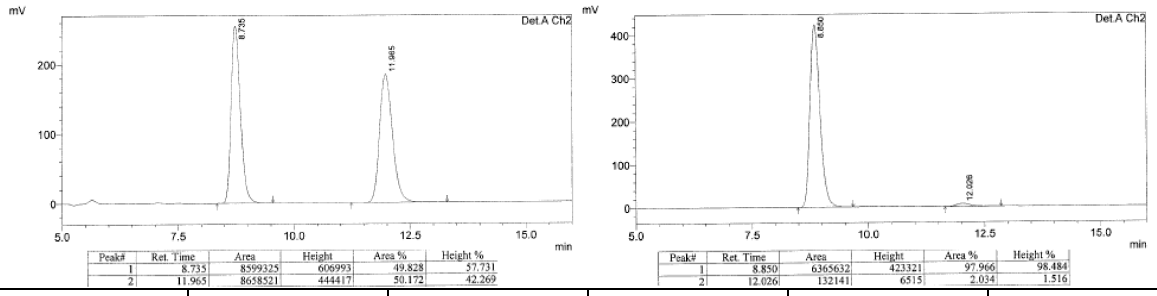
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.146	9911056	509842	49.485	82.897
2	19.592	10117320	105186	50.515	17.103

Peak #	Ret. Time	Area %
1	9.1	49.485
2	19.6	50.515

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.110	13309254	753172	91.606	98.265
2	19.236	1219500	13299	8.394	1.735

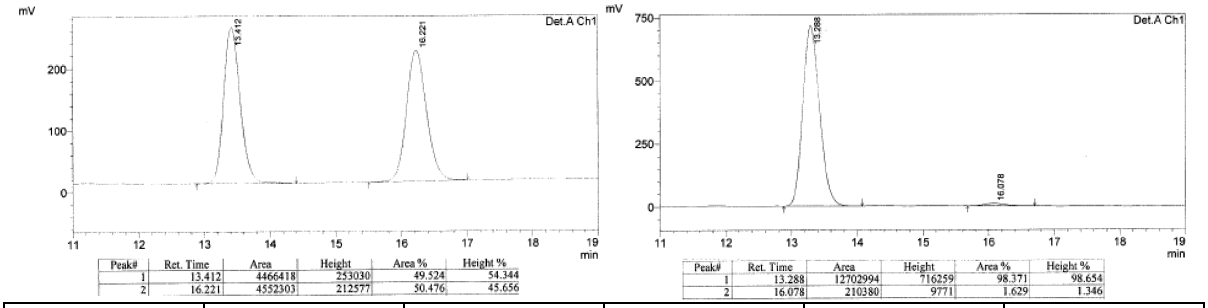
Peak #	Ret. Time	Area %
1	9.1	91.606
2	19.2	8.394

(*R*)-3-Allyl-1-(*tert*-butyldimethylsilyl)-3-hydroxy-5-methoxyindolin-2-one (16, Figure 5a): The title compound is synthesized in the same manner as described for **S17** (except reaction time is four h) and purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in dichloromethane and eluted with 10 mL dichloromethane, 15 mL 30:1 dichloromethane:diethyl ether, 30 mL 20:1 dichloromethane:diethyl ether), affording *N*-TBS-protected hydroxyoxindole **16** (31.2 mg, 0.0932 mmol, 93% yield) as a pale orange oil. IR (neat): 3400 (w, br), 2953 (w), 2930 (w), 2858 (w), 1699 (s), 1594 (m), 1482 (s), 1255 (s), 1197 (s), 1120 (w), 1081 (m), 911 (m), 840 (s), 790 (m), 730 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.96 (1H, d, J = 2.8 Hz), 6.89 (1H, d, J = 8.7 Hz), 6.75 (1H, app dd, J = 8.7, 2.7 Hz), 5.54 (1H, dddd, J = 16.9, 10.1, 9.0, 6.1 Hz), 5.11–5.07 (2H, m), 3.79 (3H, s), 2.99 (1H, s), 2.70–2.56 (2H, m), 0.98 (9H, s), 0.50 (3H, s), 0.48 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.2, 155.8, 138.9, 132.8, 130.8, 120.3, 114.5, 113.7, 110.7, 76.7, 55.9, 44.0, 26.6, 19.8, –3.2, –3.4; HRMS Calcd for $C_{18}H_{28}NO_3Si$ $[M + H]^+$: 334.18384; Found: 334.18318. $[\alpha]^{20}_D$ = +11 (c = 1.3, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel AD-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 254 nm): t_R of **16**: 9 min (major) and 12 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	8.7	49.828	1	8.9	97.966
2	12.0	50.172	2	12.0	2.034

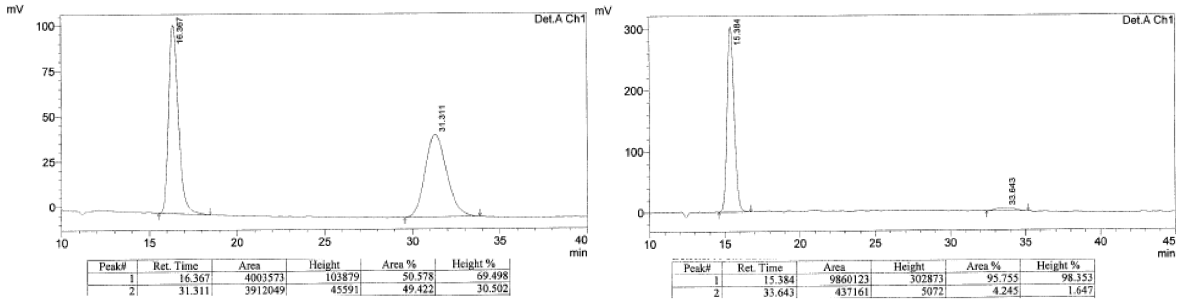
(*R*)-3-Allyl-1-benzyl-3-hydroxy-5-methylindolin-2-one (17, Figure 5a): The title compound is synthesized in the same manner as that described for **S17** except for the following changes: 1) Reaction time is two h. 2) The catalytic enantioselective allyl addition is quenched with 3 mL of a solution of saturated aqueous $NaIO_4$ (to remove excess pinacol) and allowed to stir for 14 h at 22 ºC. The aqueous layer is washed with ethyl acetate (4 x 4 mL) and the combined organic layers are dried over Na_2SO_4 and concentrated *in vacuo* to provide yellow oil. The product **17** is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in hexanes and eluted with 10 mL hexanes, 10 mL 6:1 hexanes:ethyl acetate, and 20 mL 4:1 hexanes:ethyl acetate), affording **17** (24.5 mg, 0.084 mmol, 84% yield) as an off-white solid. The analytical data are fully consistent with those reported previously.[16] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31–7.22 (6H, m), 6.99 (1H, d, J = 7.9 Hz), 6.57 (1H, d, J = 8.0 Hz), 5.69–5.58 (1H, m), 5.18–5.09 (2H, m), 4.99 and 4.70 (2H, ABq, J_{AB} = 15.7 Hz), 3.18 (1H, br s), 2.83–2.78 (1H, m), 2.73–2.68 (1H, m), 2.31 (3H, s); HRMS Calcd for $C_{19}H_{20}NO_2$ $[M + H]^+$: 294.14940; Found: 294.14905. $[\alpha]^{20}_D$ = +5.1 (c = 0.95, $CHCl_3$) for a 98.5:1.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OJ-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **15b**: 13 min (major) and 16 min (minor).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	13.4	49.524	1	13.3	98.654
2	16.2	50.476	2	16.1	1.346

(16) Itoh, J.; Han, S. B; Krische, M. J. *Angew. Chem. Int. Ed.* **2009**, *48*, 6313–6316.

(*R*)-1-Benzyl-3-hydroxy-3-(2-methylallyl)indolin-2-one (18, Figure 5a): The title compound is synthesized in the same manner as described for **S17** except for the following changes: 1) Reaction time is one h. 2) Allylboronate **1b** is employed as the nucleophile instead of allylboronate **1a**. 3) The catalytic enantioselective allyl addition process is quenched with 3 mL of a solution of saturated aqueous $NaIO_4$ (to remove excess pinacol) and allowed to stir for 14 h at 22 ºC. The aqueous layer is washed with ethyl acetate (4 x 4 mL), dried over Na_2SO_4, and concentrated *in vacuo* to provide yellow oil. The product is purified by silica gel chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in dichloromethane and eluted with 34 mL dichloromethane followed by 26 mL 9:1 dichloromethane:ethyl acetate), affording **18** (28.7 mg, 0.0976 mmol, 98% yield) as a white solid. M.p. = 52–54 ºC. IR (neat): 3399 (w, br), 3366 (w, br), 1692 (s), 1614 (m), 1466 (m), 1350 (m), 1196 (m), 991 (m), 756 (s), 727 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.41 (1H, d, J = 7.3 Hz), 7.31–7.22 (5H, m), 7.20 (1H, t, J = 7.7 Hz), 7.06 (1H, t, J = 7.5 Hz), 6.69 (1H, d, J = 7.7 Hz), 5.02 and 4.72 (2H, ABq, J_{AB} = 15.7 Hz), 4.79 (1H, s), 4.68 (1H, s), 2.93 (1H, s), 2.77 (2H, s), 1.50 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 178.0, 142.9, 139.1, 135.5, 129.9, 129.8, 128.9, 127.8, 127.4, 124.6, 123.1, 116.5, 109.6, 76.5, 46.3, 44.0, 24.1; HRMS Calcd for $C_{19}H_{20}NO_2$ $[M + H]^+$: 294.14940; Found: 294.14930. $[\alpha]^{20}_D$ = +22 (c = 1.3, $CHCl_3$) for a 96:4 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OJ-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **15e**: 15 min (major) and 34 min (minor).

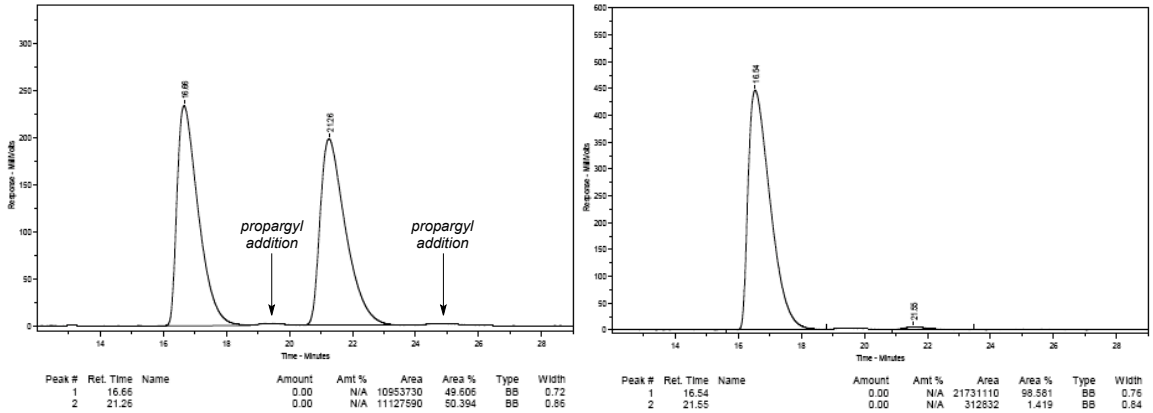


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.4	50.578	1	15.4	95.755
2	31.3	49.422	2	33.6	4.245

■ **Representative Procedure for *Small Scale* Catalytic Enantioselective Allene Group Additions to Isatins (Figure 5c)**: An oven-dried vial equipped with a stir bar is charged with aminophenol **2g** (6.1 mg, 20 μmol) and NaO*t*-Bu (1.9 mg, 20. μmol). The vial is sealed with a septum and Teflon tape and purged with N_2. Anhydrous toluene (2.0 mL) is added and the mixture is allowed to stir for 10 min under N_2 at 22 °C. A separate oven-dried vial equipped with a stir bar is charged with isatin **14c** (53.4 mg, 0.200 mmol). The vial is sealed with a septum and Teflon tape and purged with N_2. Toluene (600. μL) and MeOH (8.1 μL, 0.20 mmol) are then transferred by syringe to the vial containing isatin

14c. An appropriate portion of the stock solution of catalyst (100. μL) is transferred to the vial. Allenyl boron **19** (50.0 μL, 0.140 mmol) is added by syringe and the mixture was allowed to stir at 22 °C until the solution becomes colorless indicating complete consumption of the highly pigmented isatin. The mixture is diluted with AcOEt and passed through a short column of silica gel. The unpurified residue obtained as a pale yellow oil was purified by silica gel chromatography (a gradient from 100% CH_2Cl_2 to 1:1 Et_2O:CH_2Cl_2 to 100 % Et_2O) to yield 56.0 mg (0.182 mmol, 91% yield) of pure **20a** as a white crystalline solid in 98.5:1.5 er.

(*R*)-1-Benzyl-3-hydroxy-5-methoxy-3-(propa-1,2-dien-1-yl)indolin-2-one (**20a, Figure 5c**): white crystalline solid: M.p. = 117–119 °C. IR (neat): 3366 (m, br), 1697 (s), 1604 (w), 1490 (s), 1435 (m), 1346 (m), 1179 (m), 1017 (m), 853 (m), 730 (m), 697 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.33–7.24 (5H, m), 7.03 (1H, d, J = 2.4 Hz), 6.73 (1H, dd, J = 8.4, 2.8 Hz), 6.60 (1H, d, J = 8.4 Hz), 5.55 (1H, t, J = 6.4 Hz), 5.01 (2H, dd, J = 6.4, 1.2 Hz), 4.93 and 4.72 (2H, ABq, J_{AB} = 15.8 Hz), 3.76 (3H, s), 3.36 (1H, br s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 207.8, 176.6, 156.4, 135.5, 135.4, 130.9, 128.9, 127.8, 127.3, 114.7, 111.7, 110.3, 93.1, 80.2, 75.1, 55.9, 44.0; HRMS Calcd for $C_{19}H_{18}NO_3$ $[M + H]^+$: 308.12867; Found: 308.12935. $[\alpha]^{20}_D$ = –37.6 (c = 1.00, $CHCl_3$) for a 98.5:1.5 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **20a**: 17 min (major) and 21 min (minor), t_R of corresponding propargyl adduct: 19 min (major) and 25 min (minor).

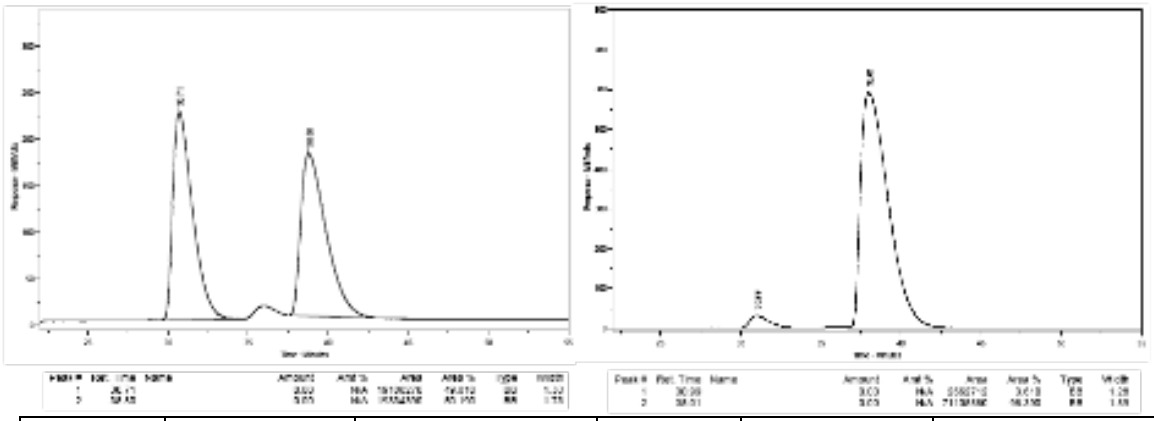


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.7 min	49.606	1	16.5 min	98.581
2	21.3 min	50.394	2	21.6 min	1.419

■ **Representative Procedure for *Gram Scale* Catalytic Enantioselective Allene Group Additions to Isatins (Figure 5c)**: An oven-dried vial equipped with a stir bar is charged with aminophenol **2g** (11.6 mg, 38. μmol) and NaO*t*-Bu (3.6 mg, 38 μmol). The vial is sealed with a septum and Teflon tape and purged with N_2. Anhydrous toluene (2.0 mL) is added and the mixture is allowed to stir for 10 min under N_2 at 22 °C. A separate flame-dried 50 mL round bottom flask equipped with a stir bar is charged with isatin **14d** (1.015

g, 3.800 mmol). The flask is sealed with a septum and Teflon tape and purged with N_2. Toluene (14.0 mL) and MeOH (307 μL, 7.60 mmol) are then transferred by syringe to the flask containing isatin **14d**. An appropriate portion of the stock solution of catalyst (1.00 mL) is transferred to the flask. Allenyl boron **19** (750. μL, 4.17 mmol) is added by syringe and the mixture is allowed to stir at 22 °C until the solution becomes colorless indicating complete consumption of the highly pigmented isatin (4.0 h). The reaction mixture is concentrated and the unpurified residue obtained as pale yellow oil is purified by silica gel chromatography (a gradient from 100% CH_2Cl_2 to 1:1 Et_2O:CH_2Cl_2 to 100 % Et_2O) to yield 1.056 g (3.43 mmol, 90% yield) of pure **20b** as a foamy white solid in 96:4 er.

(*R*)-3-Hydroxy-1-(4-methoxybenzyl)-3-(propa-1,2-dien-1-yl)indolin-2-one (20b, Figure 5c): clear oil. IR (neat): 3367 (m, br), 1701 (s), 1612 (m), 1512 (m), 1467 (m), 1350 (m), 1246 (m), 1175 (m), 1031 (m), 810 (m), 749 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.41–7.39 (1H, m), 7.23–7.19 (3H, m), 7.08–7.04 (1H, m), 6.85–6.81 (2H, m), 6.73 (1H, d, J = 7.6 Hz), 5.55 (1H, t, J = 6.4 Hz), 4.98 (2H, d, J = 6.8 Hz), 4.92 and 4.73 (2H, ABq, J_{AB} = 15.6 Hz), 3.76 (3H, s), 3.43 (1H, br s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 207.8, 176.6, 159.3, 142.3, 129.9, 129.6, 128.7, 127.5, 124.8, 123.3, 114.3, 109.8, 93.0, 80.3, 74.7, 55.4, 43.5; HRMS Calcd for $C_{19}H_{18}NO_2$ $[M + H]^+$: 292.13375; Found: 292.13468. $[\alpha]^{20}_D$ = –2.92 (c = 1.00, $CHCl_3$) for a 96:4 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 95:5 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **20b**: 31 min (minor) and 38 min (major), t_R of corresponding propargyl adduct: 36 min.

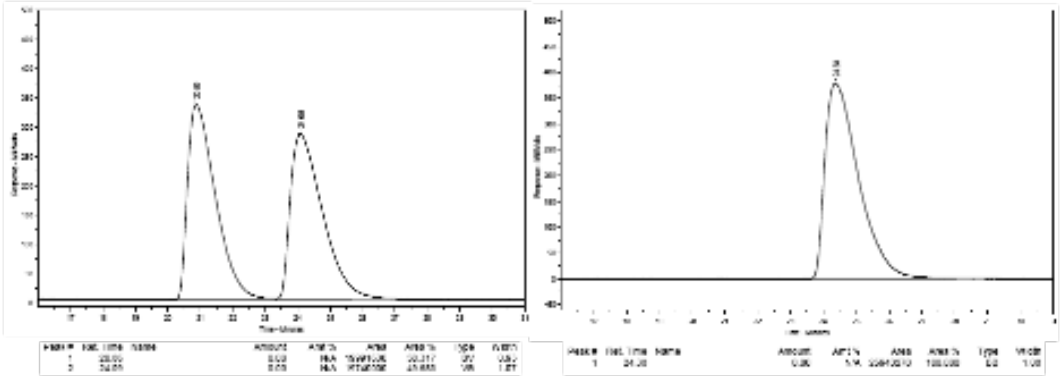


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	30.7 min	49.810	1	31.0 min	3.610
2	38.8 min	50.190	2	38.0 min	96.390

Procedure for One-Pot Aminophenol-Catalyzed Enantioselective Allene Group Addition/Desilylation of *N*-TBS-protected-Isatin 14a on Gram Scale (Figure 5c): On a bench-top, an oven-dried vial equipped with a stir bar is charged with aminophenol **2g** (6.1 mg, 20. μmol) and NaO*t*-Bu (3.1 mg, 32 μmol). The vial is sealed with a septum and Teflon tape and purged with N_2. Anhydrous toluene (2.0 mL) is added and the mixture is

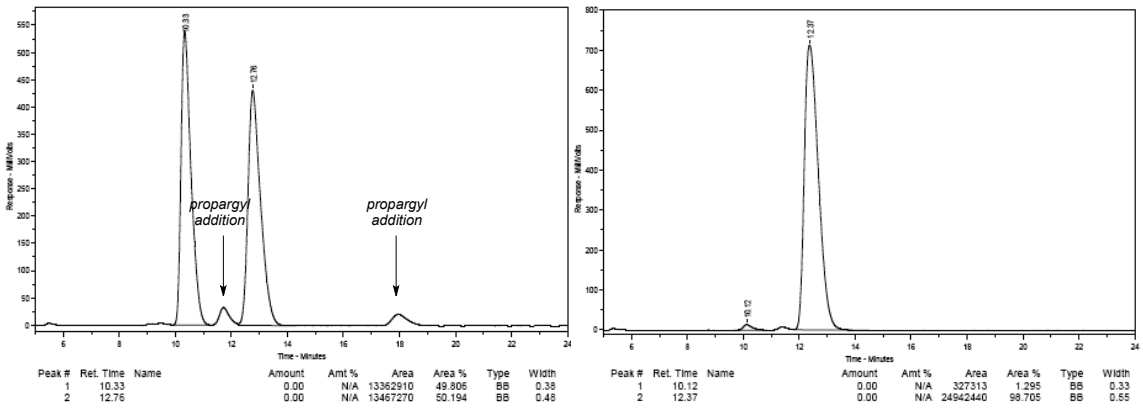
allowed to stir for 10 min under N_2 at 22 °C. A separate flame-dried 50 mL round bottom flask equipped with a stir bar is charged with isatin **14a** (1.045 g, 4.000 mmol). The flask is sealed with a septum and Teflon tape and purged with N_2. Toluene (9.0 mL) and MeOH (325 μL, 8.00 mmol) are then transferred by syringe to the flask containing *N*-TBS-protected isatin **14a**. An appropriate portion of the stock solution of catalyst (1.00 mL) is transferred to the flask. Allenylboron reagent **19** (750. μL, 4.17 mmol) is added by syringe and the mixture is allowed to stir at 22 °C until the solution becomes colorless indicating complete consumption of intensely orange **14a** (2.0 minutes). The mixture is concentrated and the unpurified residue is re-dissolved in MeOH (20.0 mL) and treated with an aqueous 1.0 M solution of HCl (5.0 mL). The solution is allowed to stir at 22 °C until TLC analysis indicated complete consumption of the silylamide (typically 2.0 h). The solution is diluted with EtOAc (20 mL) and H_2O (20 mL) and the organic layer is separated. The aqueous layer is further washed with EtOAc (3 x 20 mL), the organic layers are combined and dried over Na_2SO_4. The volatiles are removed yielding white solid which is recrystallized from EtOAc/hexanes (2 crops) to yield 675.8 mg of hydroxyindole **21** (3.61 mmol, 90% yield) as a white crystalline solid in >99:1 er.

(*R*)-3-Hydroxy-3-(propa-1,2-dien-1-yl)indolin-2-one (**21, Figure 5c**): white crystalline solid, M.p. = 189–190 °C. IR (neat): 3316 (s, br), 1955 (w), 1691 (s), 1619 (m), 1469 (m), 1377 (m), 1355 (m), 1181 (m), 1103 (m), 1068 (m), 928 (m), 852 (m), 782 (m), 731 (m), 642 (s), 559 (m), 497 (m) cm^{-1}; ^1H NMR (400 MHz, CD_3OD): δ 7.33–7.31 (1H, m), 7.26–7.22 (1H, m), 7.05–7.01 (1H, m), 6.88–6.86 (1H, m), 5.51 (1H, t, J = 6.4 Hz), 4.90–4.75 (2H, m); ^{13}C NMR (100 MHz, CD_3OD): δ 209.5, 180.6, 142.5, 132.3, 130.8, 126.3, 123.7, 111.3, 93.5, 78.9, 76.3; HRMS Calcd for $C_{11}H_{10}NO_2$ $[M + H]^+$: 188.07115; Found: 188.07196. $[\alpha]^{20}_D$ = –35.2 (c = 1.00, MeOH) for a >99:1 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 90:10 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **21**: 21 min (minor) and 24 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	20.9 min	50.317	1	24.4 min	100.000
2	24.1 min	49.683			

If the TBS-protected hydroxyindole is desired instead, the unpurified residue, obtained as a pale yellow oil after the allene addition protocol, can be purified by silica gel chromatography directly (a gradient from 100% CH_2Cl_2 to 1:4 Et_2O:CH_2Cl_2 to 100 % Et_2O) to obtain a 92% to >98% yield of **(*R*)-1-(*tert*-Butyldimethylsilyl)-3-hydroxy-3-(propa-1,2-dien-1-yl)indolin-2-one** (**S19, not shown in manuscript, see Chart S1**): pale yellow oil. IR (neat): 3398 (m, br), 2929 (w), 2858 (w), 1955 (w), 1703 (s), 1613 (m), 1464 (m), 1256 (m), 1172 (m), 1101 (m), 939 (m), 829 (s), 746 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.38–7.36 (1H, m), 7.23–7.19 (1H, ddd, J = 7.6, 7.6, 1.6 Hz), 7.07–7.00 (2H, m), 5.44 (1H, t, J = 6.4 Hz), 4.96 (2H, d, J = 6.4 Hz), 3.13 (1H, br s), 1.00 (9H, s), 0.54 (3H, s), 0.52 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 207.6, 183.9, 145.6, 131.5, 129.6, 125.1, 122.7, 113.2, 93.7, 79.9, 74.9, 26.6, 19.8, –3.1, –3.2; HRMS Calcd for $C_{17}H_{24}NO_2Si$ $[M + H]^+$: 302.15763; Found: 302.15757. $[\alpha]^{20}_D$ = +25.9 (c = 1.00, $CHCl_3$) for a 98:2 er sample. The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 96:4 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of 10 min (minor) and 13 min (major), t_R of corresponding propargyl adduct: 12 and 18 min.

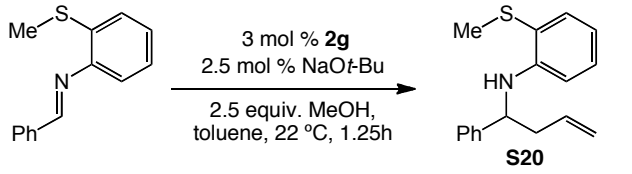


Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	10.4 min	49.806	1	10.1 min	1.295
2	12.8 min	50.194	2	12.4 min	98.705

Procedure for Two-step Conversion of Allenic Alcohol 21 to α–Hydroxy Alcohol 22 (Figure 5c): A vial equipped with a stir bar is charged with allenyl carbinol **21** (37.4 mg, 0.200 mmol) to which is added enough MeOH to ensure complete dissolution of the solid (~2 mL). The solution is allowed to cool to –78 °C, before a flow of O_3 (10 mL/min) is bubbled through the solution until TLC analysis indicated complete consumption of the allene (typically between 1 and 5 minutes). Upon complete oxidative cleavage, the solution is purged with O_2 before the addition of $NaBH_4$ (76.0 mg, 2.00 mmol) at –78 °C. The solution is allowed to warm to 22 °C and stir for 20 min during the reduction. A drop of acetyl chloride is added and the mixture is concentrated *in vacuo*. The residue is redissolved in MeOH and a drop of acetyl chloride is added and reconcentrated. This procedure is repeated twice more to ensure protonation to the diol with concomitant

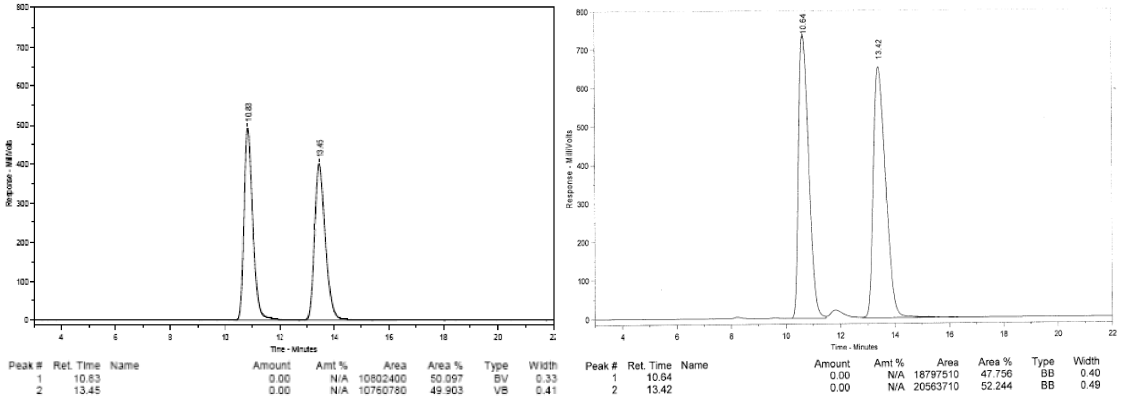
removal of $B(OMe)_3$. The maroon solid is purified by silica gel chromatography (gradient from 1:1 EtOAc:Et_2O to 100% EtOAc to 4:1 EtOAc:MeOH) to afford 31.8 mg of diol **22** (0.177 mmol, 89% yield) as a pale yellow solid.

(*S*)-3-Hydroxy-3-(hydroxymethyl)indolin-2-one (**22, Figure 5c**): sticky pale yellow solid. IR (neat): 3248 (s, br), 1701 (s), 1620 (m), 1470 (m), 1334 (w), 1184 (m), 1118 (m), 1052 (s), 810 (m), 749 (m), 670 (m), 489 (m) cm^{-1}; ^1H NMR (400 MHz, CD_3OD): δ 7.39 (1H, ddd, J = 7.6, 1.2, 0.8 Hz), 7.25 (1H, ddd, J = 7.6, 7.6, 1.2 Hz), 7.25 (1H, ddd, J = 7.6, 7.6, 1.2 Hz), 6.90–6.87 (1H, m), 3.83 and 3.80 (2H, ABq, J_{AB} = 10.8 Hz), 3.35 (1H, s); ^{13}C NMR (100 MHz, CD_3OD): δ 181.5, 143.7, 131.7, 130.7, 125.8, 123.7, 111.2, 78.1, 66.9; HRMS Calcd for $C_9H_{10}NO_3$ $[M + H]^+$: 180.06607; Found: 180.06614. $[\alpha]^{20}_D$ = +43.9 (*c* = 1.00, MeOH) for a >99:1 er sample.



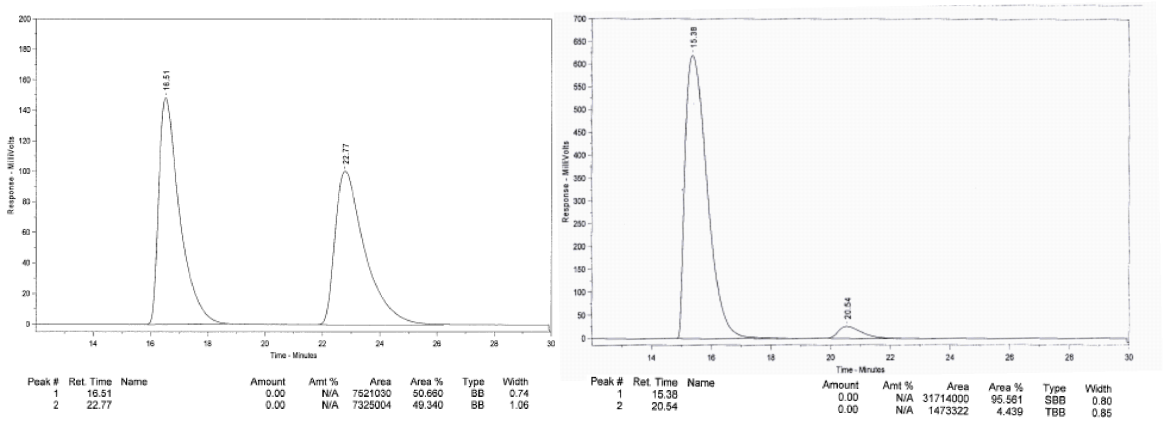
90% conv., 78% yield,
52:48 e.r.

■ **Aminophenol-Catalyzed Enantioselective Allyl Additions to *o*-Thiomethylaniline-derived Aldimines: 2-(methylthio)-*N*-(1-phenylbut-3-en-1-yl)aniline (S20)** is synthesized analogously to **4b** and purified by column chromatography (10 mm diameter column slurry packed with 2.5 g of silica gel in 95:5 hexanes:triethylamine and eluted with 50 mL hexanes and 20 mL 50:1 hexanes:diethyl ether) to afford 21 mg (0.078 mmol, 78% yield) of **S20** as a yellow oil. The analytical data are fully consistent with those reported previously.[13] The enantiomeric purity of this compound was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 98:2 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **S20**: 11 min (minor) and 13 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	10.8 min	50.097	1	10.6 min	47.756
2	13.5 min	49.903	2	13.4 min	52.244

■ **Representative Example of Utilization of DBU as the Base Instead of NaO*t*-Bu for the Enantioselective Allyl Addition to Aldimine *3a***: The reaction is performed following the representative procedure for *small scale* catalytic enantioselective allyl additions to aryl-, heteroaryl-, alkenyl-, and alkynyl *N*-diphenylphosphinoyl imines except for the following changes: 1) 2.5 mol % DBU is used (instead of 2.5 mol % NaO*t*-Bu) 2) Reaction time is 75 min. The conversion to desired product is 83% (judged by 400 MHz ^{1}H NMR spectra of unpurified reaction mixture vs. an internal standard of 9-methylanthracene) which is lower than the >98% conversion obtained when using the same amount of NaO*t*-Bu. The enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 92:8 hexanes:*i*-PrOH, 0.5 mL/min, 220 nm): t_R of **4a**: 15 min (major) and 21 min (minor).



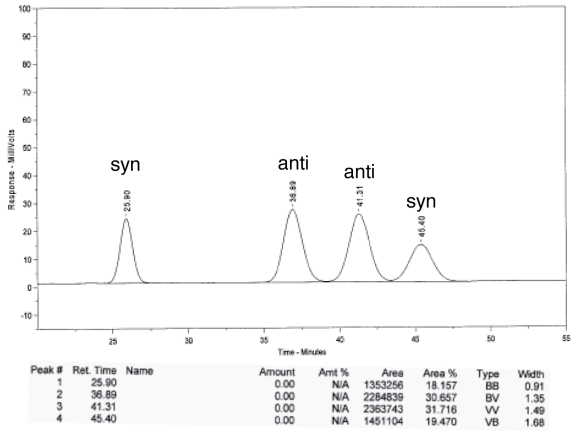
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	16.5 min	50.660	1	15.4 min	95.561
2	22.8 min	49.340	2	20.5 min	4.439

■■ PROOF of ABSOLUTE STEREOCHEMISTRY of PRODUCTS

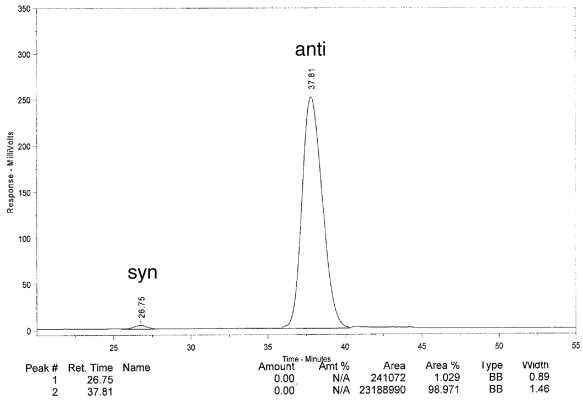
Absolute configuration of homoallylamide S7: Please see Part D of the Supplementary Information for X-ray crystallographic data.

Absolute configuration of homoallylamide S12: Please see Part D of the Supplementary Information for X-ray crystallographic data. For the catalytic enantioselective allyl additions to aldimines, it should be noted that the absolute stereochemical identities of the major product enantiomers are inferred from the obtained X-ray crystal structures of homoallylic amides **S7** and **S12**.

Absolute configuration of homoallylamide 10: Please see Part D of the Supplementary Information for X-ray crystallographic data. The absolute stereochemistry of the obtained crystal was further verified by HPLC analysis in comparison with authentic racemic material



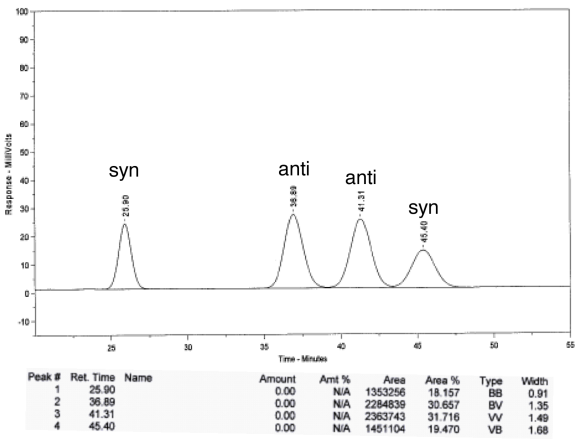
Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.90		0.00	N/A	1353256	18.157	BB	0.91
2	36.89		0.00	N/A	2284839	30.657	BV	1.35
3	41.31		0.00	N/A	2363743	31.716	VV	1.49
4	45.40		0.00	N/A	1451104	19.470	VB	1.68



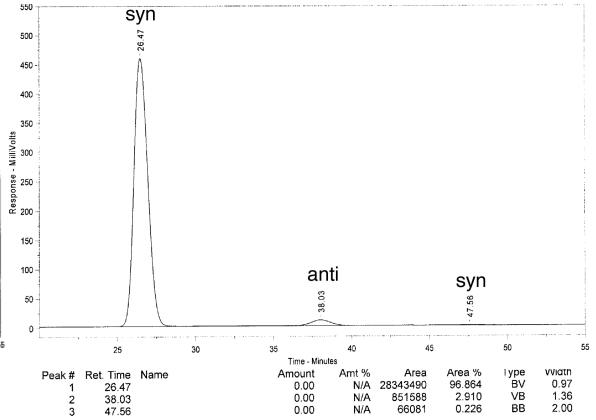
Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	26.75		0.00	N/A	241072	1.029	BB	0.89
2	37.81		0.00	N/A	23188990	98.971	BB	1.46

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	25.9	18.157	1 (syn)	26.8	1.029
2 (anti)	36.9	30.657	2 (anti)	37.8	98.971
3 (anti)	41.3	31.716	3 (anti)	-	-
4 (syn)	45.4	19.470	4 (syn)	-	-

Absolute configuration of homoallylamide 11: Please see Part D of the Supplementary Information for X-ray crystallographic data. The absolute stereochemistry of the obtained crystal was further verified by HPLC analysis in comparison with authentic racemic material.

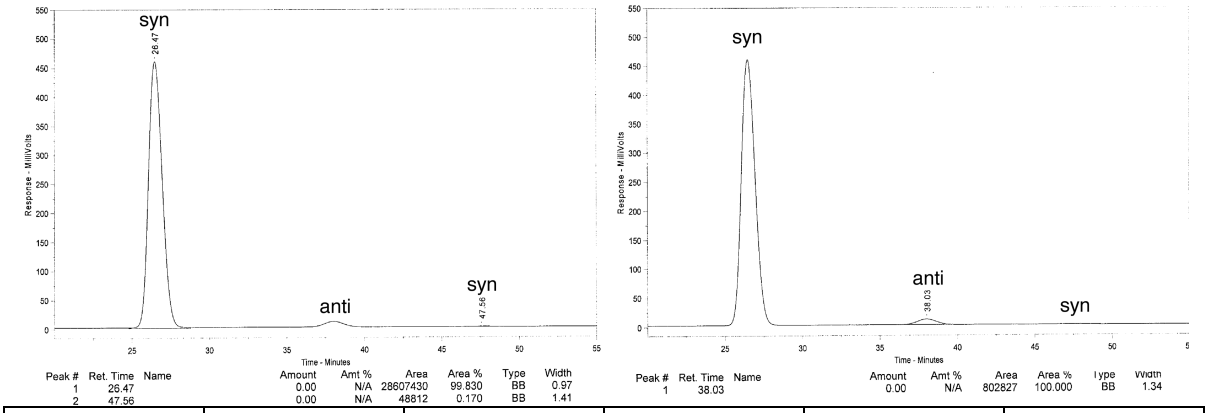


Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	25.90		0.00	N/A	1353256	18.157	BB	0.91
2	36.89		0.00	N/A	2284839	30.657	BV	1.35
3	41.31		0.00	N/A	2363743	31.716	VV	1.49
4	45.40		0.00	N/A	1451104	19.470	VB	1.68



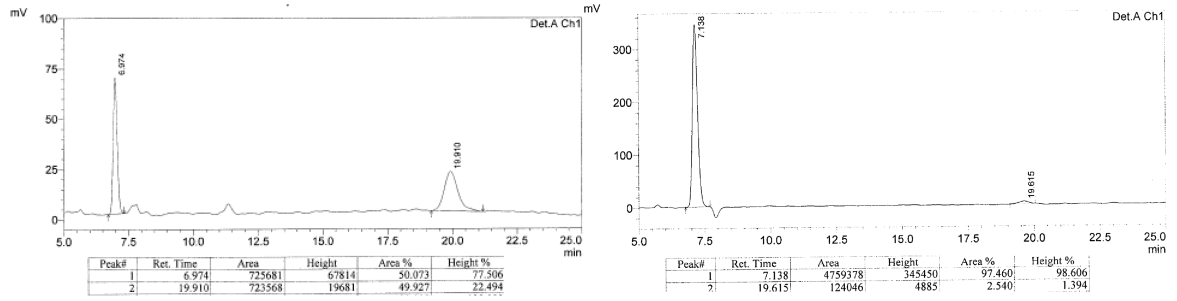
Peak #	Ret. Time	Name	Amount	Amt %	Area	Area %	Type	Width
1	26.47		0.00	N/A	28343490	96.864	BV	0.97
2	38.03		0.00	N/A	851588	2.910	VB	1.36
3	47.56		0.00	N/A	66081	0.226	BB	2.00

Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	25.9	18.157	1 (syn)	26.5	96.864
2 (anti)	36.9	30.657	2 (anti)	38.0	2.910
3 (anti)	41.3	31.716	3 (anti)	-	-
4 (syn)	45.4	19.470	4 (syn)	47.6	0.226



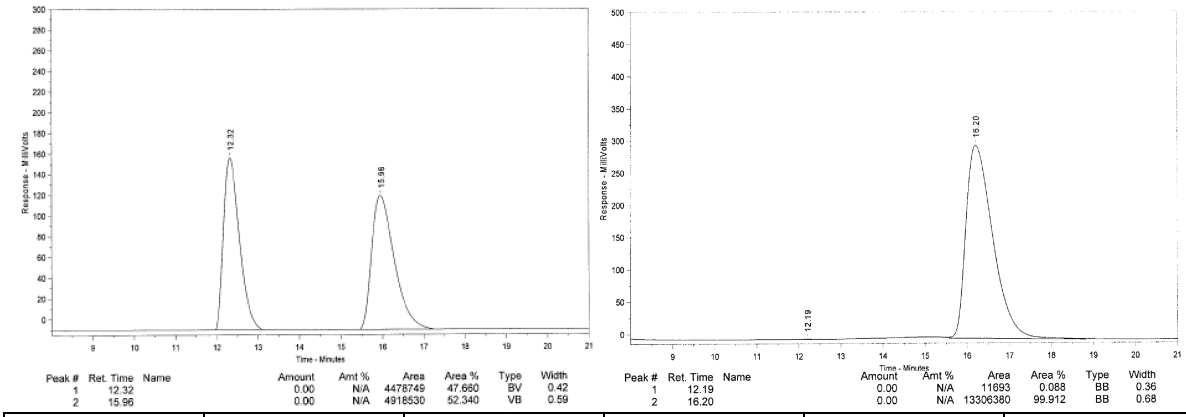
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1 (syn)	26.5	99.830	1 (anti)	38.0	100.000
2 (syn)	41.7	0.170	2 (anti)	-	-

Absolute configuration of homoallylamide 13: Please see Part D of the Supplementary Information for X-ray crystallographic data. The absolute stereochemistry the obtained crystal was further verified by HPLC analysis in comparison with authentic racemic material.



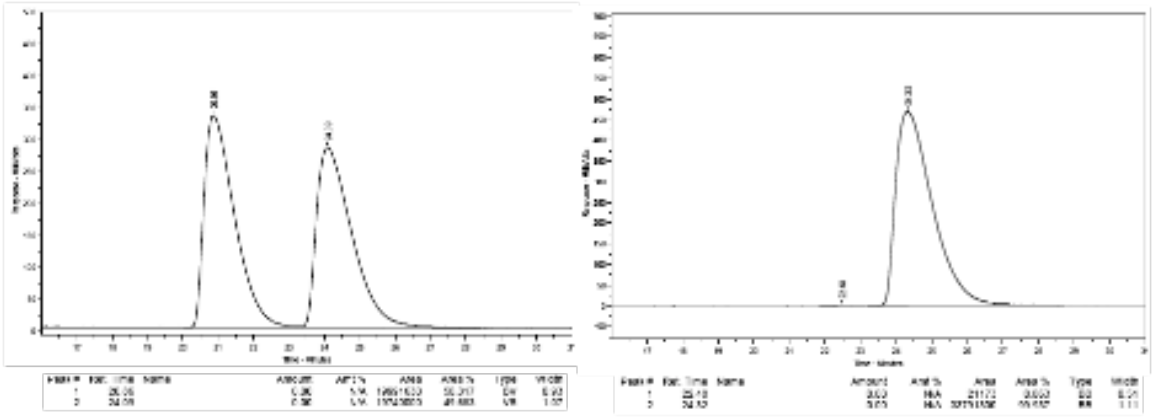
Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	7.0	50.073	1	7.1	97.460
2	19.9	49.927	2	19.6	2.540

Absolute configuration of homoallylic alcohol 15a: For the aminophenol catalyzed enantioselective allyl additions to isatin, please note that the absolute stereochemistries of the major product enantiomers are inferred from the obtained X-ray crystal structure (see Part D of the Supplementary Information) of homoallylic alcohol **15a.** The absolute stereochemistry of the obtained crystal was also verified by HPLC analysis in comparison with authentic racemic material (Chiracel OD-H, 90:10 hexanes:*i*-PrOH, 0.8 mL/min, 220 nm): t_R of **15a**: 12 min (minor) and 16 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	12.3	47.660	1	12.2	0.088
2	16.0	52.340	2	16.2	99.912

Absolute configuration of allenyl alcohol 21: For the catalytic enantioselective allene additions to isatin, please note that the absolute stereochemistries of the major product enantiomers are inferred from the obtained X-ray crystal structure (see Part D of the Supplementary Information) of allenyl alcohol **21.** The absolute stereochemistry of the obtained crystal was further verified by HPLC analysis in comparison with authentic racemic material (Chiracel OD, 90:10 hexanes:*i*-PrOH, 0.6 mL/min, 220 nm): t_R of **21**: 21 min (minor) and 24 min (major).



Peak #	Ret. Time	Area %	Peak #	Ret. Time	Area %
1	20.9 min	50.317	1	22.5 min	0.063
2	24.1 min	49.683	2	24.3 min	99.937

Simple Organic Molecules as Catalysts for Enantioselective Synthesis of Amines and Alcohols

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SUPPLEMENTARY INFORMATION; PART B

Table of Contents ***Page***

■ Investigation of the Level of Brønsted Acidity of the Complex Derived from Allylboron Reagent (1a) and MeOH

General Information Specific to the Following Study (for further information; see Part A of the Supplementary Information). All vials, stir bars, and NMR tubes were oven-dried (135 ºC) overnight prior to use. The ^{1}H NMR spectra were recorded on a Varian Unity INOVA 400 (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (d_8-toluene: δ 7.09 ppm).

Preparation of samples for NMR spectroscopy: In a nitrogen-filled glovebox, aminophenol **2g** (7.7 mg, 25 μmol) is weighed into a one-dram vial and dissolved in 700. μL of d_8-toluene. The solution is transferred to an NMR tube and sealed with a cap and Teflon tape; it is then used to obtain **Spectrum 1**.

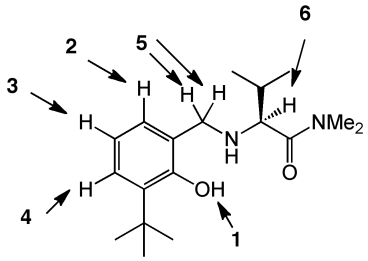
A separate one-dram vial equipped with a stir bar is charged with **2g** (30.8 mg, 0.101 mmol) and 2.8 mL of a stock solution of NaO*t*-Bu in d_8-toluene (9.6 mg, 0.10 mmol NaO*t*-Bu/2.8 mL d_8-toluene) to afford a translucent solution. A 700. μL aliquot of this solution (containing NaO*t*-Bu [2.4 mg, 25 μmol] and aminophenol [7.7 mg, 25 μmol]) is added to an NMR tube and sealed with a cap and Teflon tape; it is then used to obtain **Spectrum 2**.

A second 700. μL aliquot is transferred to a one-dram vial containing allylboronic acid pinacol ester (10. μL, 53 μmol) **1a** and this mixture is then used to obtain **Spectrum 3**.

Methanol (10. μL, 250 μmol) is added to the remaining 1.4 mL of NaO*t*-Bu and **2g** mixture and a 700. μL aliquot (containing NaO*t*-Bu [2.4 mg, 25 μmol], aminophenol **2g** [7.7 mg, 25 μmol], and methanol [5.0 μL, 130 μmol]) of the resultant solution is added to an NMR tube and sealed with a cap and Teflon tape; it is then used to obtain **Spectrum 4**.

Allylboronic acid pinacol ester **1a** (10. μL, 53 μmol) is added to the remaining solution (containing NaO*t*-Bu [2.4 mg, 25 μmol], aminophenol **2g** [7.7 mg, 25 μmol], and methanol [5.0 μL, 130 μmol]), which results in formation of a white precipitate, causing the toluene solution to become cloudy. The latter solution is added to an NMR tube and sealed with a cap and Teflon tape; it is then used to obtain **Spectrum 5**.

Spectrum 1 (^{1}H NMR, 400 MHz, d_8-toluene): Aminophenol **2g**



1: 11.11 ppm (1H, br s)

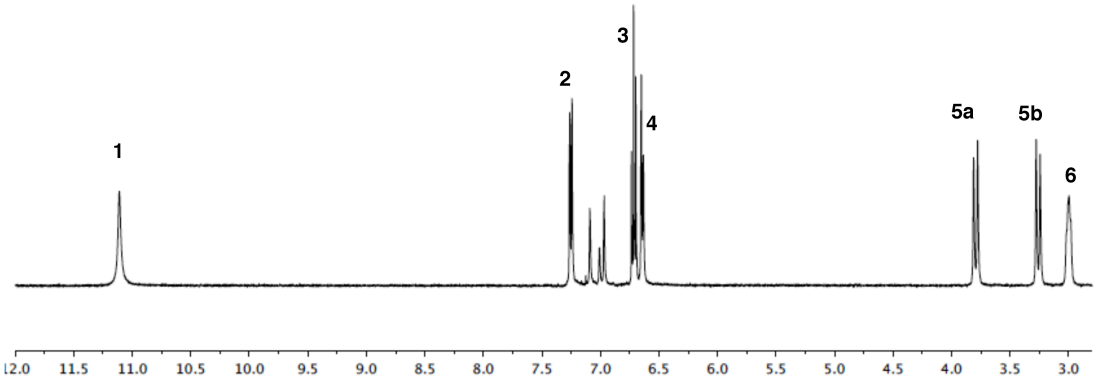
2: 7.27–7.24 ppm (1H, m)

3: 6.72 ppm (1H, t, J = 7.6 Hz)

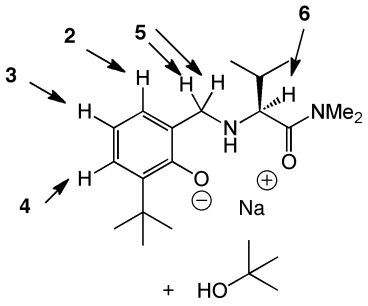
4: 6.65–6.63 ppm (1H, m)

5a, 5b: 3.79, 3.26 ppm (2H, ABq, J_{AB} = 13.5 Hz)

6: 3.02–2.98 ppm (1H, br m)



Spectrum 2 (^{1}H NMR, 400 MHz, d_8-toluene): Aminophenol **2g** (25 μmol, 1 equiv.) and NaO*t*-Bu (25 μmol, 1 equiv.)



2: 7.35–7.33 ppm (1H, m)

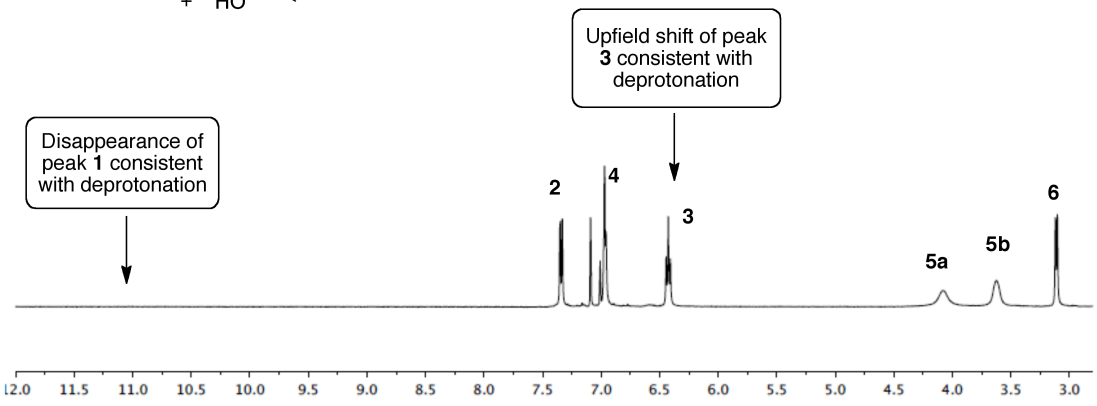
3: 6.43 ppm (1H, t, J = 7.3 Hz)

4: 6.98–6.96 ppm (1H, m)

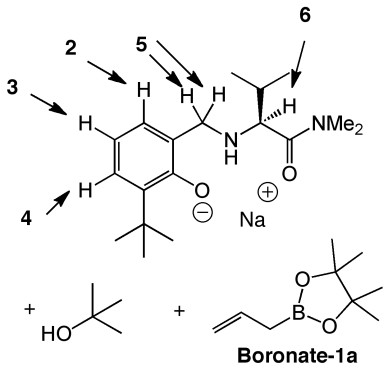
5a: 4.09 ppm (1H, br s)

5b: 3.63 ppm (1H, br s)

6: 3.11 ppm (1H, d, J = 6.4 Hz)



Spectrum 3 (^{1}H NMR, 400 MHz, d_8-toluene): Aminophenol **2g** (25 μmol, 1 equiv.), NaO*t*-Bu (25 μmol, 1 equiv.), and Allylboronate **1a** (53 μmol, 2 equiv.)



2: 7.32 ppm (1H, d, J = 7.4 Hz)

3: 6.42–6.38 ppm (1H, br m)

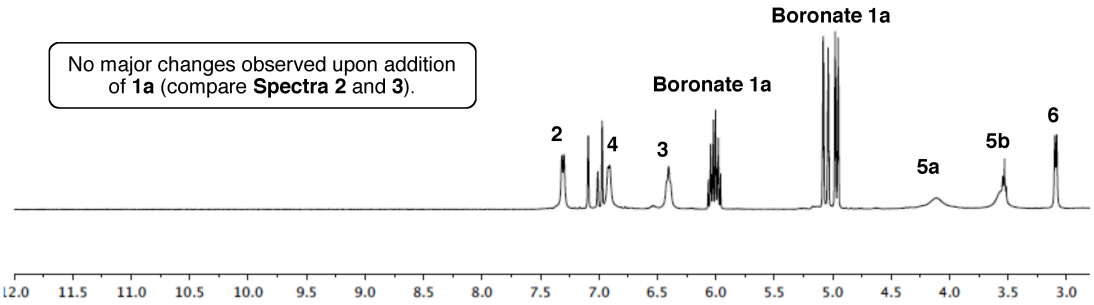
4: 6.92 ppm (1H, br s)

5a: 4.12 ppm (1H, br s)

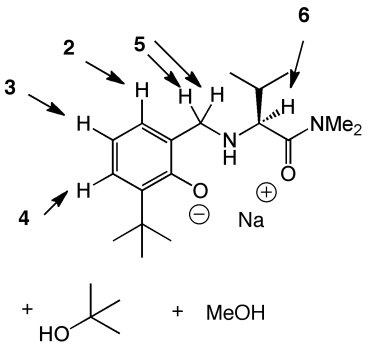
5b: 3.80–3.66 ppm (1H, br m [overlaps with new unknown peak].

6: 3.09 ppm (1H, d, J = 6.3 Hz)

No major changes observed upon addition of **1a** (compare **Spectra 2** and **3**).



Spectrum 4 (^{1}H NMR, 400 MHz, d_8-toluene): Aminophenol **2g** (25 μmol, 1 equiv.), NaO*t*-Bu (25 μmol, 1 equiv.), and MeOH (130 μmol, 5 equiv.)



2: 7.40–7.35 ppm (1H, m)

3: 6.52 ppm (1H, t, J = 7.4 Hz)

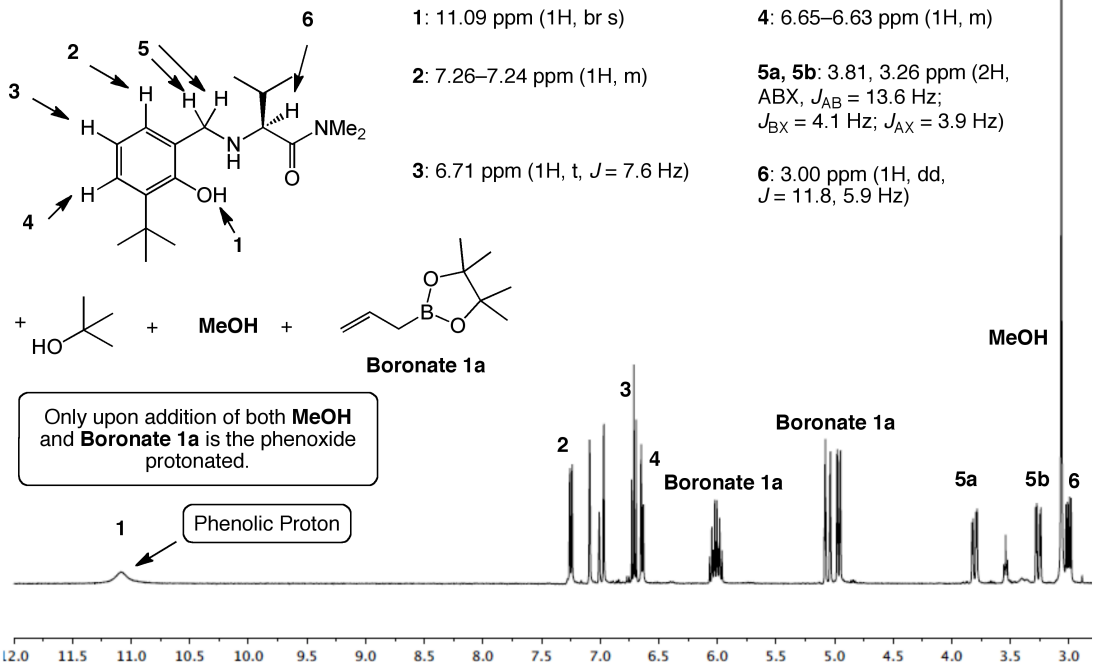
4: 6.97–6.95 ppm (1H, m)

5a, 5b: 3.80, 3.66 ppm (2H, ABq, J_{AB} = 10.9 Hz)

6: 3.14 ppm (1H, d, J = 6.5 Hz)

Absence of peak **1** and chemical shifts of peaks **2-4** indicate addition of MeOH does not protonate the phenoxide of **2g**.

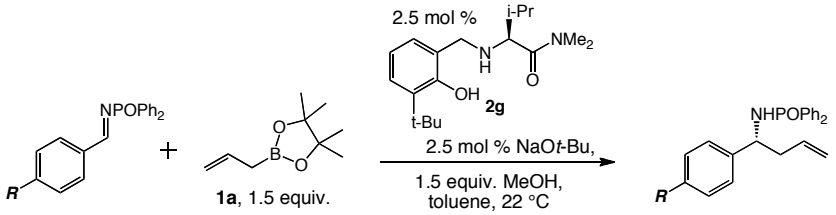
Spectrum 5 (^{1}H NMR, 400 MHz, d_8-toluene): Aminophenol **2g** (25 μmol, 1 equiv.), NaO*t*-Bu (25 μmol, 1 equiv.), Allylboronate **1a** (53 μmol, 2 equiv.), and MeOH (130 μmol, 5 equiv.)



■ Generation of a Hammett Plot for the Aminophenol Catalyzed Enantioselective Allyl Addition to a Series of Aryl-Substituted Aldimines

The electronic effect of the aryl substituent on the reaction rate of the aminophenol catalyzed enantioselective allyl addition to aryl-substituted aldimines was determined by React-IR measurements of conversion of imine [%] as a function of time [min] (Scheme S1).

Scheme S1: Reaction Conditions for the Enantioselective Allylation of Imines Applied in React-IR Measurements to Generate the Hammett Plot



	Hammett σ_p-constant	
R = Br	***R*** = Br	0.23
R = H	***R*** = H	0.00
R = Me	***R*** = Me	-0.17
R = OMe	***R*** = OMe	-0.27
R = N(*n*-Bu)$_2$	***R*** = N(*n*-Pr)$_2$	-0.93*

Increasing rate of reaction

*The σ_p-constant for -N(*n*-Pr)$_2$ has been used for -N(*n*-Bu)$_2$.

General Procedure (for further information; see Part A of the Supplementary Information): The preparation of stock solutions of reagents (allylboronate **1a**, MeOH, aminophenol **2g**, and NaO*t*-Bu) and weighing of imines were performed in a nitrogen-filled glovebox. All vials and stir bars were oven-dried (135 ºC) overnight prior to use. Rubber septa and caps were oven-dried (60 ºC) overnight prior to use. An 8 mL vial equipped with a stir bar is charged with the desired aldimine (0.200 mmol) and the vial is sealed with a cap. To prepare the stock solution of allylboronate **1a**, a 4 mL vial is charged with **1a** (0.450 mL, 2.40 mmol) and toluene (3.55 mL) and sealed with a cap containing a teflon septum. To prepare the stock solution of MeOH, a 4 mL vial is charged with MeOH (0.120 mL, 3.00 mmol) and toluene (3.88 mL) and sealed with a cap containing a teflon septum. To prepare the stock solution of aminophenol **2g**, 4 mL vial is charged with aminophenol **2g** (15.3 mg, 0.0499 mmol) and toluene (4.00 mL) and sealed with a cap containing a Teflon septum. To prepare the stock solution of NaO*t*-Bu, a 4 mL vial is charged with NaO*t*-Bu (19.2 mg, 0.200 mmol) and toluene (4.00 mL). The NaO*t*-Bu solution is diluted further by charging a 4 mL vial with toluene (3.00 mL) and 1.00 mL of the original stock solution. The vial was sealed with a cap containing a teflon septum. The prepared solutions and vials containing the imines were taken out of the glovebox and stored in a desiccator for the duration of React-IR measurements.

React-IR measurements: Measurements were performed on a ReactIR iC10 instrument equipped with a 6.3 mm AgX DiComp Fiber probe. Spectra were recorded from 2000 cm^{-1} to 650 cm^{-1} at standard resolution (8 cm^{-1}) in 15 s intervals. The vial containing imine is equipped with a 14/20 rubber septum with a 4 mm diameter hole and attached to the probe, which had been dried with a heat gun (T_{max} = 200 °C). The rubber septum is further sealed with electrical tape. Toluene (0.3 mL) is added with a syringe, followed by the addition of the stock solutions of allylboronate **1a** (0.50 mL) and MeOH (0.40 mL). After 3 min, the reaction is started by the simultaneous addition of the solutions of aminophenol **2g** (0.4 mL) and NaO*t*-Bu (0.4 mL).

Data processing: The decrease in concentration of imine was monitored as a function of time [min] (Figures 1a and 1b). The following IR absorption frequencies characteristic of the imines in this study were used: 834–822 cm^{-1} for R = Br, 836–824 cm^{-1} for R = H, 842–830 cm^{-1} for R = Me, 835–823 cm^{-1} for R = OMe, and 1592–1580 cm^{-1} for R = N(*n*-Bu)$_2$. The intensities were calibrated as following: the difference between the intensities at the start of the reaction and the intensities at the end of the reaction (i.e. when no further change was observed in the concentration of imine) was set to the conversion [%] determined by 400 MHz ^{1}H NMR (100% except for 95% in the case of R = N(*n*-Bu)$_2$).

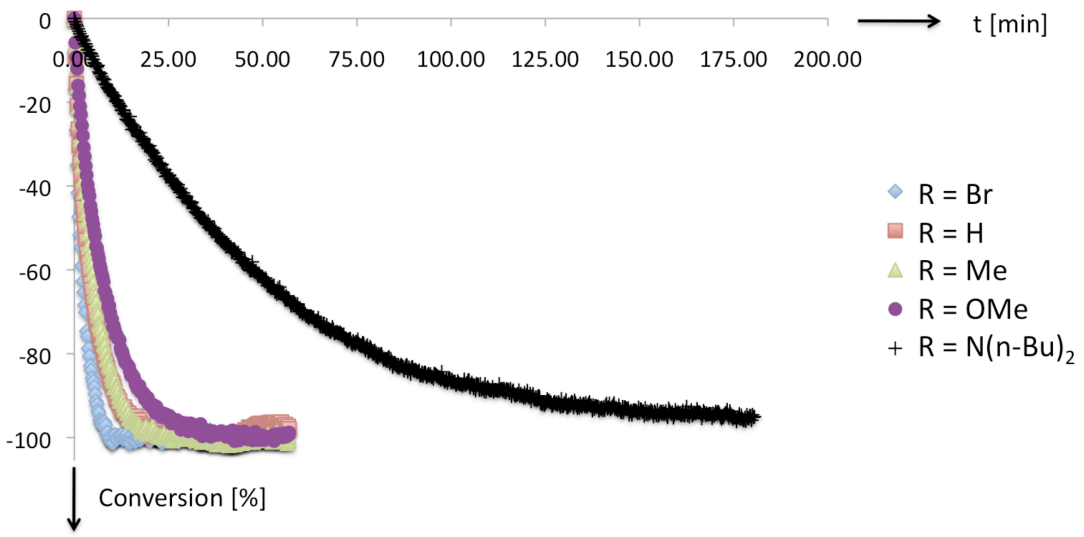


Figure S1a: Conversion of Imine [%] vs Time [min]

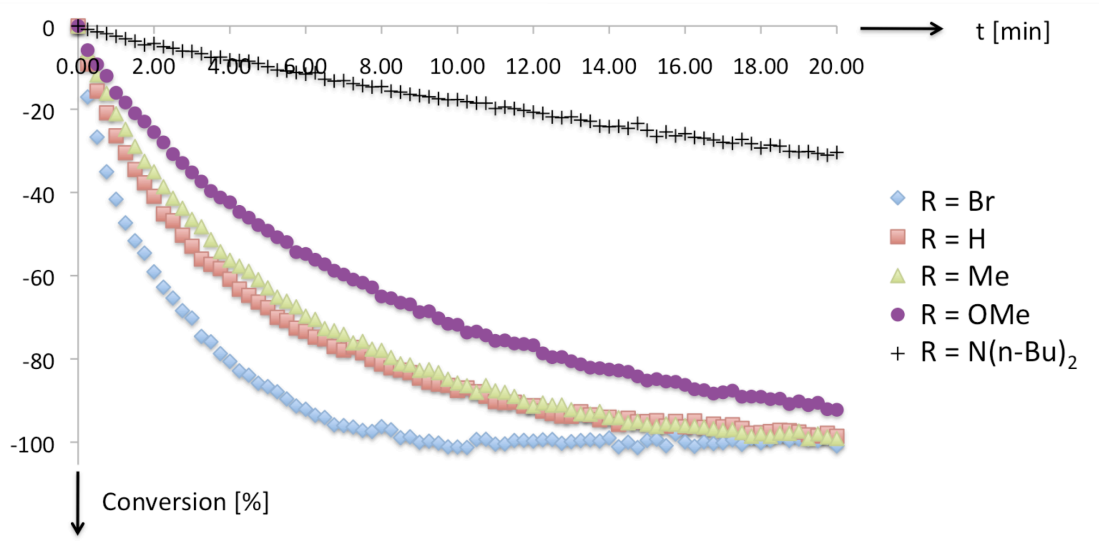
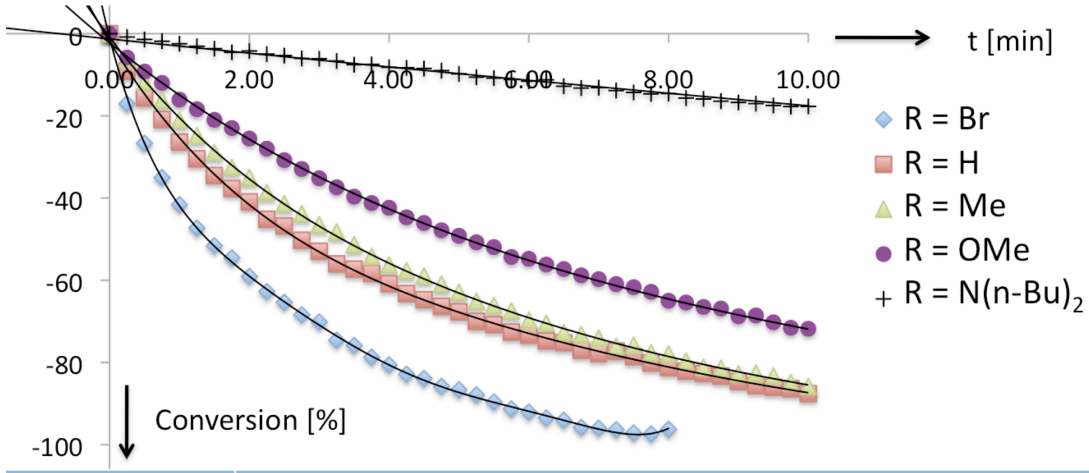


Figure S1b: Conversion of Imine [%] vs Time [min] (Zoomed in Region).

The curves in Figures S1a and S1b were fitted with a 6th-order polynomial function through the use of Microsoft Excel (Figure S1c). In order to obtain a reasonable fit, the curves were truncated after a maximum time (8 min for R = Br, 20 min for R = H, 20 min for R = Me, 40 min for R = OMe, and 180 min for R = N(*n*-Bu)$_2$). The relative rates k_X (for time → 0 min) can be read directly from the equations of the polynomials (values in red), which are used for the generation of the Hammett plot in Graph S1 (plot of $\log(k_X/k_H)$ vs σ_p-constant). Linear regression results in a ρ-value of 1.3 (slope), indicating a faster reaction with more electron deficient aryl substituted aldimines.

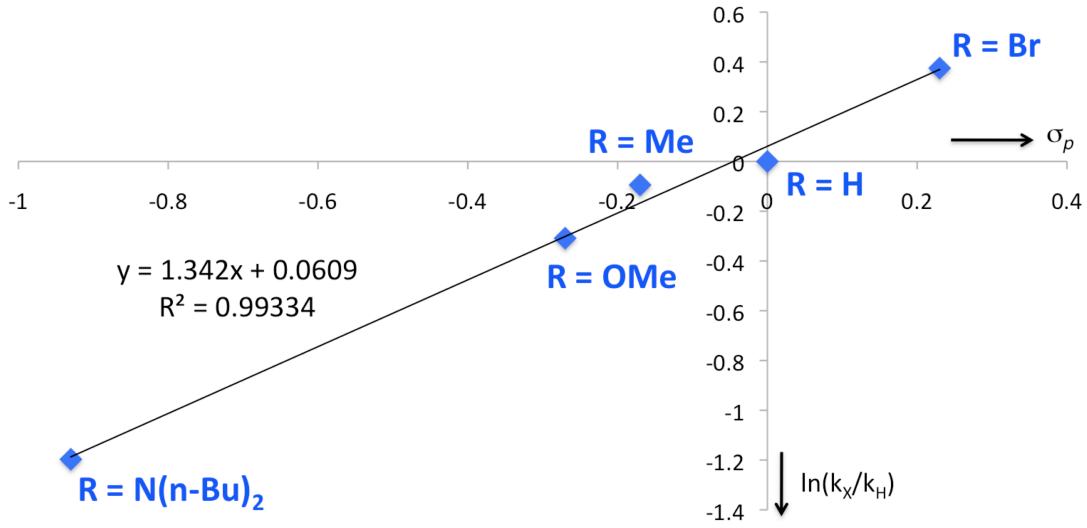


R = Br	y = 0.0088x^6 - 0.23x^5 + 2.3827x^4 - 12.444x^3 + 35.757x^2 - **66.425**x - 0.9584
R = H	y = 2E-05x^6 - 0.0013x^5 + 0.0396x^4 - 0.5957x^3 + 5.1132x^2 -**28.015**x -1.8831
R = Me	y = 9E-06x^6 - 0.0007x^5 + 0.0204x^4 - 0.3258x^3 + 3.216x^2 - **22.544**x - 0.8435
R = OMe	y = 3E-07x^6 - 4E-05x^5 + 0.0022x^4 - 0.0642x^3 + 1.1379x^2 - **13.766**x - 2.2367
R = N(n-Bu)$_2$	y = 6E-12x^6 - 3E-09x^5 + 6E-07x^4 - 8E-05x^3 + 0.0138x^2 - **1.7579**x - 1.2783

Figure S1c: Plot of Conversion of Imine [%] vs Time [min] Including 6th-Order Polynomial Fits

Please Note: The relative rates at t = 0 can be read directly from the polynomial functions (values in **red**).

Graph S1: Hammett Plot [log(k_X/k_H) vs σ_p-constant] Indicating the Electronic Substituent Dependence for the Enantioselective Allylation Under the Conditions Shown in Scheme S1.



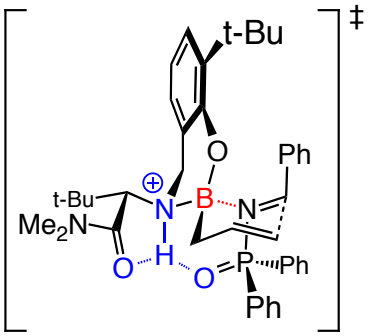
■ **DFT Calculations**: All geometry and frequency calculations of the transition states shown in Scheme S2 were carried out employing the hybrid functional B3LYP[1] and the split-valence 6-31G** basis set. The calculations were carried out in toluene, which was simulated by the polarizable dielectric continuum solvation model PCM.[2] Frequency calculations were carried out on the fully optimized geometries. All computed frequencies are real except for the transition state structures, which have one imaginary frequency. Free energies were computed at 298.15 K and 1.0 atm. with harmonic, unscaled frequencies. All quantum chemical calculations were carried out with the Gaussian 09 computer program.[3]

(1) (a) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648-5652; Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*. **1988**, *37*, 785–789. (b) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys*. **1980**, *58*, 1200–1211. (c) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, 98, 11623–11627.

(2) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev*. **2005,** *105*, 2999−3093.

(3) Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

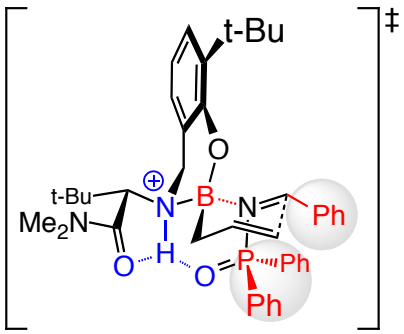
Scheme S2a: Calculated Transition State Complex Which Leads to the *R* (Major) Enantiomer



R-TS (Labeled I in Figure 2d)

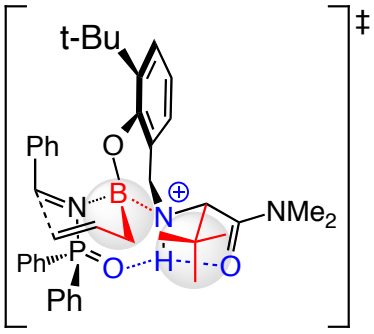
0.0 kcal/mol

Scheme S2b: Calculated Transition State Complexes Which Lead to the *S* (Minor) Enantiomer and their Energies Relative to *R*-TS



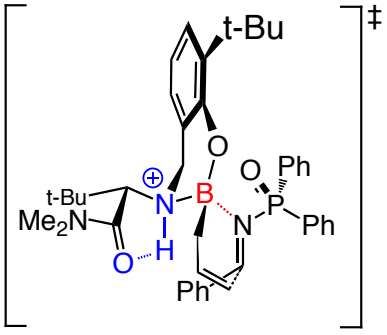
***S*-TS1**

+2.4 kcal/mol



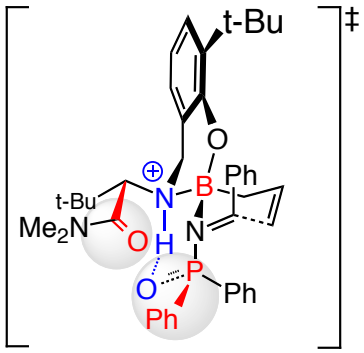
***S*-TS2** (labeled III in Figure 2d)

+5.9 kcal/mol



***S*-TS3**

+7.5 kcal/mol

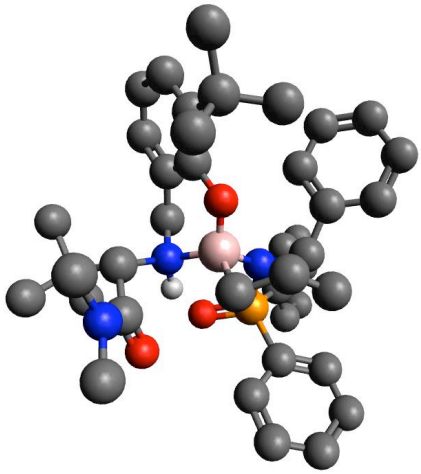


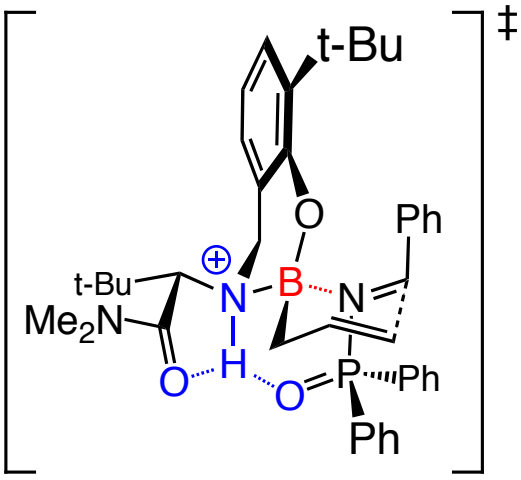
***S*-TS4**

+10.8 kcal/mol

Please Note: (a) The energy of complex ***R*-TS** is used as a zero point reference. (b) The aminophenol derived from L-*tert*-leucine **2h** (Table 1) was modeled instead of **2g** due to fewer possible conformers present in **2h**.

Transition State Energy for Complex *R*-TS (Scheme S2a; Labeled I in Figure 2d of the Manuscript)





Cartesian coordinates (Angstroms):

H	-1.997	5.662	-2.432
H	2.845	3.498	-3.033
C	-1.530	4.983	-1.725
H	-2.465	3.254	-2.572
H	5.208	3.571	-2.438
H	-0.497	6.545	-0.652
H	-1.613	1.457	-3.522
C	-1.786	3.619	-1.808
C	-0.689	5.479	-0.724
C	2.573	3.276	-1.995
H	2.401	4.227	-1.484
H	4.283	1.440	-3.143
C	4.982	3.358	-1.389
H	1.634	2.723	-1.994
H	4.852	4.319	-0.882
H	0.707	0.874	-3.068
C	-1.391	0.596	-2.902
H	-5.918	-1.106	-2.868
C	3.713	2.484	-1.315
C	4.005	1.190	-2.114
C	-0.079	0.199	-2.737
H	5.856	2.856	-0.960
C	-1.189	2.716	-0.908
H	-2.184	-0.140	-2.815
C	-0.116	4.598	0.192
H	-5.159	-3.355	-3.599
H	3.135	0.532	-2.147
C	-5.062	-1.574	-2.391
H	4.839	0.639	-1.667
C	-4.636	-2.840	-2.799
C	-1.614	1.287	-0.936
C	-0.361	3.228	0.101

H	0.524	4.972	0.985
H	-4.759	0.058	-1.029
H	-2.692	1.219	-1.082
C	-4.398	-0.911	-1.359
C	3.350	2.117	0.142
C	0.298	-0.915	-1.906
H	-2.085	2.015	1.781
H	4.935	3.270	1.022
O	1.420	0.816	-0.501
H	1.301	-1.278	-2.131
C	-3.548	-3.449	-2.171
H	-0.423	-1.730	-1.893
H	-3.599	3.312	3.221
C	4.114	2.594	1.219
H	0.076	2.562	0.832
H	-3.226	-4.439	-2.477
C	2.276	1.256	0.479
N	-1.101	0.313	-0.104
C	-3.293	-1.514	-0.733
B	0.412	-0.198	-0.346
C	-3.060	1.611	2.023
C	-2.876	-2.795	-1.139
C	-3.918	2.348	2.839
P	-2.343	-0.731	0.604
H	-2.035	-3.269	-0.642
C	3.872	2.228	2.544
C	-3.464	0.367	1.515
C	2.067	0.822	1.796
H	2.858	-1.505	0.475
H	4.490	2.633	3.339
N	0.828	-1.158	0.907
C	-5.179	1.847	3.164
H	0.004	0.282	2.178
C	2.862	1.319	2.831
C	0.982	-0.187	2.060
H	-5.845	2.422	3.800
H	-0.019	-1.726	1.131
O	-1.674	-1.763	1.479
C	1.999	-2.122	0.728
H	4.078	-2.097	-0.846
O	0.453	-3.555	-0.377
C	-4.733	-0.137	1.856
C	1.592	-3.076	-0.411
H	2.128	-3.964	-3.385
H	4.232	-1.923	2.414
C	-5.584	0.603	2.674
H	2.686	0.991	3.852
N	2.486	-3.397	-1.388
H	1.101	-4.757	-2.160
H	2.911	-1.394	3.453
H	1.172	-0.740	2.975
C	2.104	-4.401	-2.382
C	3.849	-2.897	-1.544
H	-5.056	-1.105	1.487
C	3.340	-2.260	2.952
H	4.042	-4.031	0.993
H	3.980	-2.510	-2.560
C	2.366	-3.004	2.009
H	-6.562	0.207	2.930
H	4.571	-3.708	-1.392
C	3.130	-4.273	1.547
H	3.671	-2.949	3.736

H 2.808 -5.240 -2.352
H 2.511 -4.935 0.939
H 0.546 -2.673 3.237
C 1.109 -3.481 2.765
H 3.433 -4.834 2.435
H 0.429 -4.015 2.098
H 1.413 -4.166 3.563

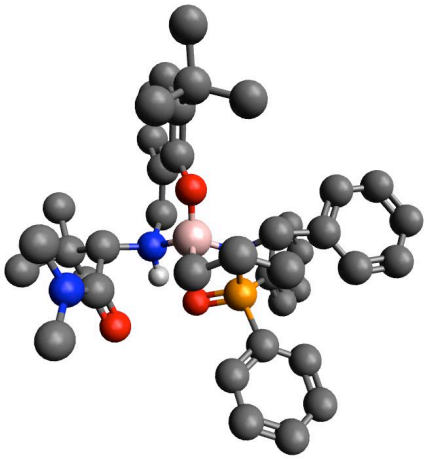
SCF Done: E(RB3LYP) = -2349.81121449 A.U. after 1 cycles

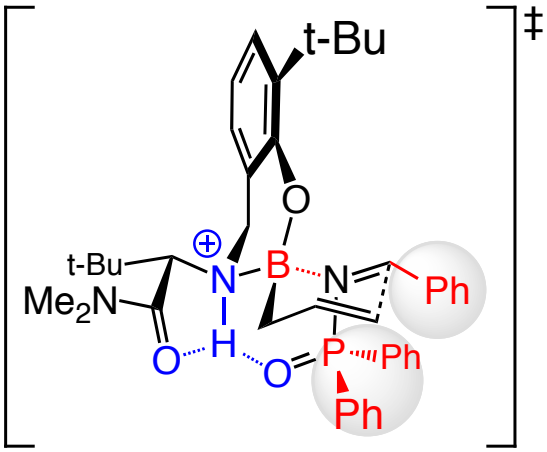
	1	2	3
	A	A	A
Frequencies --	-309.7171	15.8257	27.8170
Red. masses --	8.1218	5.5670	3.9897

Zero-point correction=	0.861950 (Hartree/Particle)
Thermal correction to Energy=	0.909242
Thermal correction to Enthalpy=	0.910186
Thermal correction to Gibbs Free Energy=	0.782800
Sum of electronic and zero-point Energies=	-2348.949264
Sum of electronic and thermal Energies=	-2348.901973
Sum of electronic and thermal Enthalpies=	-2348.901028
Sum of electronic and thermal Free Energies=	-2349.028414

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000450	YES
RMS Force	0.000000	0.000300	YES

Transition State Energy for Complex *S*-TS1 (not shown in manuscript; see Scheme S2b)





Cartesian coordinates (Angstroms):

H 3.751 2.814 -3.386
H 1.600 4.186 -3.258
H 3.742 5.158 -2.730
C 3.627 2.506 -2.342
H 4.626 2.381 -1.911
C 1.458 3.814 -2.238

H	3.123	1.538	-2.327
C	3.618	4.902	-1.674
H	0.874	2.895	-2.297
H	0.874	4.561	-1.689
H	4.618	4.824	-1.236
C	2.830	3.581	-1.563
H	3.096	5.737	-1.195
H	2.587	-4.468	-1.957
O	1.682	-3.320	-0.246
H	3.273	-3.522	-3.306
C	3.431	-3.861	-2.276
H	4.349	-4.459	-2.244
O	1.449	1.133	-0.699
C	2.650	3.137	-0.094
H	3.638	4.856	0.738
H	1.839	-1.100	-2.200
C	2.645	-2.557	-0.383
C	2.006	1.929	0.274
H	-1.628	0.879	-3.621
B	0.744	-0.105	-0.450
C	-1.216	0.149	-2.933
N	3.558	-2.710	-1.382
C	3.149	3.916	0.961
H	3.444	-0.616	0.298
C	0.790	-0.944	-1.951
C	2.813	-1.429	0.653
H	1.687	-2.174	3.275
C	0.155	-0.027	-2.868
H	3.597	-0.206	3.217
N	1.422	-0.830	0.837
H	0.273	-1.895	-1.838
C	1.949	1.506	1.609
H	4.733	-0.973	-1.039
C	4.706	-1.856	-1.672
C	3.055	3.531	2.299
H	4.661	-1.527	-2.715
C	2.456	-2.812	2.833
H	0.784	0.715	-3.355
C	4.233	-0.973	2.778
H	1.952	-3.587	2.253
C	3.480	-2.051	1.964
H	3.456	4.172	3.077
H	4.978	-0.464	2.158
C	1.301	0.191	1.946
C	2.470	2.314	2.622
H	5.639	-2.412	-1.531
H	2.983	-3.295	3.662
H	0.231	0.304	2.121
H	4.767	-1.457	3.602
H	1.712	-0.222	2.862
H	2.412	1.985	3.656
C	4.563	-3.080	1.545
H	5.336	-2.637	0.910
H	4.140	-3.947	1.034
H	5.060	-3.444	2.448
H	-1.867	-0.684	-2.686
H	0.768	-1.597	1.104
H	-3.176	2.810	3.452
H	-5.140	1.636	4.419
C	-3.423	1.804	3.128
C	-4.525	1.143	3.672
C	-2.633	1.174	2.168

H -1.775 1.696 1.758
C -4.831 -0.156 3.263
H -5.679 -0.679 3.693
H -1.790 3.507 -0.374
C -2.945 -0.124 1.736
C -4.043 -0.792 2.306
H -0.558 1.797 -1.282
H -3.908 4.769 -0.355
C -2.705 3.024 -0.706
C -1.313 1.041 -1.102
O -0.852 -1.903 1.512
H -4.278 -1.811 2.017
C -3.901 3.739 -0.697
P -1.806 -1.069 0.689
C -2.671 1.683 -1.129
N -0.830 0.110 -0.202
C -5.078 3.138 -1.145
H -0.955 -3.432 -0.608
C -2.716 -2.183 -0.429
C -3.852 1.102 -1.607
H -6.008 3.696 -1.151
C -1.990 -3.291 -0.906
C -5.046 1.823 -1.609
H -3.843 0.099 -2.011
H -4.663 -1.241 -0.357
C -4.077 -2.064 -0.749
C -2.610 -4.233 -1.726
H -2.042 -5.083 -2.090
H -5.950 1.357 -1.989
C -4.694 -3.018 -1.559
C -3.960 -4.096 -2.056
H -5.750 -2.923 -1.793
H -4.443 -4.836 -2.687

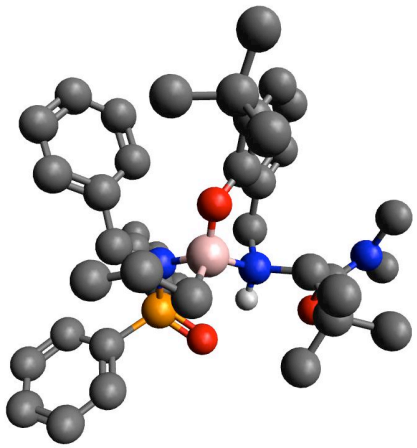
SCF Done: E(RB3LYP) = -2349.80692498 A.U. after 1 cycles

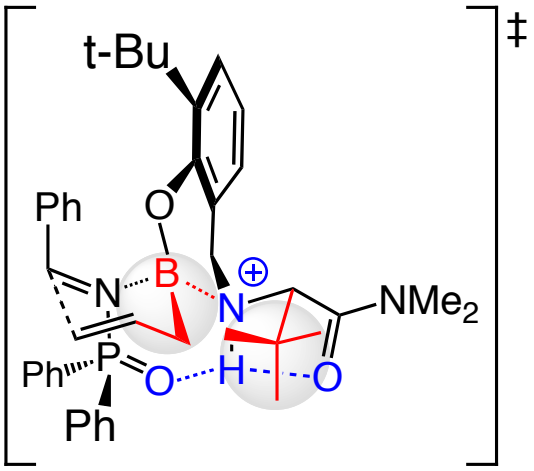
	1	2	3
	A	A	A
Frequencies --	-344.5655	12.7728	18.2767
Red. masses --	9.0648	5.1910	4.1843

Zero-point correction= 0.862291 (Hartree/Particle)
Thermal correction to Energy= 0.909628
Thermal correction to Enthalpy= 0.910572
Thermal correction to Gibbs Free Energy= 0.782402
Sum of electronic and zero-point Energies= -2348.944634
Sum of electronic and thermal Energies= -2348.897297
Sum of electronic and thermal Enthalpies= -2348.896353
Sum of electronic and thermal Free Energies= -2349.024523

Item	Value	Threshold	Converged?
Maximum Force	0.000001	0.000450	YES
RMS Force	0.000000	0.000300	YES

Transition State Energy for Complex (*S*)-TS2 (Scheme S2b; Labeled III in Figure 2d of the Manuscript)





Cartesian coordinates (Angstroms):

H	-0.181	3.850	2.912
H	-3.556	3.322	-2.949
C	0.467	3.883	2.042
H	0.240	1.790	1.642
H	-4.343	5.027	-1.425
H	0.893	5.988	2.223
H	2.342	2.756	-2.636
C	0.693	2.714	1.313
C	1.070	5.079	1.658
C	-3.425	2.604	-2.133
H	-4.351	2.024	-2.048
H	-1.941	4.884	-1.814
C	-4.278	4.343	-0.574
H	-2.618	1.923	-2.406
H	-5.244	3.835	-0.485
H	-0.031	2.235	-2.882
C	2.005	1.735	-2.495
H	3.305	0.613	4.518
C	-3.119	3.353	-0.814
C	-1.829	4.189	-0.974
C	0.680	1.422	-2.758
H	-4.123	4.951	0.323
C	1.527	2.721	0.186
H	2.761	0.974	-2.660
C	1.920	5.096	0.548
H	3.407	-1.655	5.523
H	-0.957	3.562	-1.159
C	3.125	-0.263	3.903
H	-1.631	4.779	-0.074
C	3.180	-1.540	4.468
C	1.920	1.442	-0.488
C	2.154	3.928	-0.172
H	2.409	6.017	0.249
H	2.775	0.891	2.132
H	3.004	1.335	-0.489
C	2.833	-0.109	2.548
C	-2.979	2.336	0.343

C	0.161	0.095	-2.581
H	4.917	0.061	0.693
H	-4.553	3.194	1.527
O	-1.128	1.179	-0.692
H	-0.764	-0.070	-3.127
C	2.938	-2.666	3.679
H	0.886	-0.692	-2.785
H	7.024	0.246	-0.574
C	-3.823	2.397	1.463
H	2.841	3.960	-1.011
H	2.971	-3.658	4.119
C	-2.034	1.281	0.337
N	1.252	0.249	-0.277
C	2.598	-1.240	1.749
B	-0.233	0.078	-0.895
C	4.968	-0.328	-0.318
C	2.648	-2.521	2.323
C	6.164	-0.234	-1.030
P	2.265	-1.174	-0.035
H	2.444	-3.391	1.708
C	-3.778	1.469	2.503
C	3.851	-0.950	-0.900
C	-2.010	0.311	1.353
H	-2.997	-1.148	-0.495
H	-4.455	1.566	3.346
N	-0.910	-1.264	-0.227
C	6.257	-0.768	-2.316
H	-1.379	-1.695	1.823
C	-2.885	0.407	2.436
C	-1.049	-0.843	1.233
H	7.192	-0.699	-2.865
H	-0.193	-2.019	-0.260
O	1.538	-2.398	-0.532
C	-2.246	-1.920	-0.643
H	-4.649	-1.587	0.296
O	-1.433	-3.843	0.502
C	3.959	-1.508	-2.187
C	-2.404	-3.096	0.352
H	-4.024	-4.150	2.877
H	-4.040	-1.215	-2.801
C	5.158	-1.411	-2.891
H	-2.859	-0.351	3.216
N	-3.579	-3.276	1.015
H	-2.764	-4.975	1.917
H	-2.500	-0.394	-2.892
H	-0.051	-0.588	1.588
C	-3.718	-4.456	1.871
C	-4.794	-2.474	0.905
H	3.116	-2.041	-2.614
C	-2.978	-1.364	-3.022
H	-4.409	-3.312	-1.719
H	-5.111	-2.152	1.902
C	-2.397	-2.474	-2.116
H	5.238	-1.847	-3.881
H	-5.602	-3.070	0.466
C	-3.446	-3.617	-2.139
H	-2.897	-1.648	-4.076
H	-4.483	-5.128	1.465
H	-3.097	-4.510	-1.614
H	-0.275	-2.366	-2.746
C	-1.088	-3.083	-2.653
H	-3.624	-3.897	-3.182

H -0.743 -3.884 -1.994
H -1.270 -3.509 -3.644

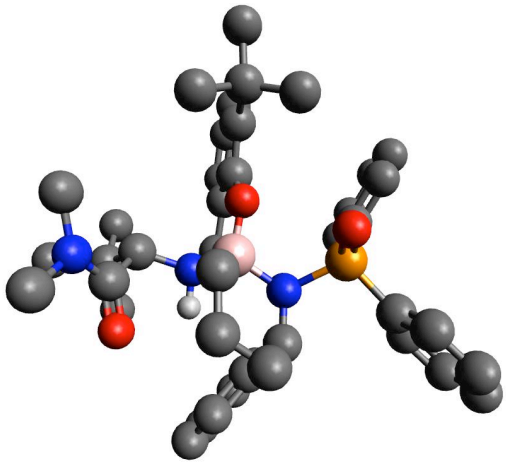
SCF Done: E(RB3LYP) = -2349.80034463 A.U. after 1 cycles

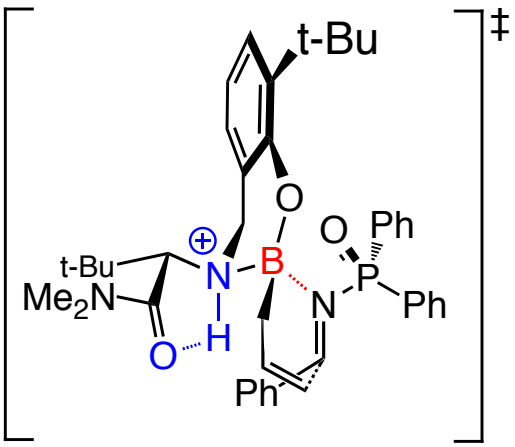
	1	2	3
	A	A	A
Frequencies --	-335.3640	16.4052	22.4182
Red. masses --	8.2371	5.2097	4.3949

Zero-point correction= 0.861454 (Hartree/Particle)
Thermal correction to Energy= 0.908946
Thermal correction to Enthalpy= 0.909890
Thermal correction to Gibbs Free Energy= 0.781405
Sum of electronic and zero-point Energies= -2348.938890
Sum of electronic and thermal Energies= -2348.891398
Sum of electronic and thermal Enthalpies= -2348.890454
Sum of electronic and thermal Free Energies= -2349.018940

Item	Value	Threshold	Converged?
Maximum Force	0.000000	0.000450	YES
RMS Force	0.000000	0.000300	YES

Transition State Energy for Complex (*S*)-TS3 (not shown in manuscript; see Scheme S2b)





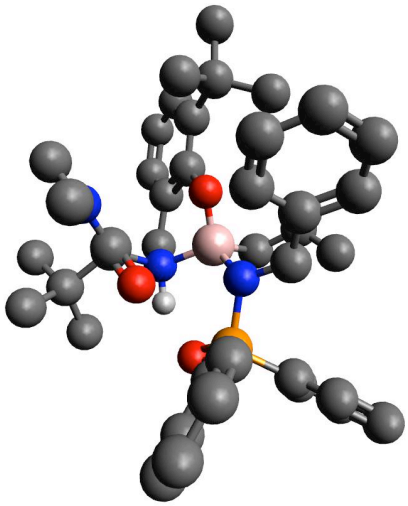
Cartesian coordinates (Angstroms):

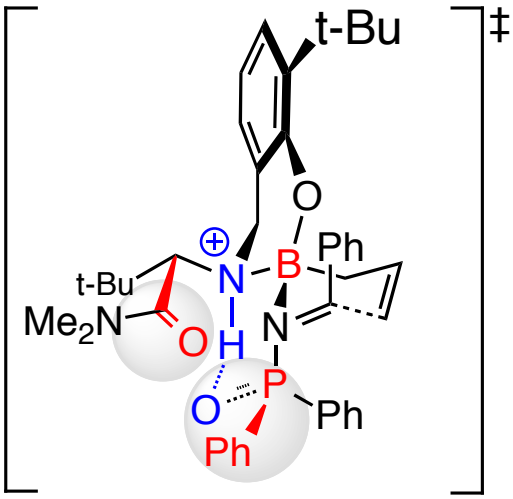
C -0.273 -3.861 2.824
C -0.769 -2.924 1.919
C 0.422 -4.980 2.362
C -0.573 -3.082 0.532
C 0.608 -5.154 0.991
C 0.110 -4.219 0.083
C 4.390 -1.903 -3.060
O 2.822 -2.546 -0.908
N 3.992 -0.944 -2.028
C 3.245 -1.383 -0.983
C 5.356 -1.119 0.771
C 4.166 0.318 2.380
C 4.497 0.410 -2.243
C 3.958 -0.849 1.388

C	2.946	-0.462	0.210
C	3.532	-2.133	2.129
B	0.358	-0.146	-0.643
N	1.453	-0.646	0.514
C	0.985	0.068	1.766
O	0.409	1.279	-0.682
C	1.056	1.562	1.598
C	0.807	2.111	0.332
C	1.369	2.396	2.673
C	-0.523	3.952	-1.935
C	0.982	3.494	0.076
C	0.897	4.102	-1.343
C	1.457	3.767	2.474
C	1.924	3.404	-2.267
C	1.288	4.289	1.190
C	1.239	5.607	-1.339
C	-2.803	2.146	2.914
C	-3.265	3.407	2.533
C	-2.513	1.186	1.945
C	-3.439	3.708	1.181
C	-2.678	1.485	0.585
C	-3.149	2.752	0.208
O	-2.312	0.865	-2.119
P	-2.483	0.276	-0.751
C	-3.964	-0.797	-0.691
C	-4.577	-1.076	-1.923
C	-4.554	-1.265	0.496
C	-5.749	-1.832	-1.968
C	-5.724	-2.021	0.444
C	-6.320	-2.308	-0.788
N	-1.092	-0.756	-0.265
C	0.562	-0.676	-2.232
C	0.267	-2.092	-2.396
C	-1.302	-2.094	-0.341
C	-1.008	-2.590	-2.474
H	-0.440	-3.719	3.887
H	-1.342	-2.079	2.287
H	0.809	-5.711	3.064
H	1.145	-6.021	0.620
H	0.269	-4.381	-0.974
H	3.913	-1.653	-4.014
H	4.091	-2.903	-2.755
H	5.476	-1.867	-3.193
H	6.062	-1.308	1.584
H	5.733	-0.258	0.210
H	5.366	-1.996	0.121
H	3.302	0.536	3.004
H	4.439	1.241	1.859
H	4.989	0.064	3.054
H	4.271	0.715	-3.270
H	5.584	0.443	-2.107
H	4.036	1.132	-1.575
H	3.069	0.594	-0.018
H	2.600	-2.025	2.690
H	4.306	-2.397	2.856
H	3.417	-2.970	1.437
H	-0.037	-0.273	1.926
H	1.571	-0.263	2.618
H	1.541	1.968	3.657
H	-1.252	4.482	-1.315
H	-0.833	2.910	-2.017
H	-0.551	4.398	-2.935

```
H   1.686   4.429   3.302
H   2.943   3.534  -1.885
H   1.885   3.847  -3.268
H   1.717   2.337  -2.362
H   1.409   5.356   1.057
H   2.247   5.804  -0.960
H   0.527   6.191  -0.747
H   1.194   5.984  -2.366
H  -2.668   1.910   3.965
H  -3.491   4.152   3.289
H  -2.163   0.208   2.257
H  -3.801   4.687   0.883
H  -3.280   2.981  -0.844
H  -4.141  -0.678  -2.833
H  -4.119  -1.030   1.462
H  -6.220  -2.039  -2.924
H  -6.175  -2.379   1.364
H  -7.234  -2.892  -0.823
H   1.573  -0.421  -2.549
H  -0.156  -0.035  -2.749
H   1.094  -2.787  -2.284
H  -2.332  -2.394  -0.516
H  -1.832  -1.944  -2.757
H  -1.186  -3.657  -2.565
H   1.332  -1.656   0.648
---------------------------------------

 SCF Done:  E(RB3LYP) =  -2349.80118264     A.U. after    1 cycles

                 1                  2                  3
                 A                  A                  A
Frequencies --  -220.1960            21.2213            23.3750
Red. masses --     6.5227            5.3294             4.2832

Zero-point correction=                          0.862703 (Hartree/Particle)
Thermal correction to Energy=                   0.909800
Thermal correction to Enthalpy=                 0.910744
Thermal correction to Gibbs Free Energy=        0.784683
Sum of electronic and zero-point Energies=          -2348.938480
Sum of electronic and thermal Energies=             -2348.891383
Sum of electronic and thermal Enthalpies=           -2348.890439
Sum of electronic and thermal Free Energies=        -2349.016500

       Item               Value     Threshold  Converged?
Maximum Force            0.000001     0.000450     YES
RMS     Force            0.000000     0.000300     YES
```

Transition State Energy for Complex (*S*)-TS4 (not shown in manuscript; see Scheme S2b)





Cartesian coordinates (Angstroms):

H	1.303	-1.944	3.939
H	3.208	-3.984	0.832
C	0.753	-2.507	3.192
H	0.359	-0.776	1.967
H	5.522	-3.454	1.165
H	0.956	-4.387	4.226
H	-1.023	-3.966	-1.454
C	0.240	-1.846	2.074
C	0.555	-3.877	3.356
C	3.104	-3.231	0.044
H	3.304	-3.723	-0.915
H	3.873	-2.143	2.448
C	5.511	-2.720	0.353
H	2.075	-2.879	0.054
H	5.774	-3.248	-0.569
H	1.063	-2.851	-2.012
C	-1.043	-2.925	-1.754
H	-5.318	3.294	2.053
C	4.108	-2.080	0.280
C	3.848	-1.399	1.644
C	0.126	-2.325	-2.182
H	6.294	-1.986	0.568
C	-0.484	-2.553	1.103
H	-1.993	-2.568	-2.138
C	-0.181	-4.587	2.402
H	-5.146	1.938	4.129
H	2.878	-0.903	1.670
C	-4.688	2.410	2.077
H	4.627	-0.656	1.850
C	-4.589	1.649	3.242
C	-1.197	-1.825	0.014
C	-0.705	-3.930	1.294
H	-0.356	-5.650	2.529
H	-4.049	2.635	0.033

H	-2.257	-2.072	0.014
C	-3.976	2.039	0.937
C	4.007	-1.021	-0.840
C	0.207	-0.946	-2.562
H	-4.543	-1.429	0.263
H	6.052	-1.254	-1.447
O	1.656	-0.573	-0.415
H	1.106	-0.749	-3.142
C	-3.769	0.520	3.271
H	-0.684	-0.548	-3.048
H	-6.177	-2.752	-1.026
C	5.131	-0.714	-1.619
H	-1.300	-4.492	0.582
H	-3.682	-0.068	4.179
C	2.818	-0.293	-1.120
N	-0.935	-0.514	-0.311
C	-3.153	0.903	0.962
B	0.418	-0.114	-0.986
C	-4.531	-1.384	-0.822
C	-3.049	0.146	2.136
C	-5.465	-2.122	-1.549
P	-2.376	0.473	-0.618
H	-2.392	-0.715	2.187
C	5.126	0.264	-2.614
C	-3.603	-0.566	-1.489
C	2.814	0.726	-2.102
H	2.303	2.214	-0.211
H	6.025	0.459	-3.190
N	0.634	1.499	-1.224
C	-5.496	-2.035	-2.943
H	1.057	1.282	-3.283
C	3.971	0.994	-2.841
C	1.590	1.578	-2.378
H	-6.229	-2.604	-3.505
H	-0.300	1.870	-1.484
O	-2.021	1.655	-1.488
C	1.235	2.374	-0.108
H	3.510	2.089	1.232
O	-0.408	1.611	1.439
C	-3.658	-0.464	-2.890
C	0.777	1.910	1.271
H	1.719	0.880	4.138
H	3.067	4.476	0.090
C	-4.598	-1.199	-3.611
H	3.952	1.781	-3.590
N	1.679	1.900	2.295
H	0.118	1.481	3.621
H	2.723	4.259	-1.629
H	1.889	2.614	-2.522
C	1.181	1.705	3.659
C	3.092	2.266	2.221
H	-2.984	0.213	-3.404
C	2.310	4.629	-0.685
H	1.186	4.522	1.813
H	3.648	1.642	2.925
C	0.970	3.954	-0.311
H	-4.637	-1.111	-4.692
H	3.251	3.315	2.497
C	0.465	4.612	0.996
H	2.166	5.708	-0.794
H	1.342	2.613	4.251
H	-0.485	4.184	1.323

H 0.213 3.937 -2.398
C -0.081 4.267 -1.397
H 0.314 5.680 0.816
H -1.056 3.832 -1.163
H -0.205 5.352 -1.452

SCF Done: E(RB3LYP) = -2349.79523369 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-335.9124	12.6240	29.5812
Red. masses --	8.2872	3.9844	5.0315

Zero-point correction= 0.862399 (Hartree/Particle)
Thermal correction to Energy= 0.909414
Thermal correction to Enthalpy= 0.910359
Thermal correction to Gibbs Free Energy= 0.783996
Sum of electronic and zero-point Energies= -2348.932835
Sum of electronic and thermal Energies= -2348.885819
Sum of electronic and thermal Enthalpies= -2348.884875
Sum of electronic and thermal Free Energies= -2349.011238

Item	Value	Threshold	Converged?
Maximum Force	0.000011	0.000450	YES
RMS Force	0.000002	0.000300	YES

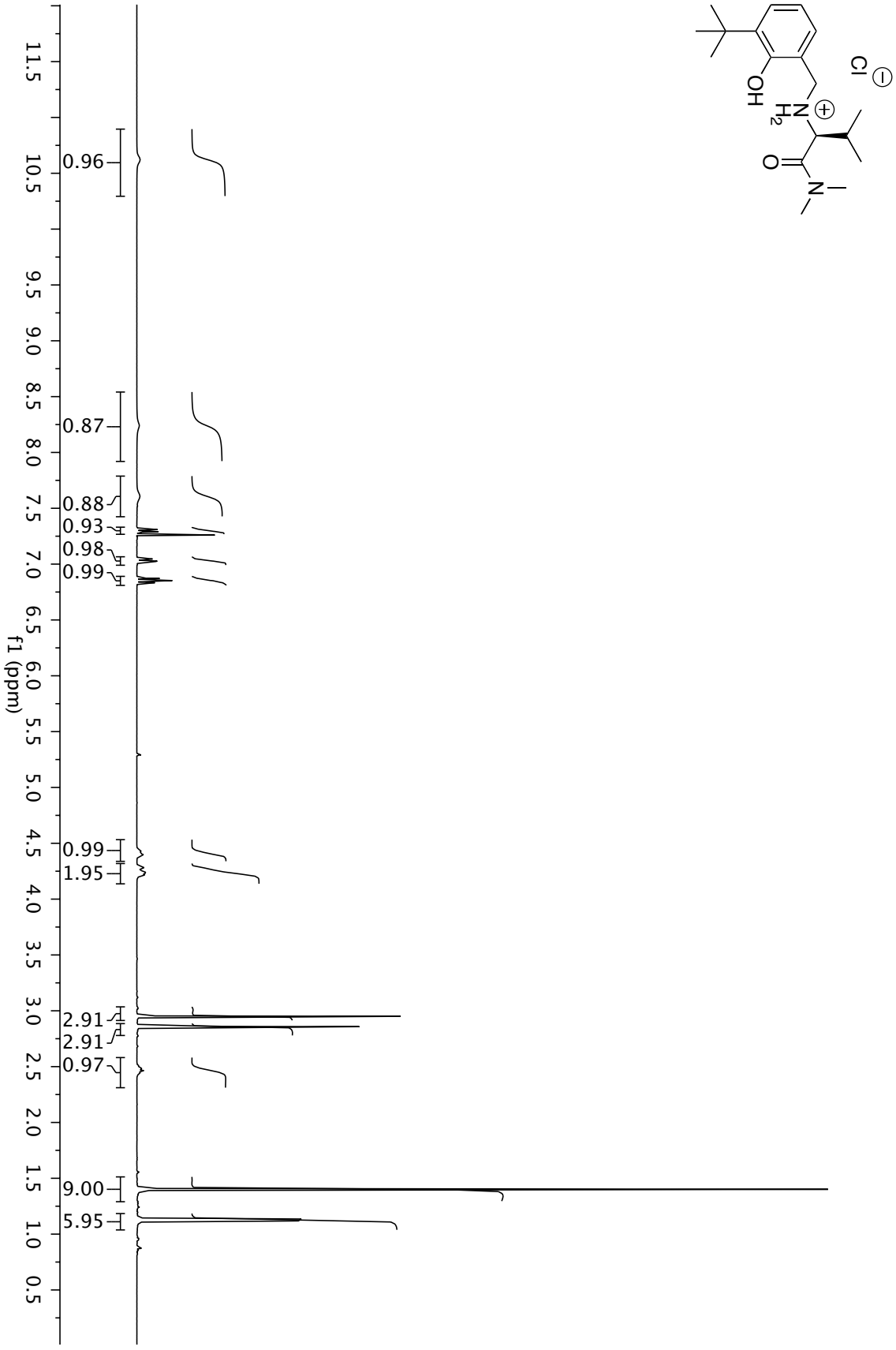
Simple Organic Molecules as Catalysts for Enantioselective Synthesis of Amines and Alcohols

Daniel L. Silverio, Sebastian Torker, Tatiana Pilyugina, Erika M. Vieira, Marc L. Snapper, Fredrik Haeffner & Amir H. Hoveyda*

Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467

SUPPLEMENTARY INFORMATION; PART C

Table of Contents ***Page***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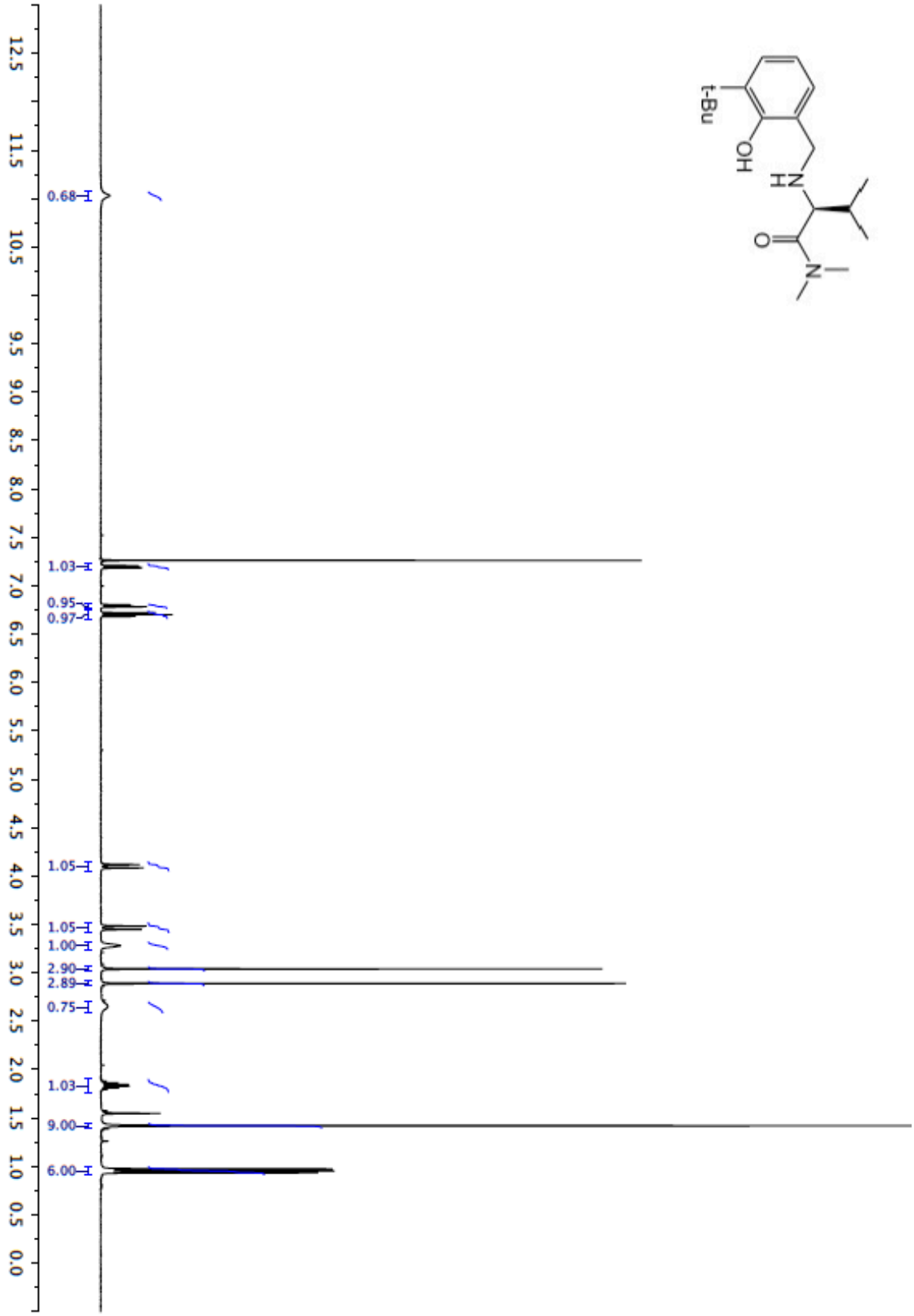
O
N
Cl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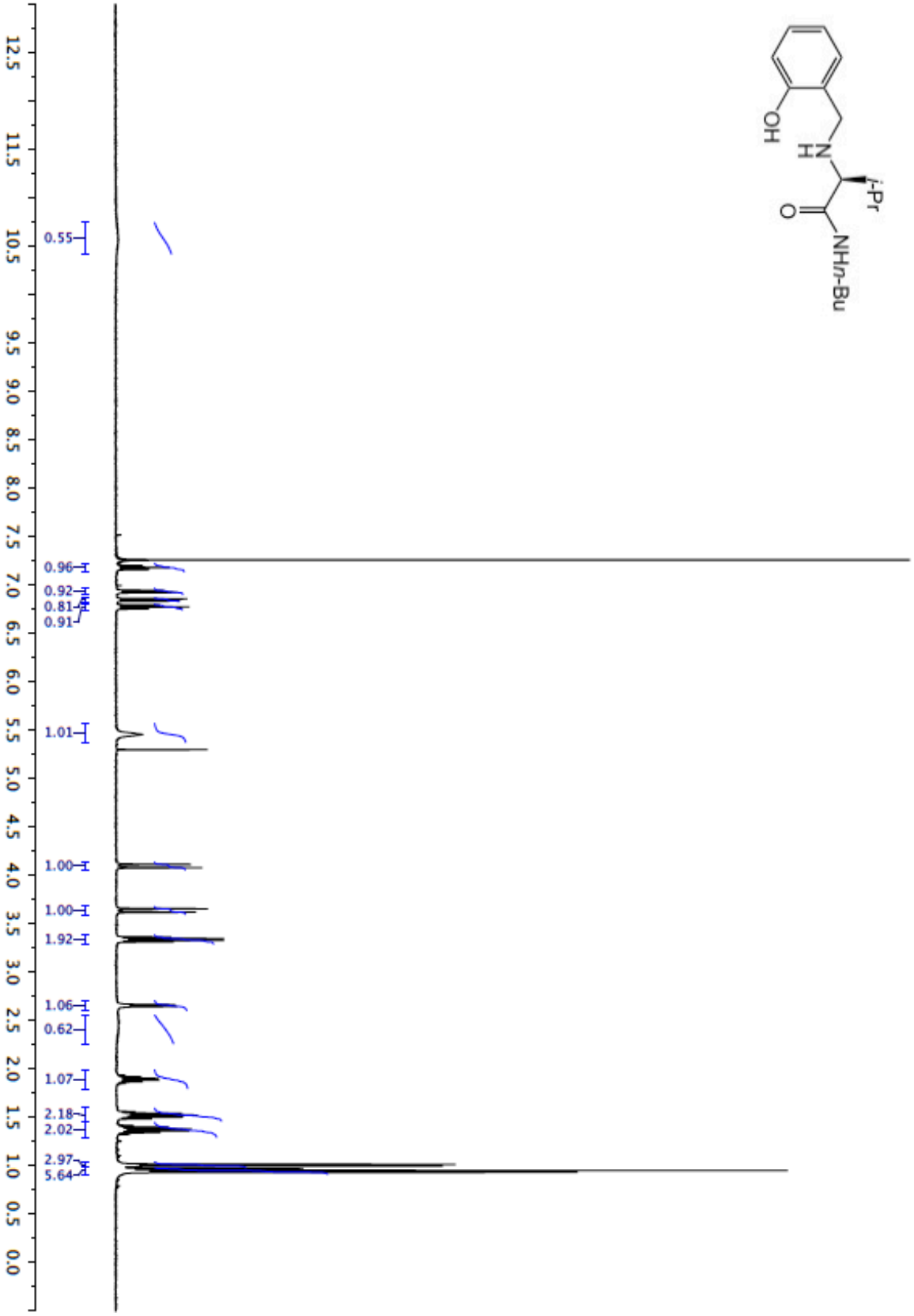
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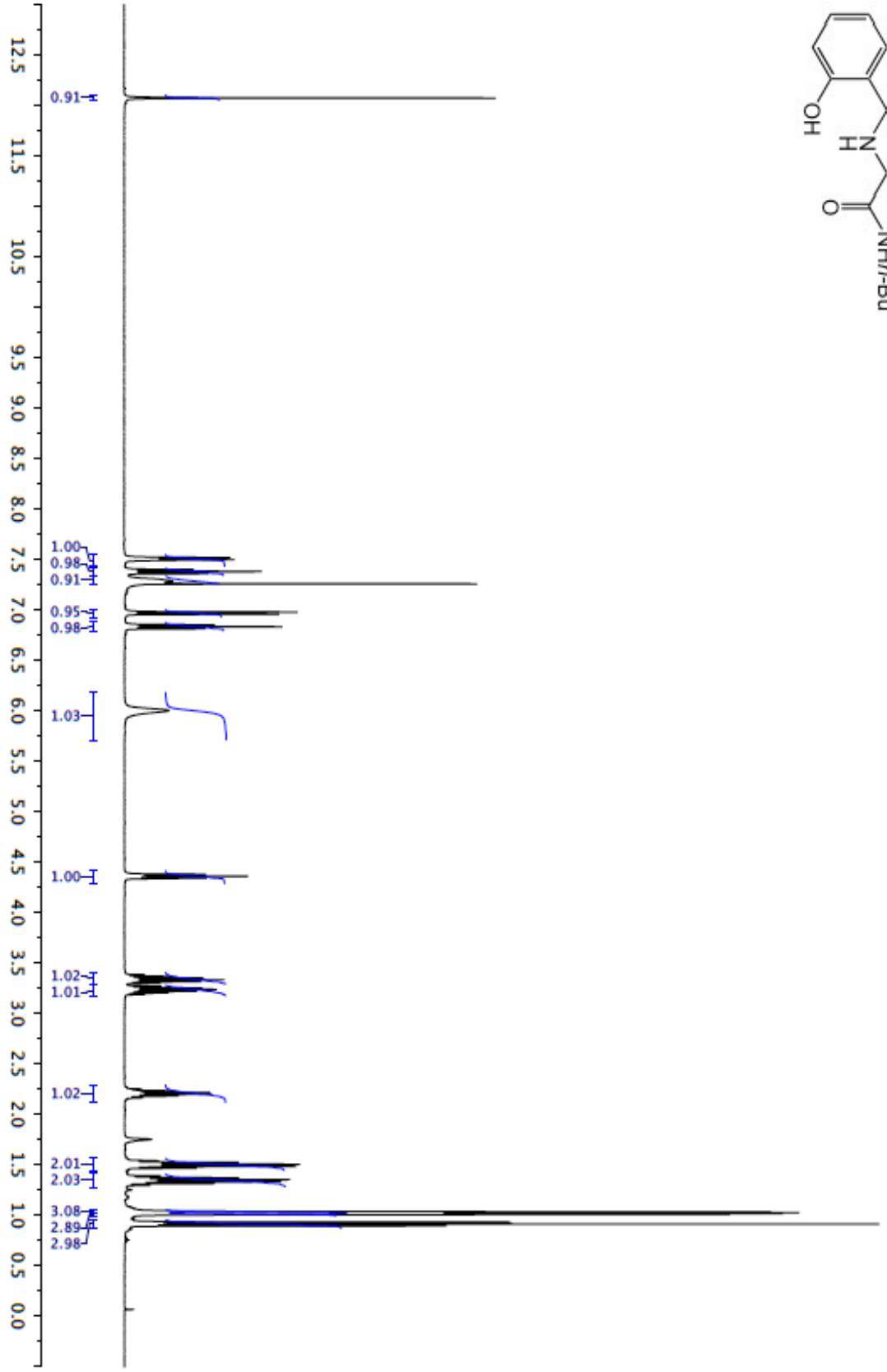
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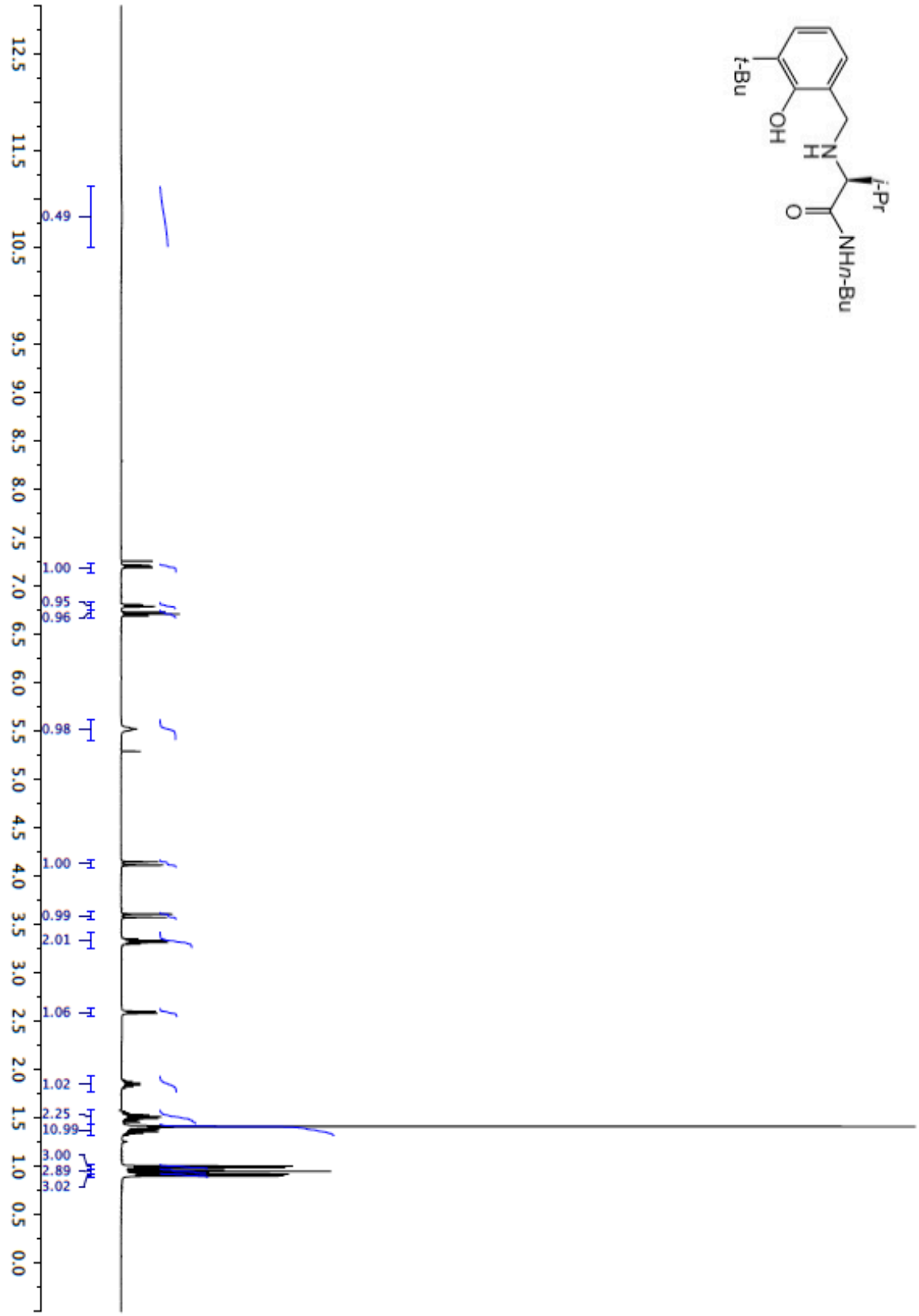
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7.5
7.0
6.5
6.0
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5.0
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4.0
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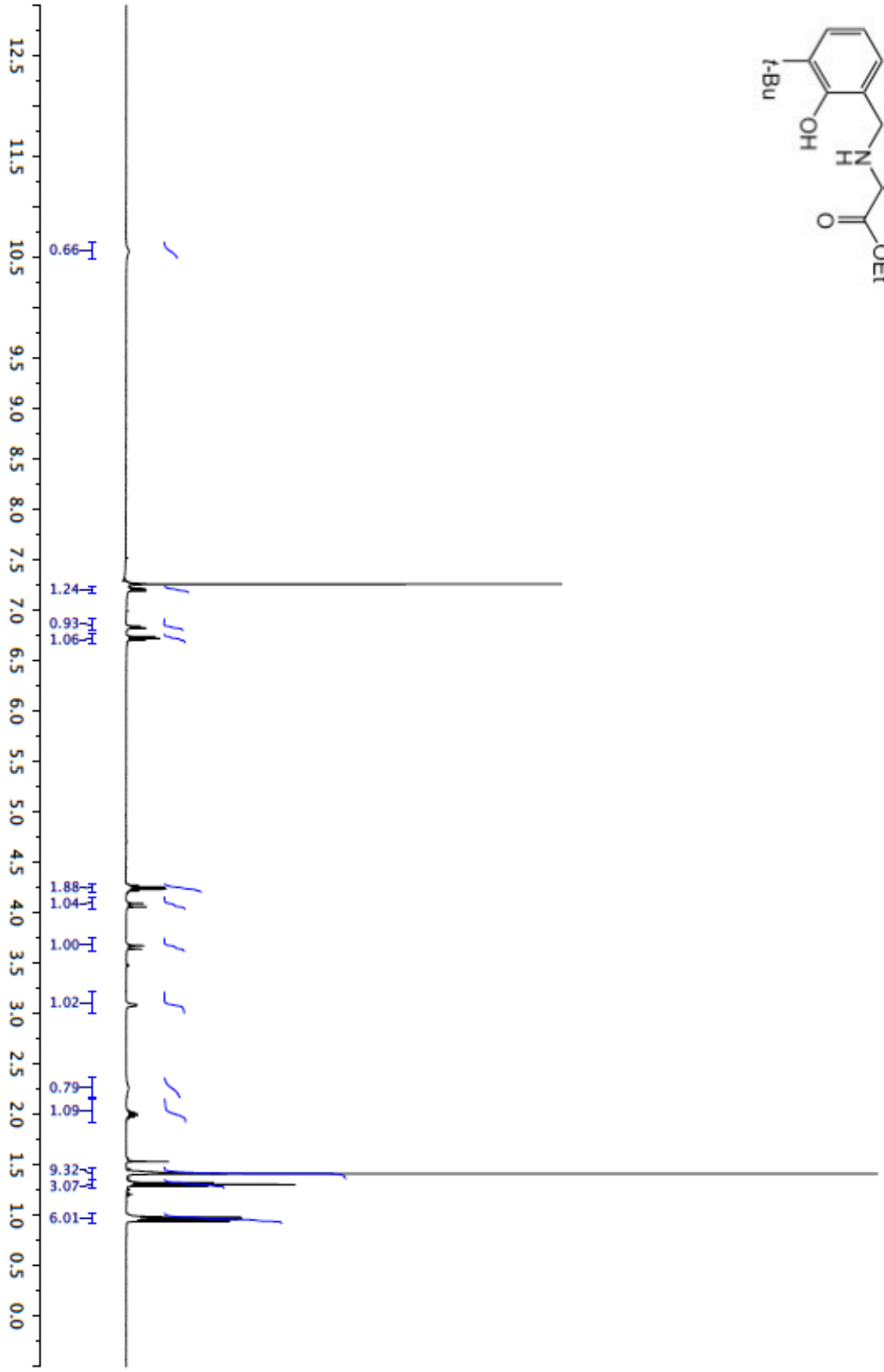
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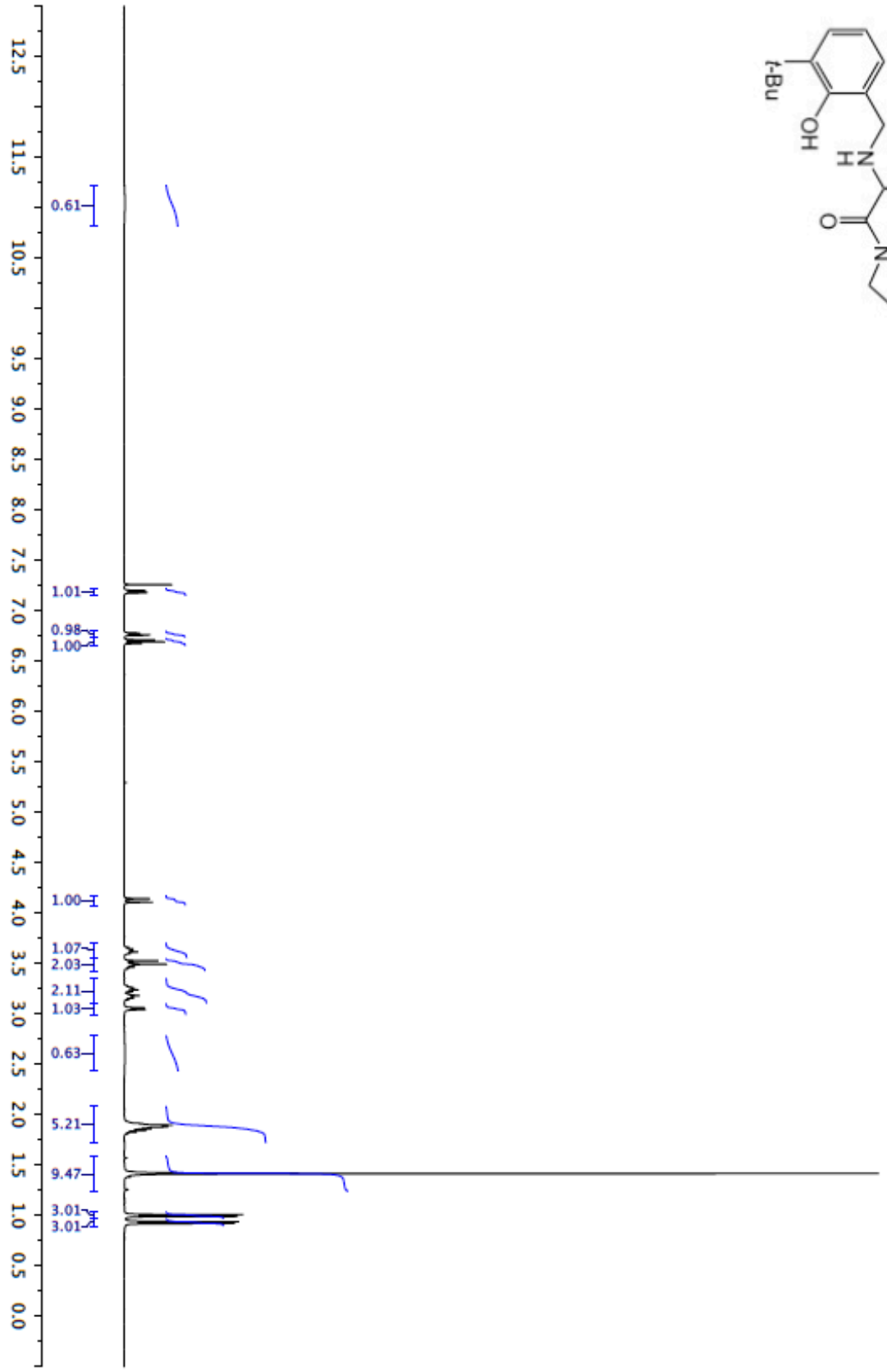
OEt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4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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0.0
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1.00
1.00
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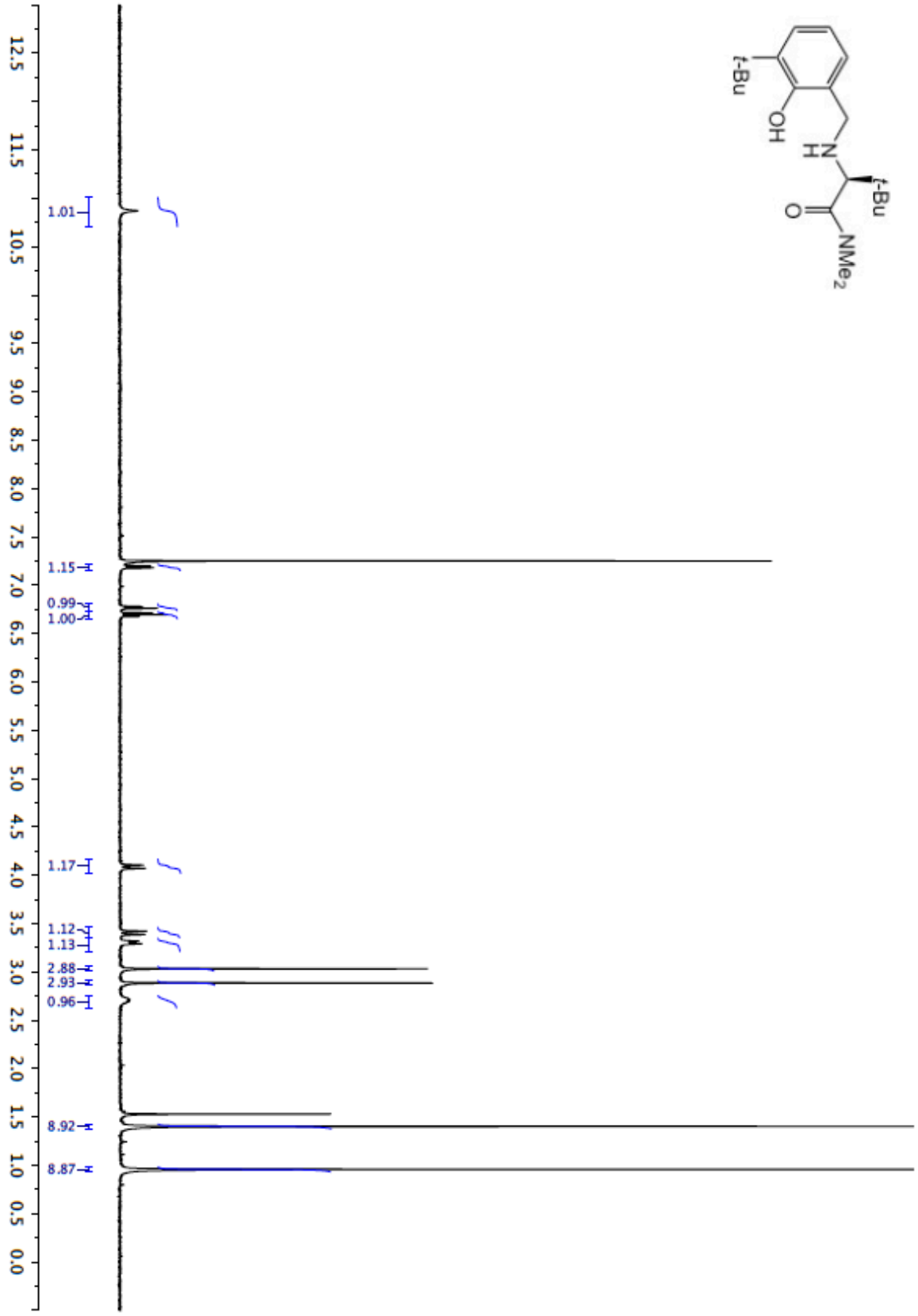
i-Pr
O
N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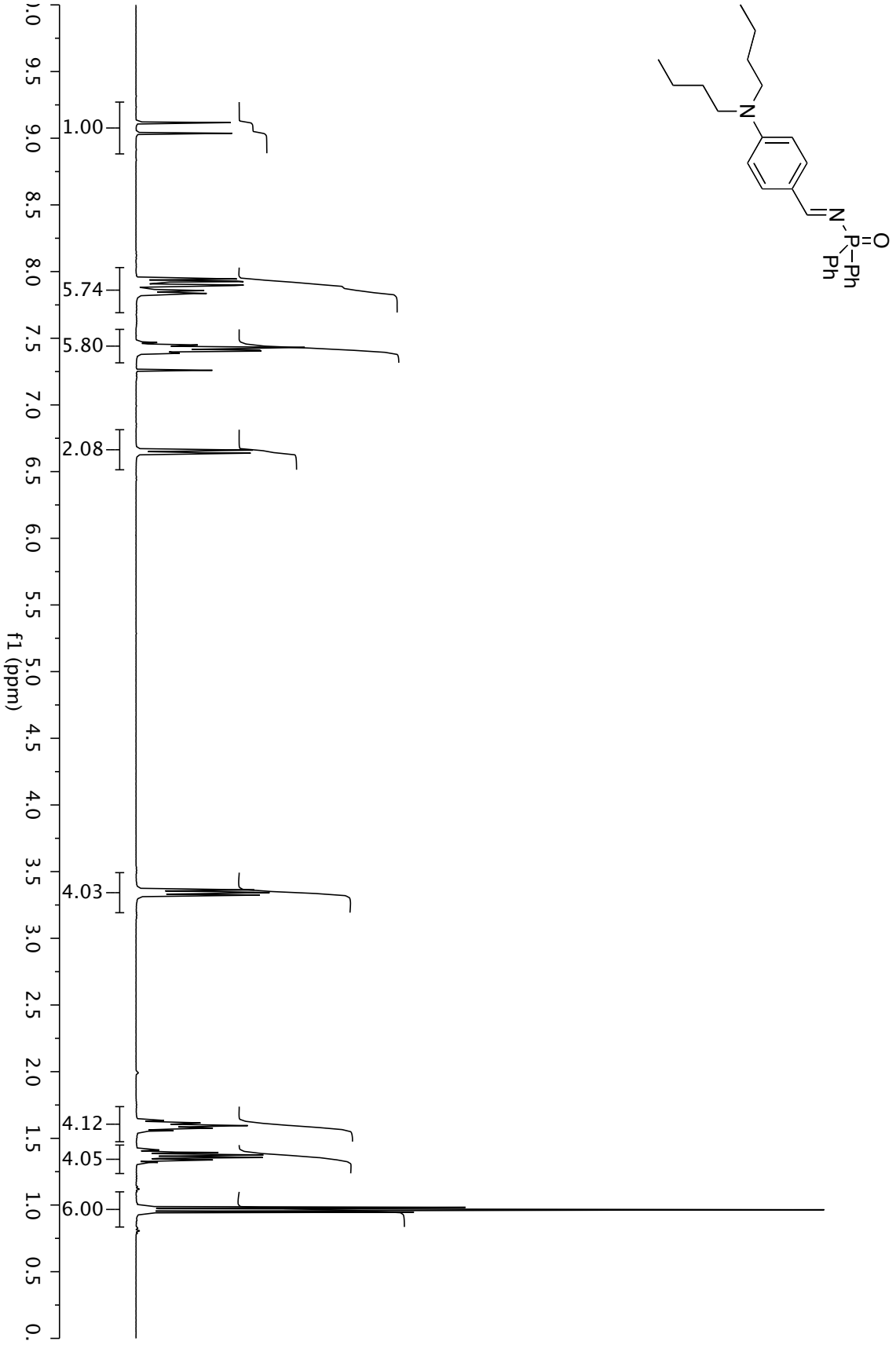
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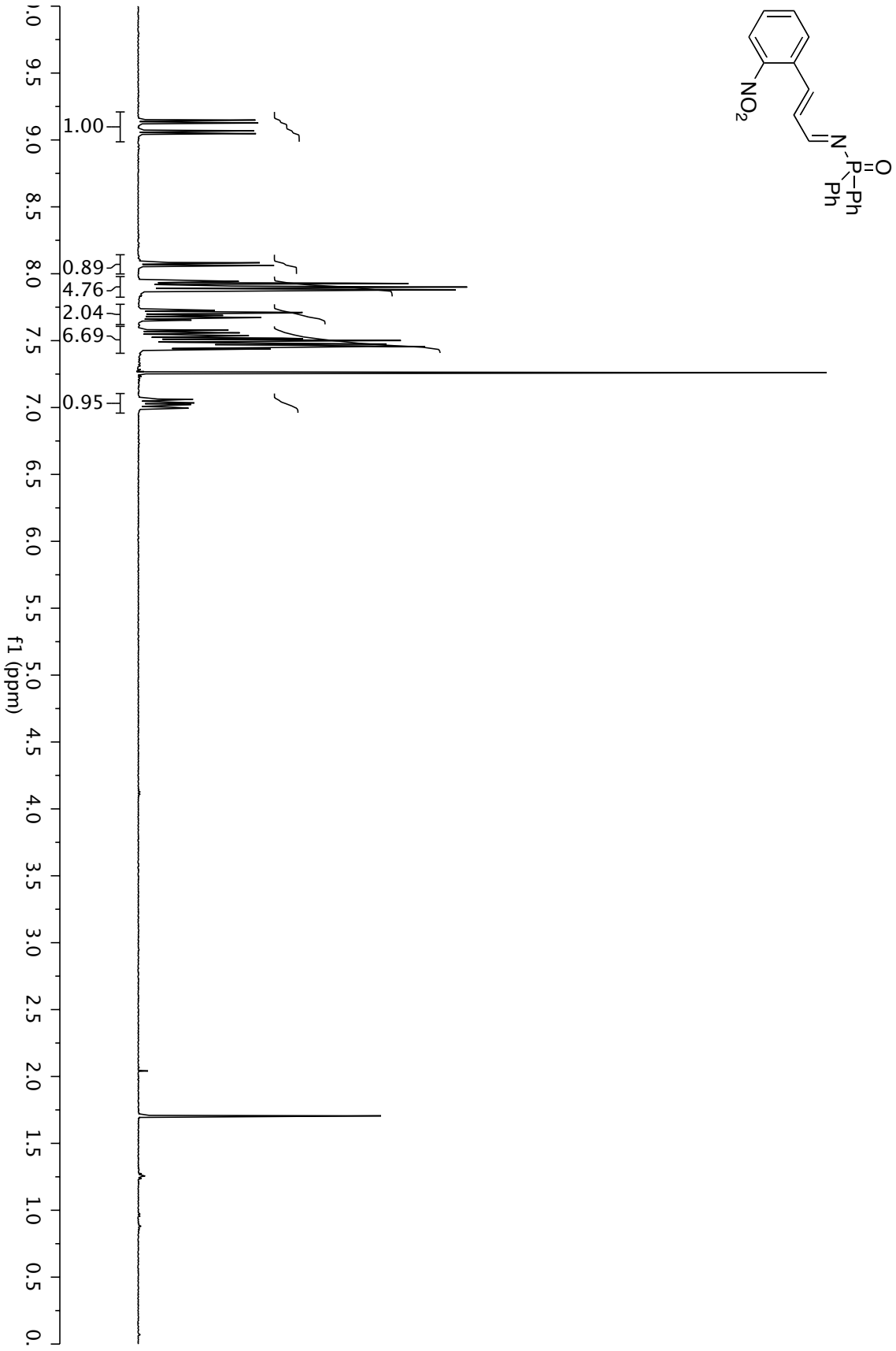
O
P
Ph
Ph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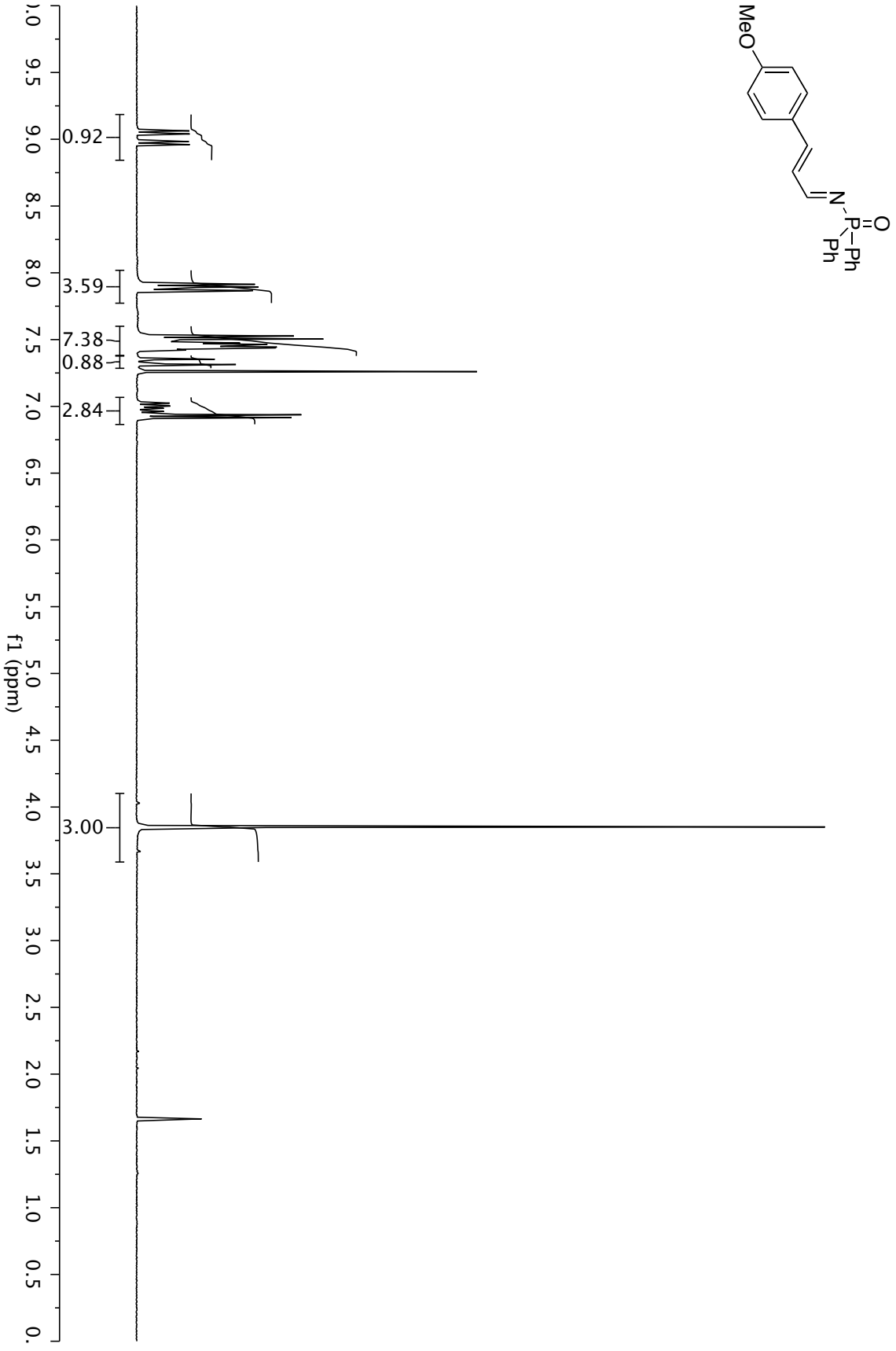
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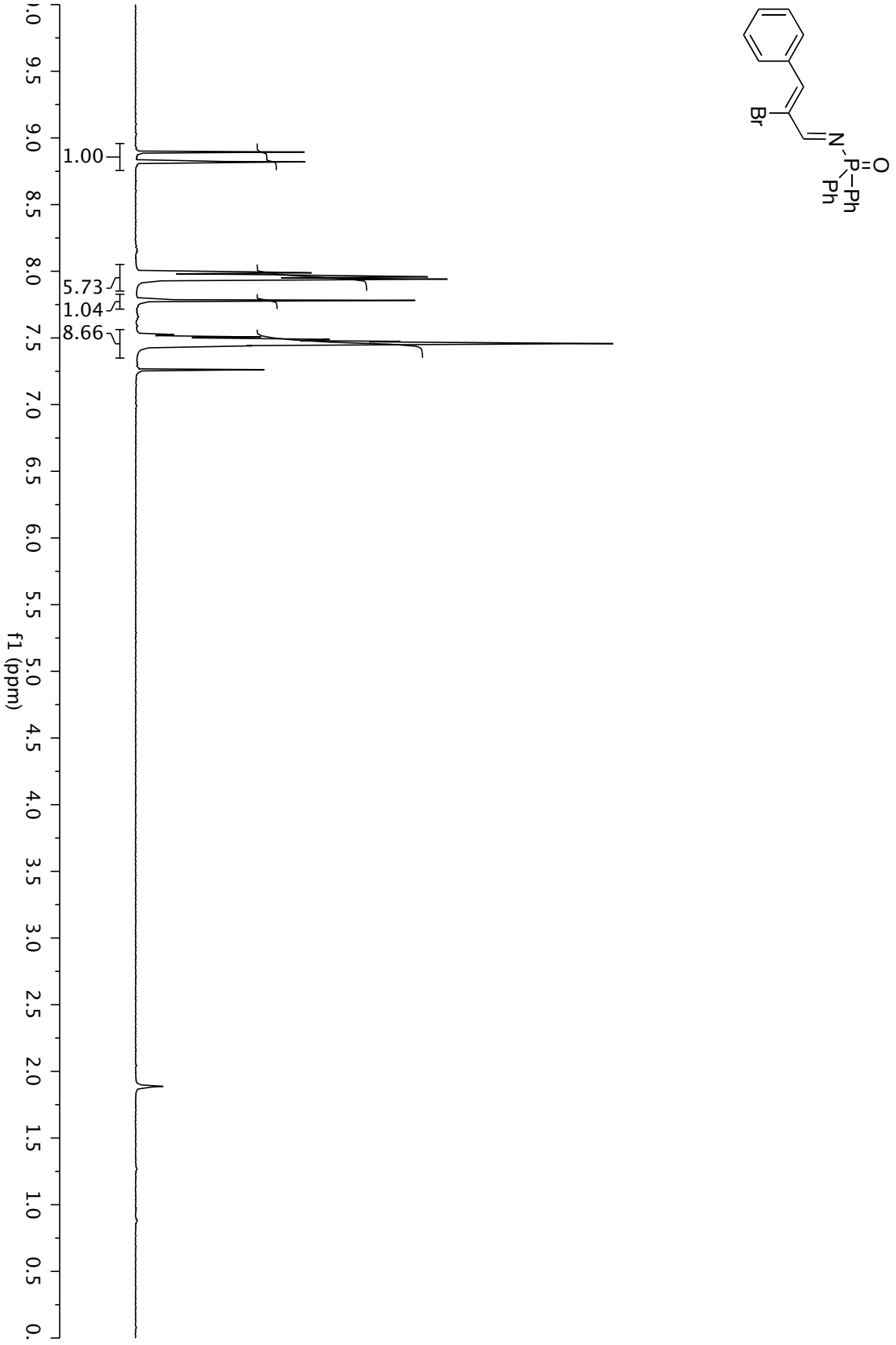
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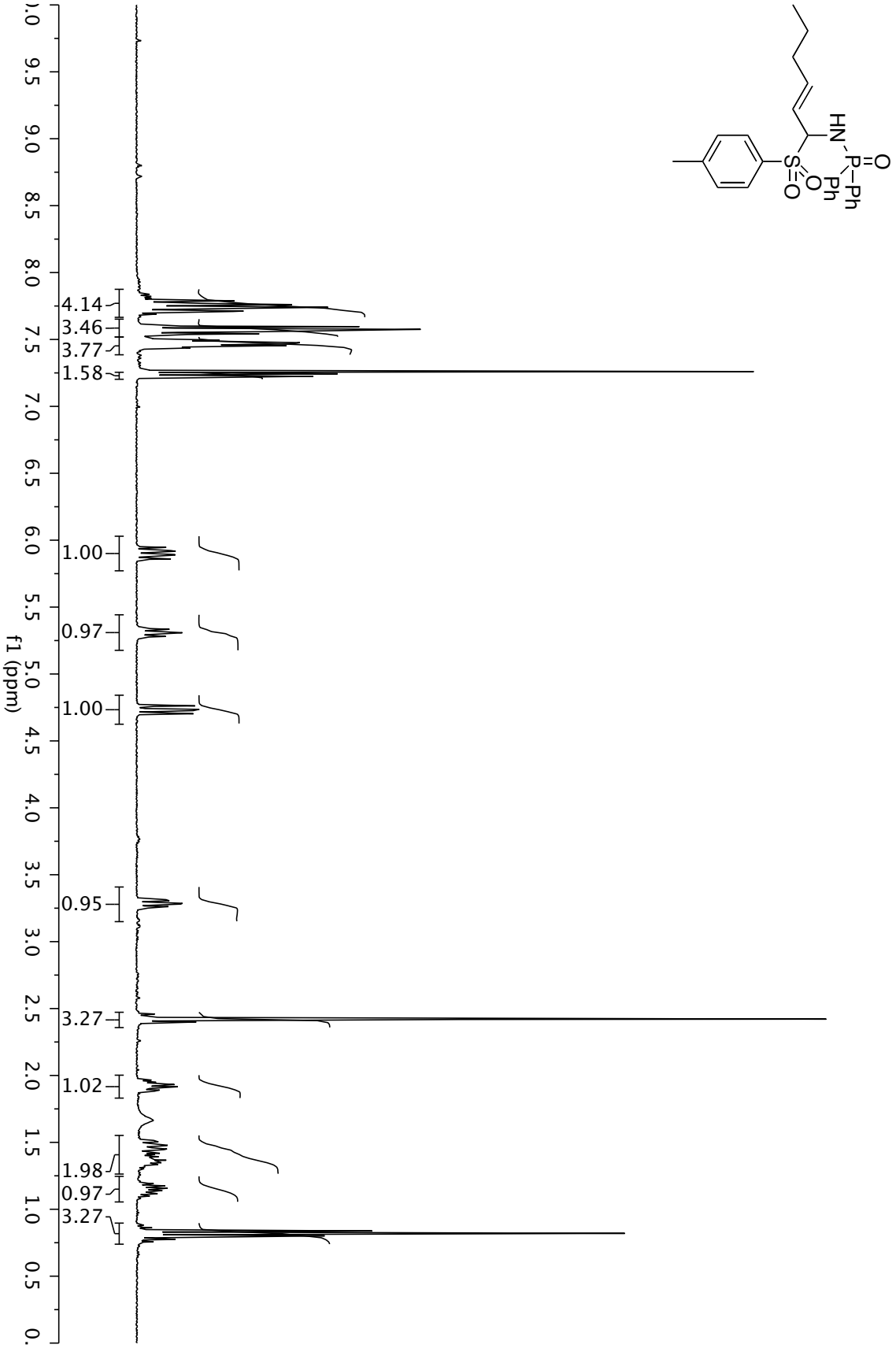
Ph
Ph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P
Ph
Ph
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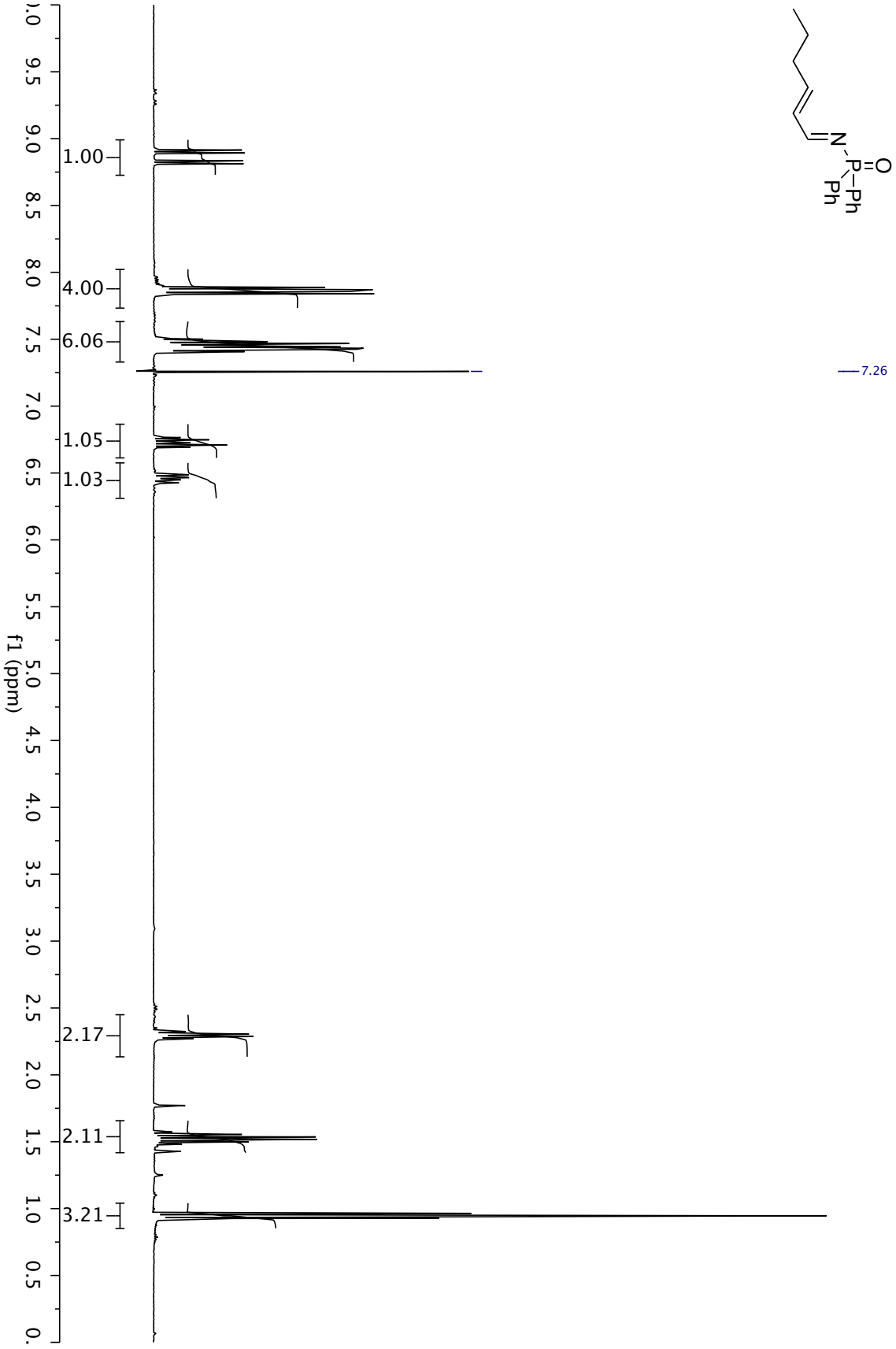
O
S
O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f1 (ppm)
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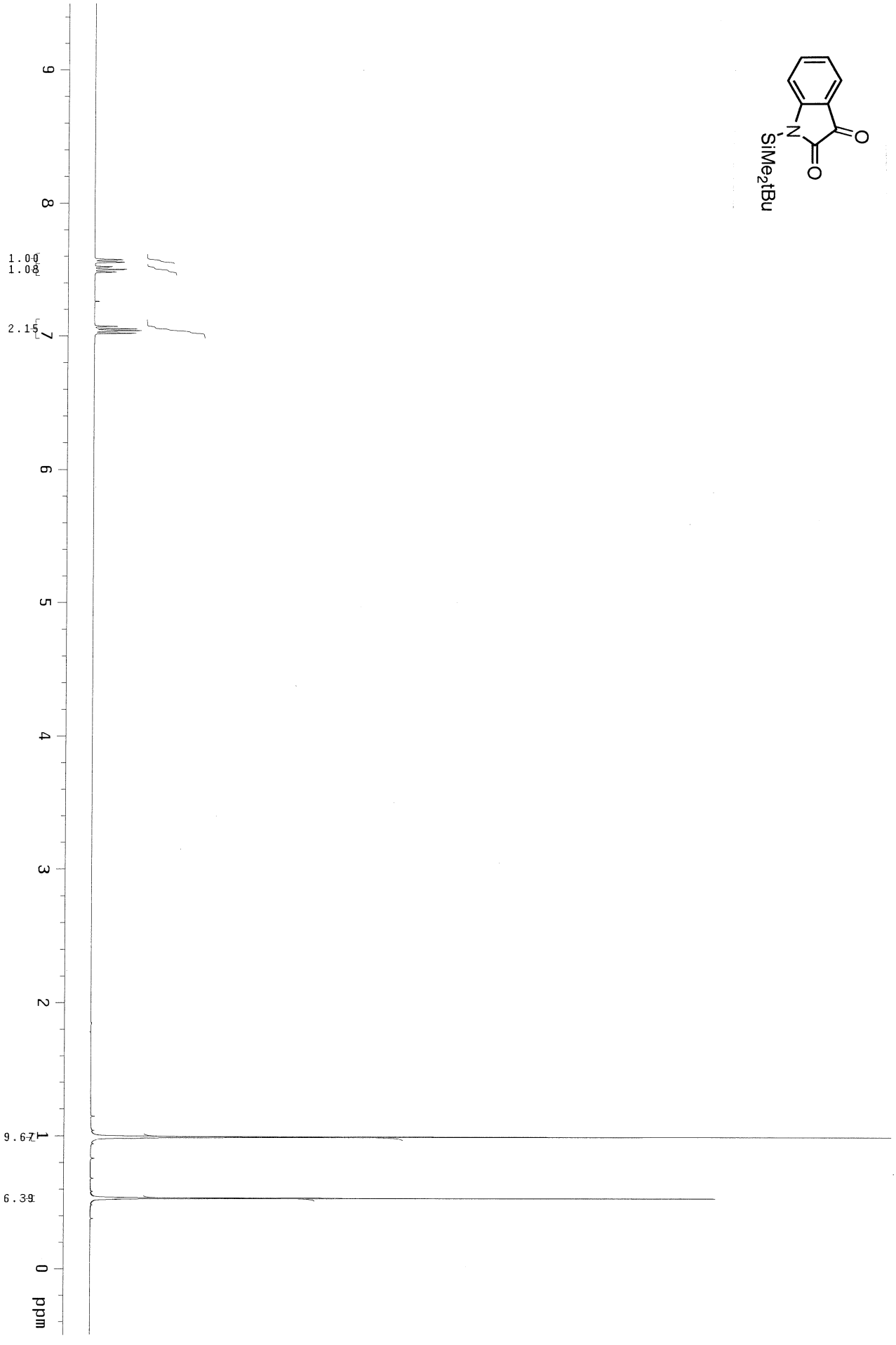
P
O
Ph
Ph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4
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2
1
0
ppm

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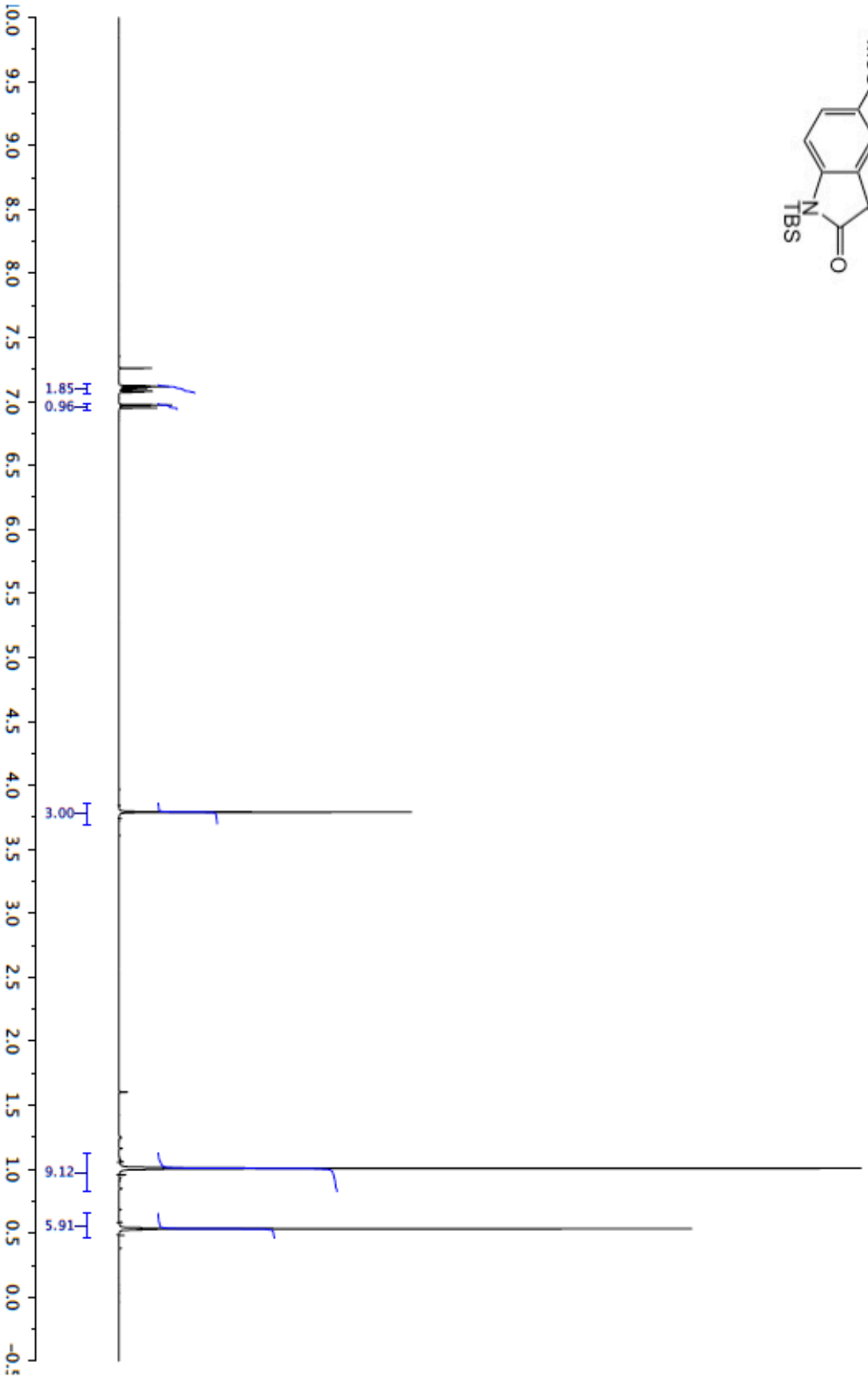
O
SiMe2tBu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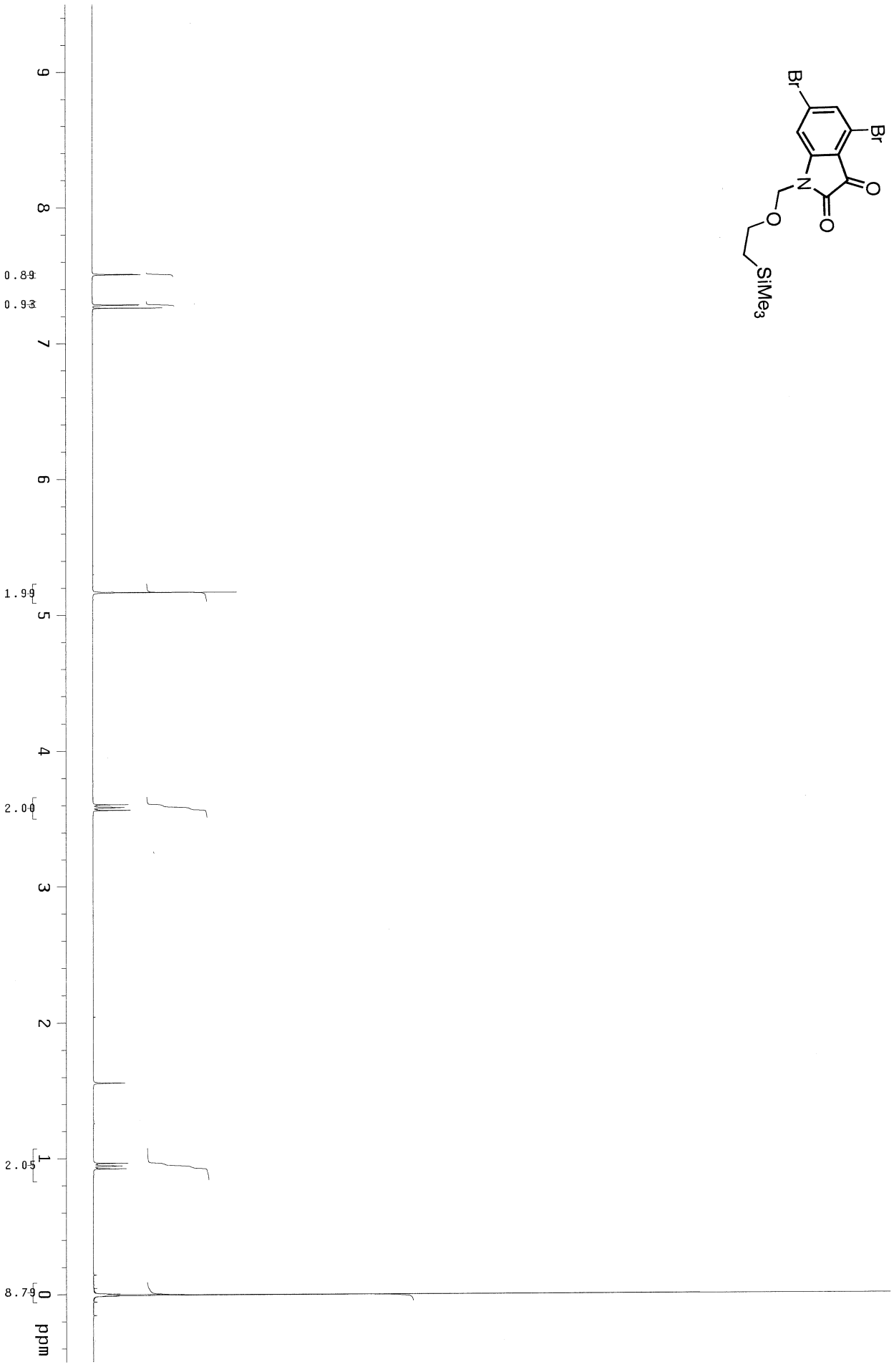
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6
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3
2
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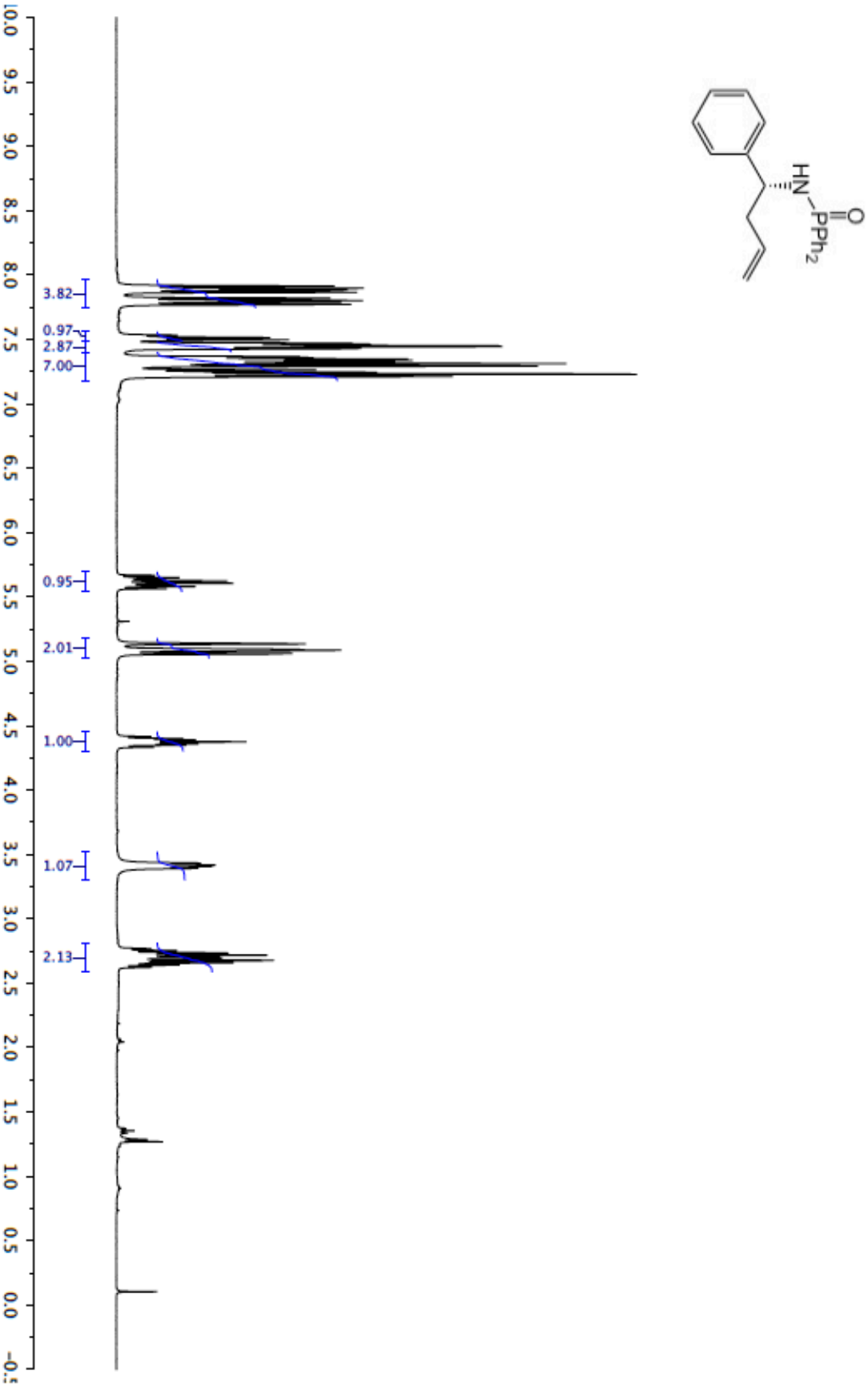
ppm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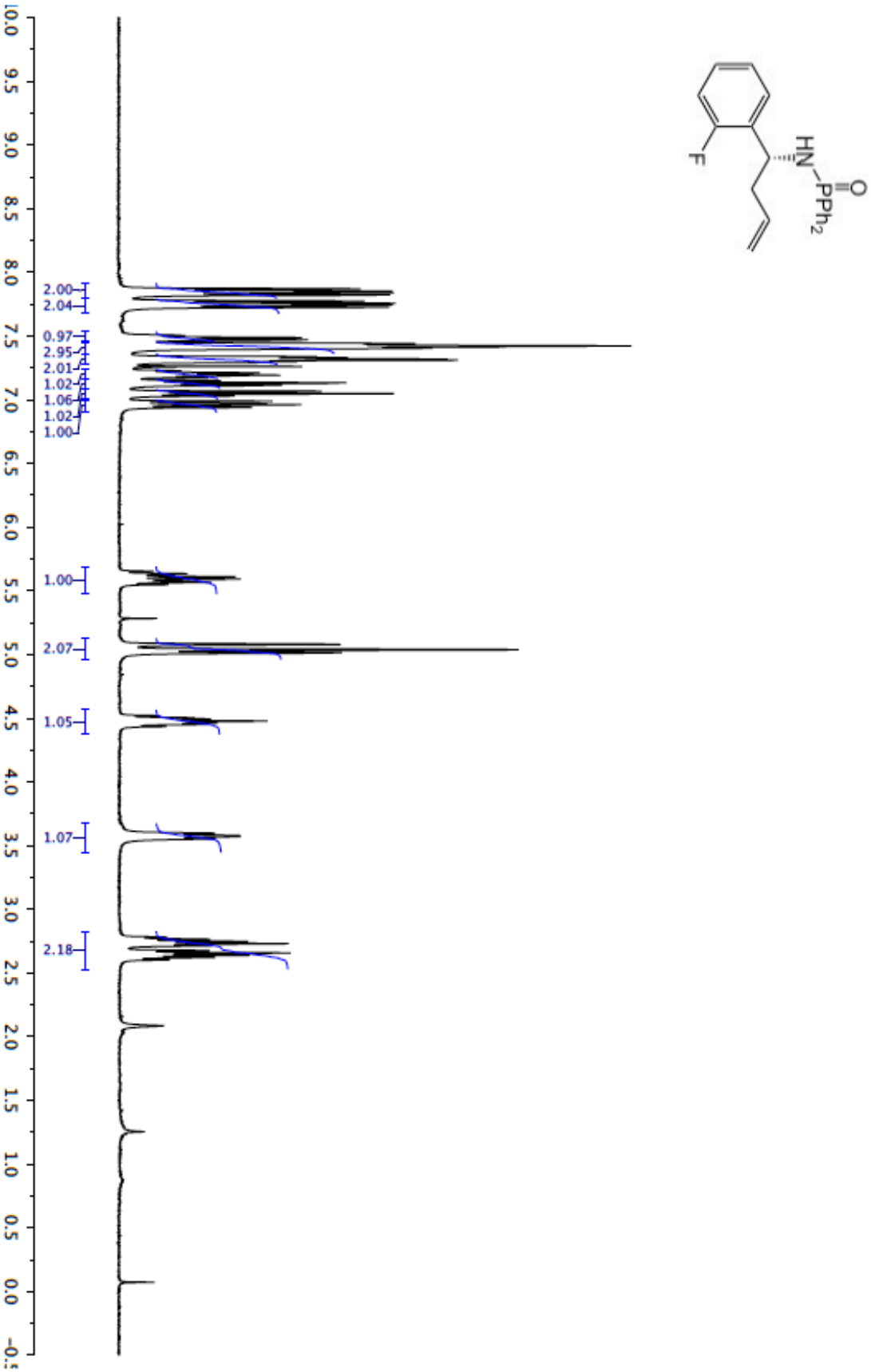
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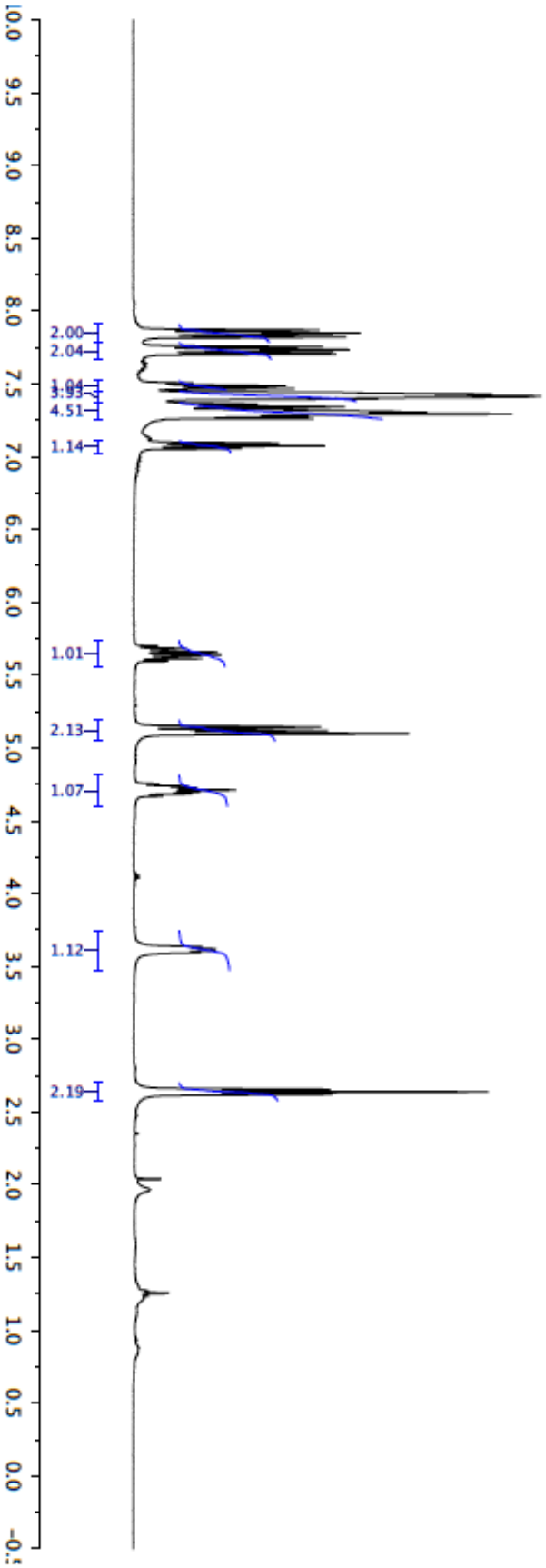
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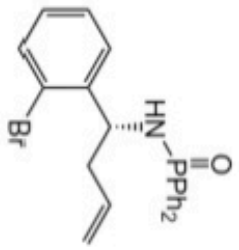
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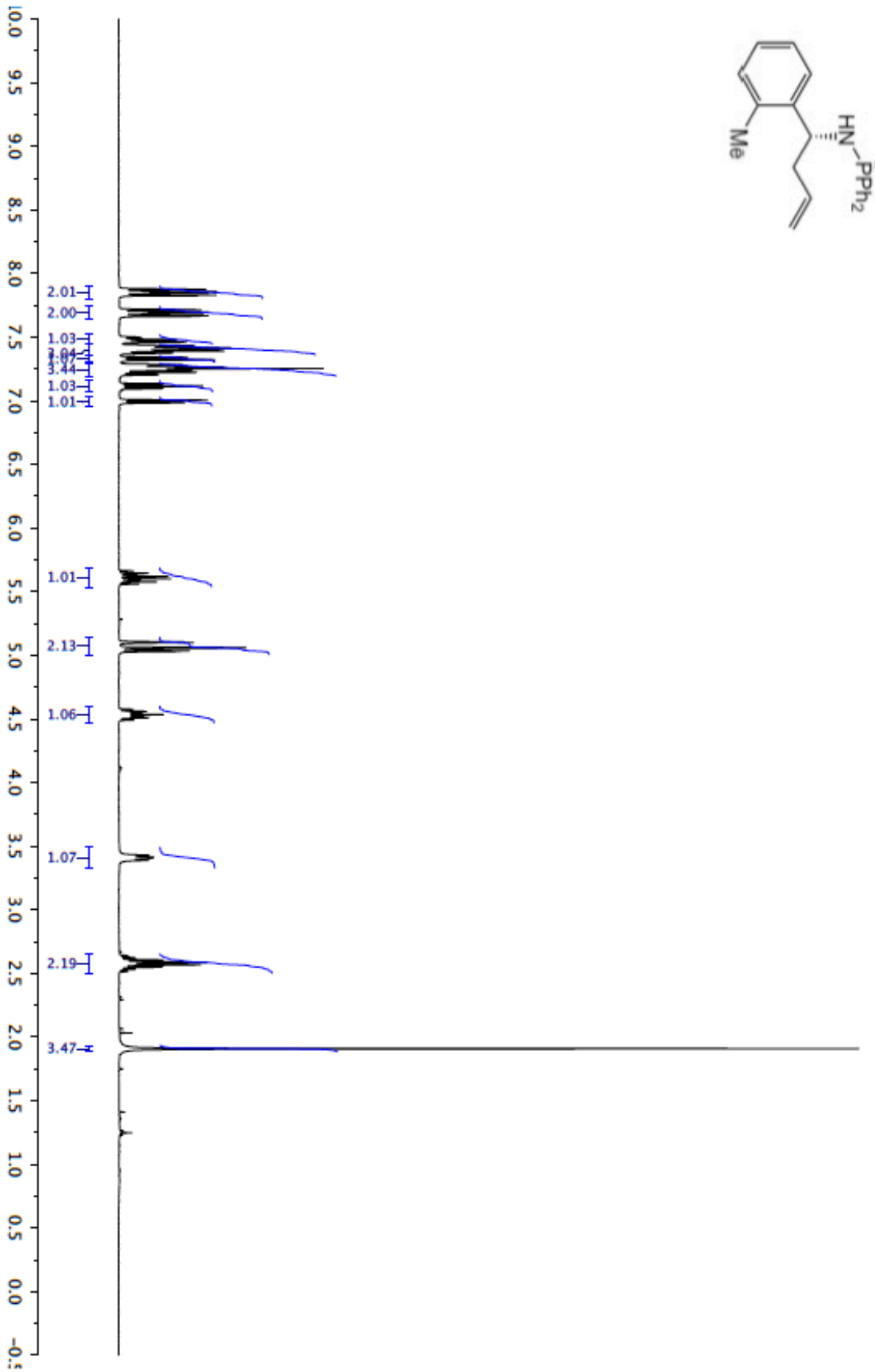
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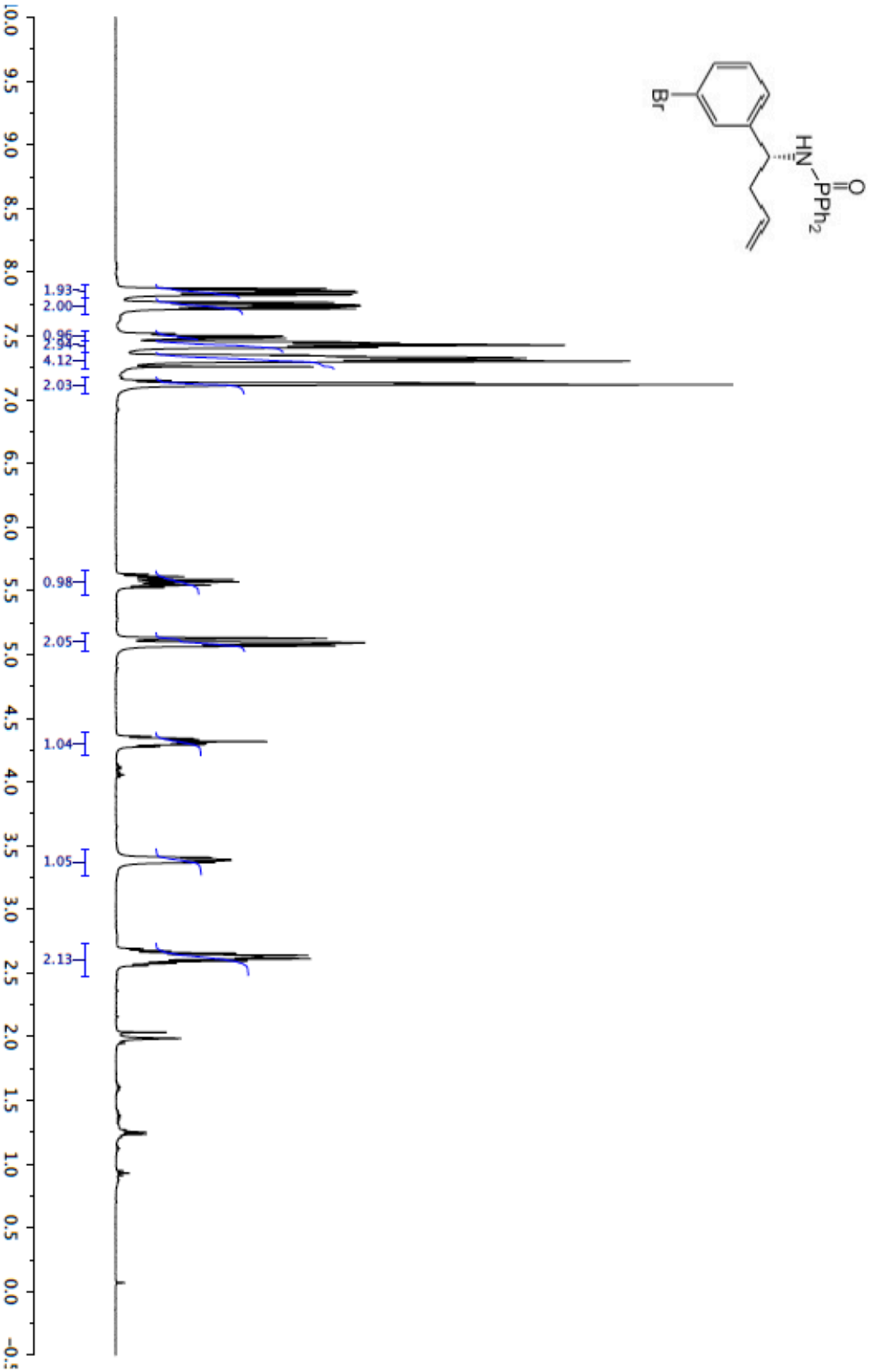
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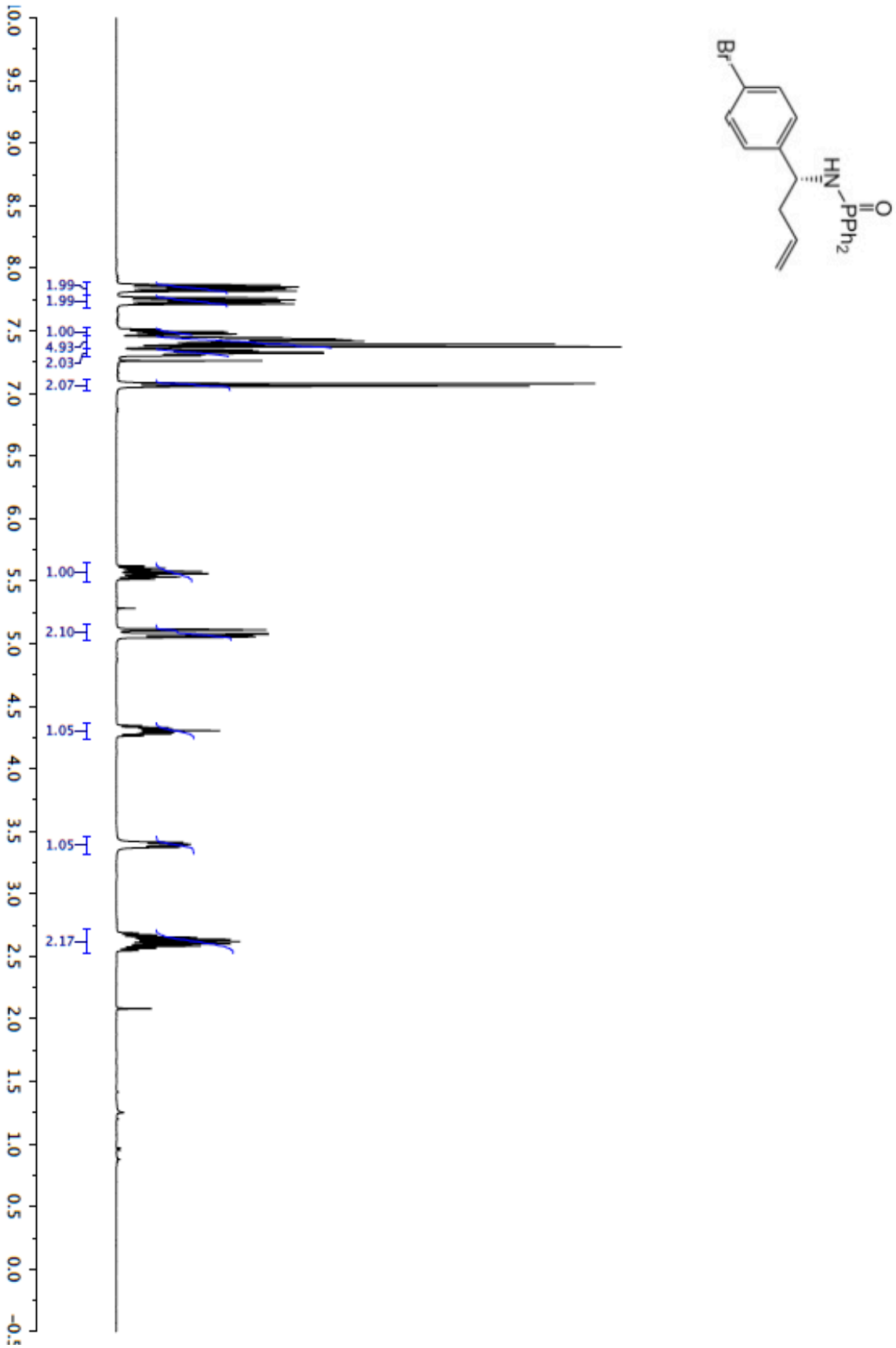
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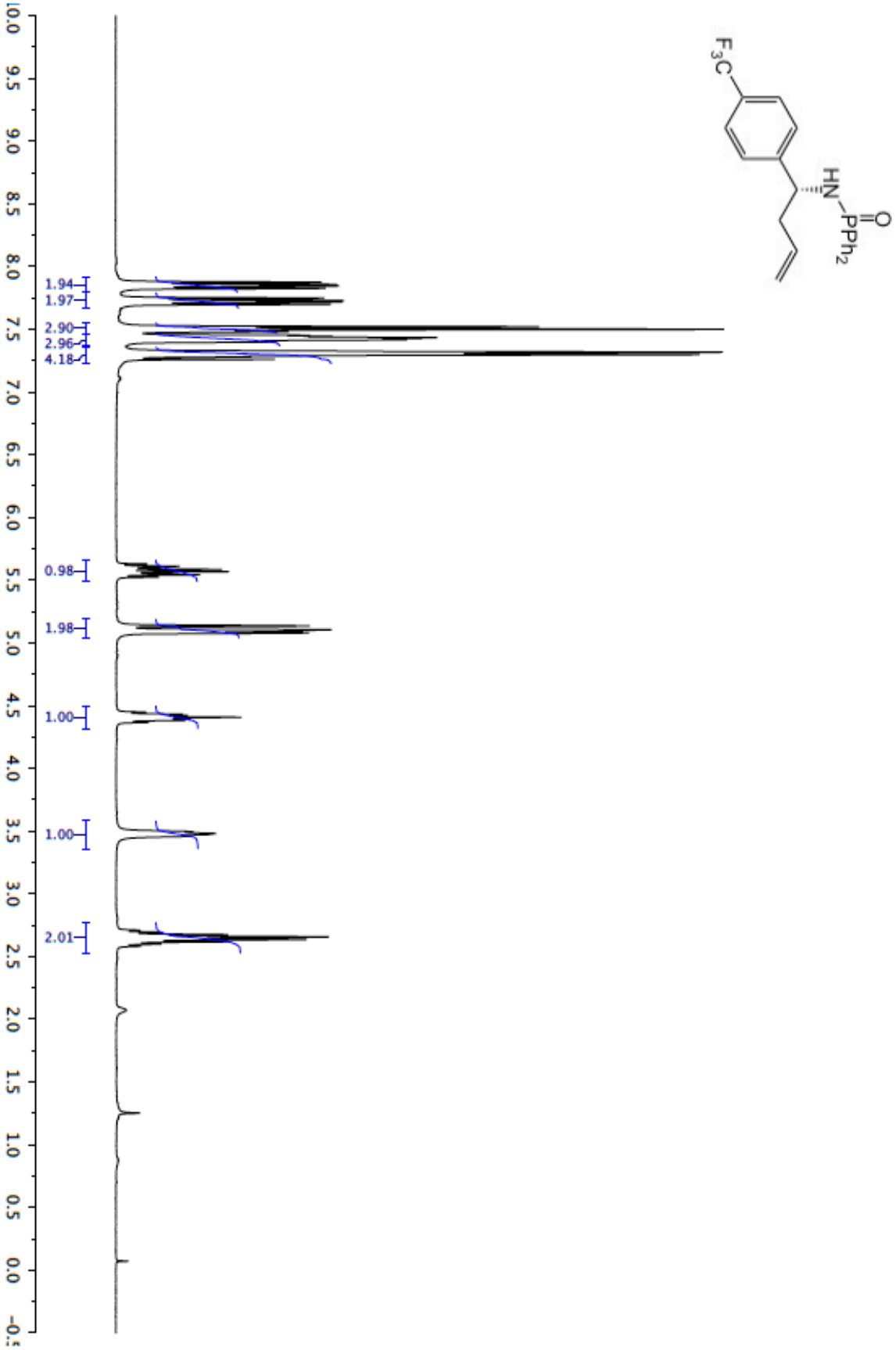
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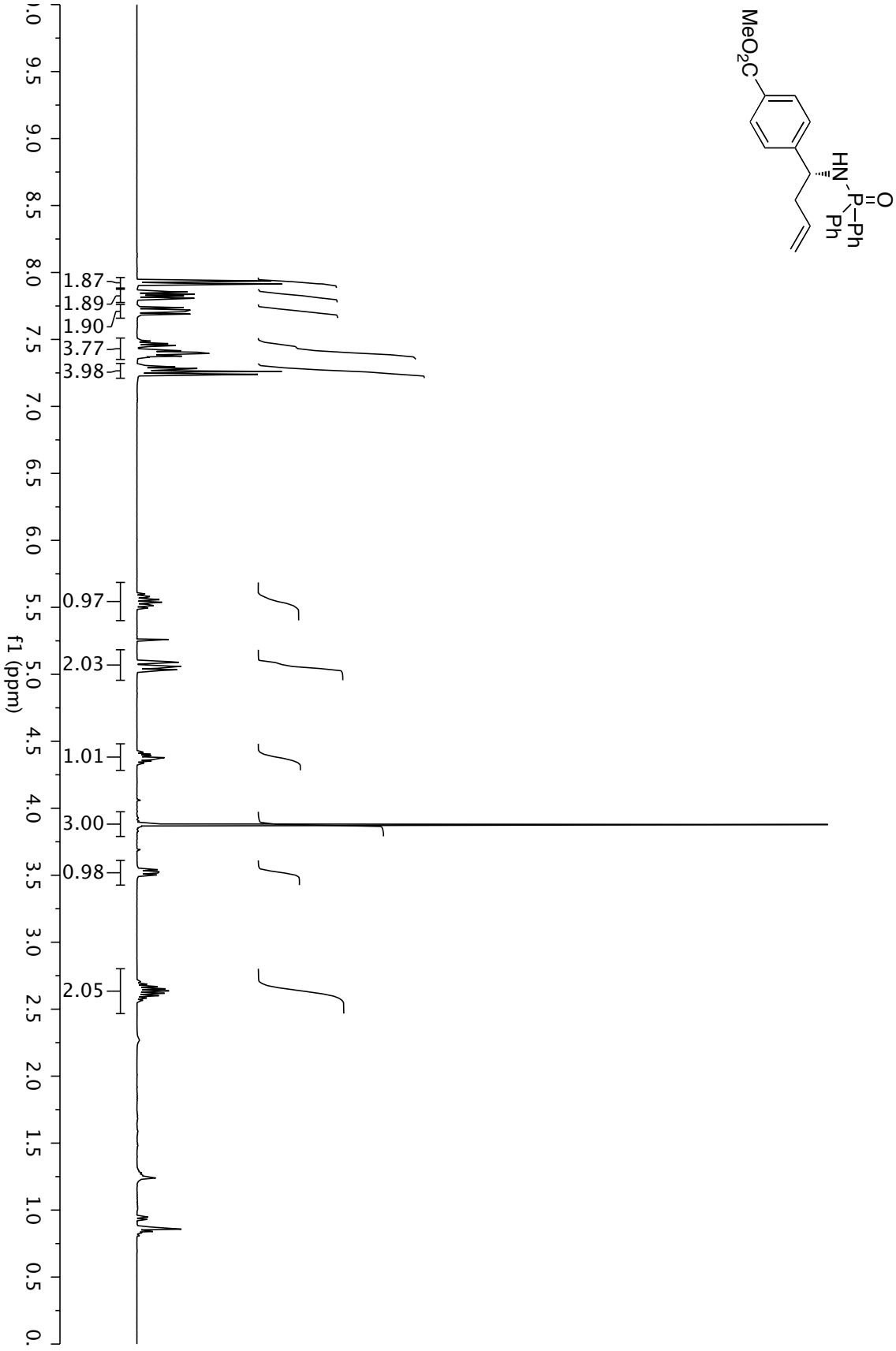
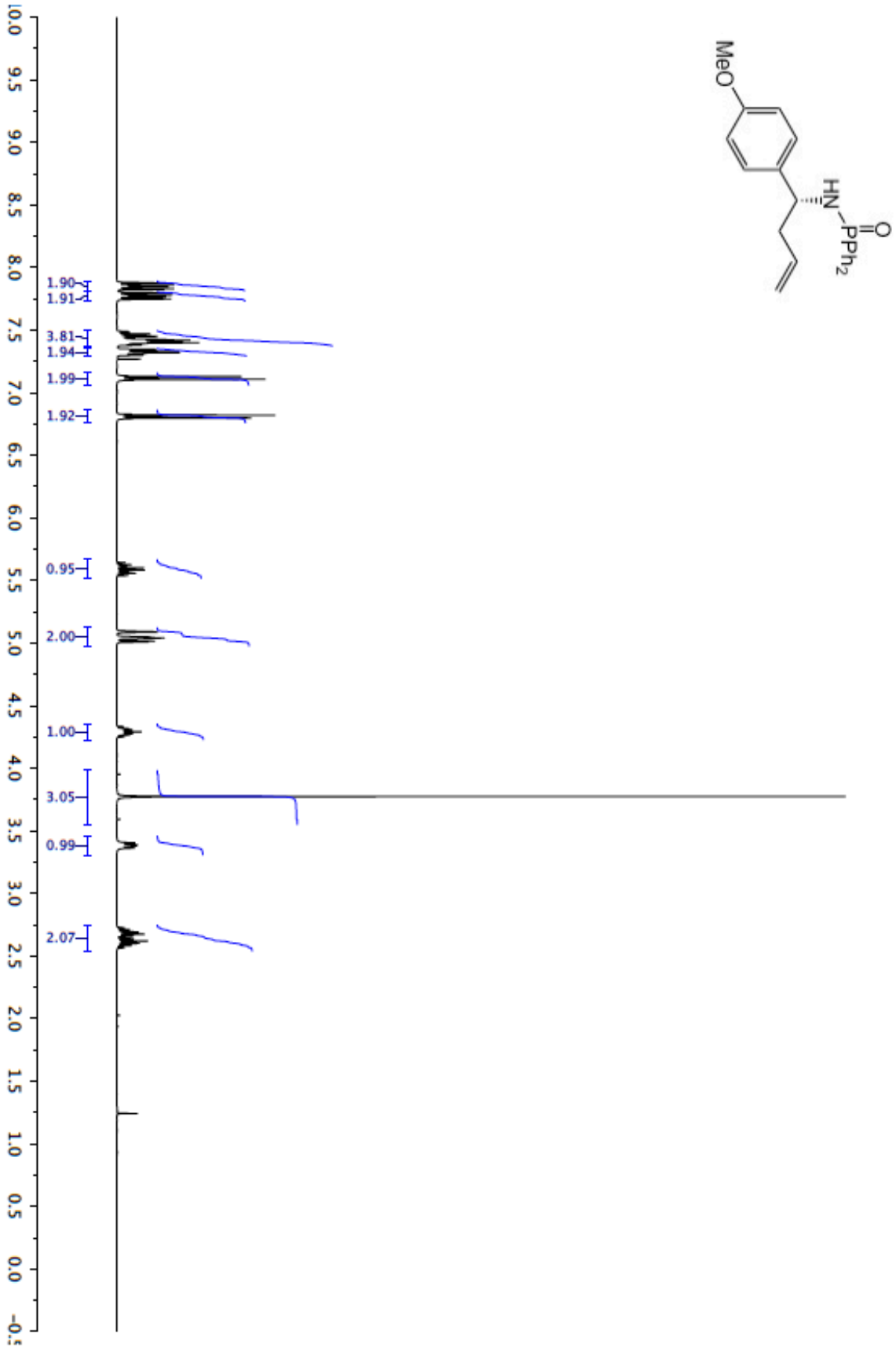
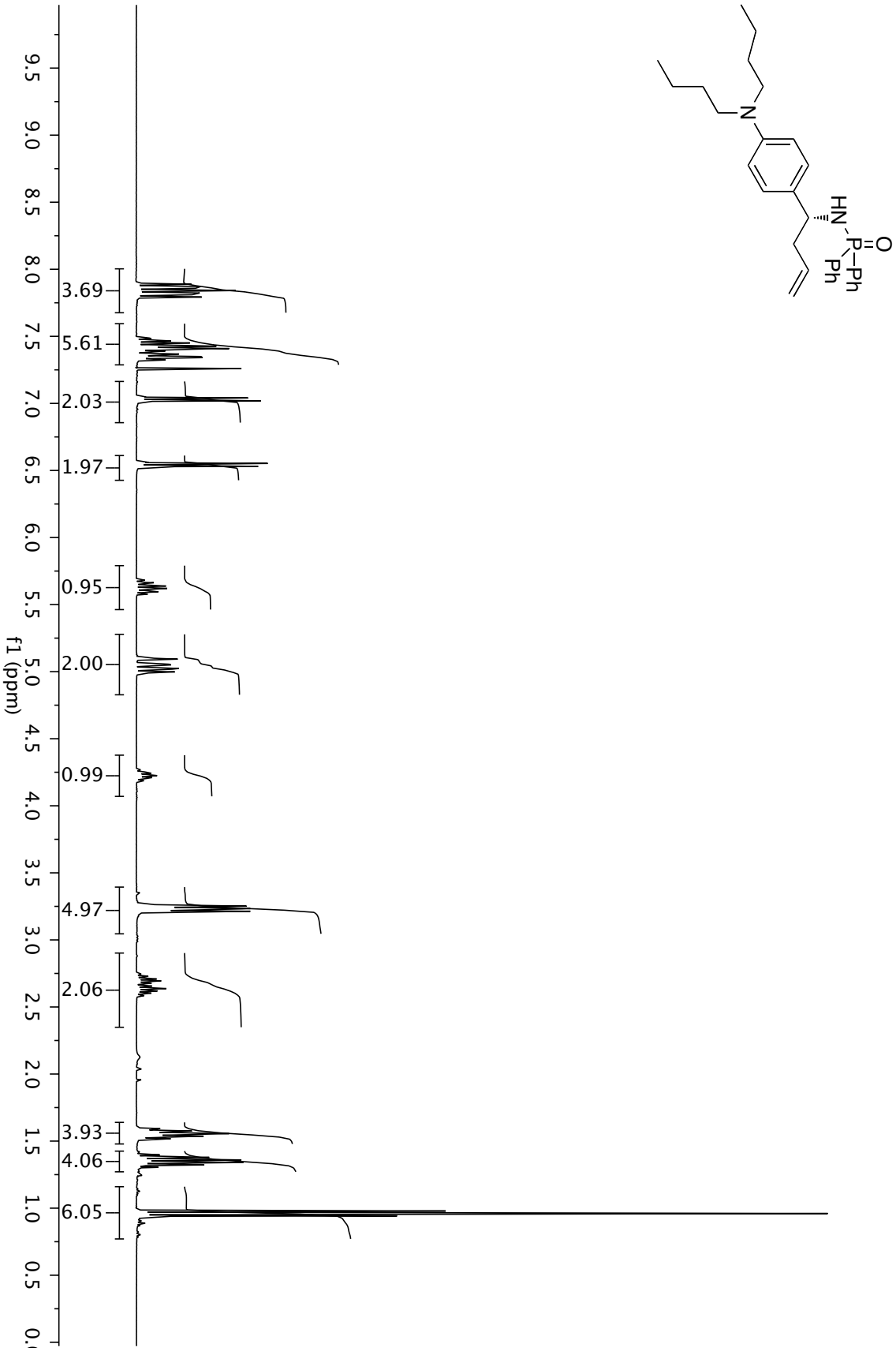
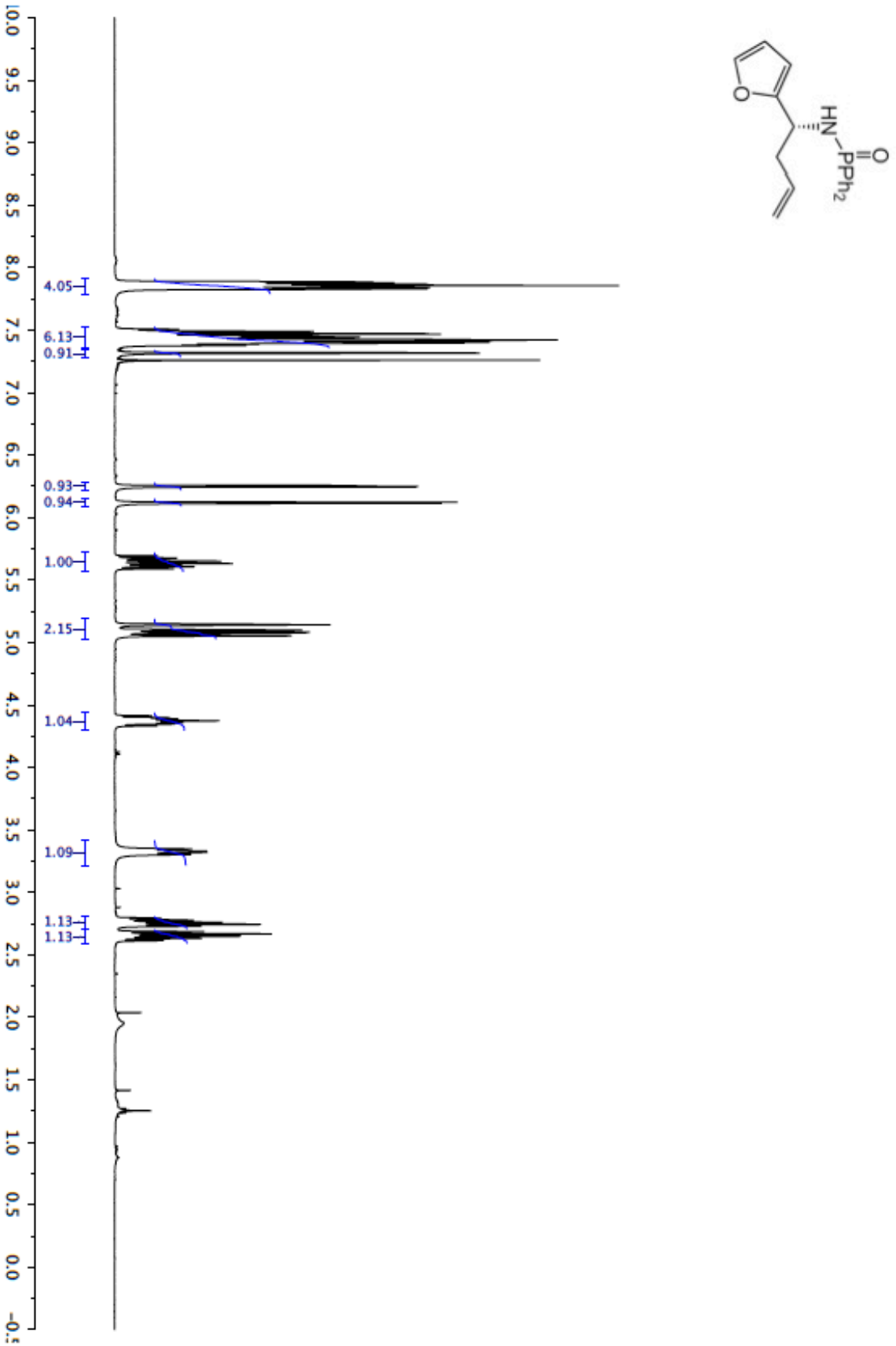
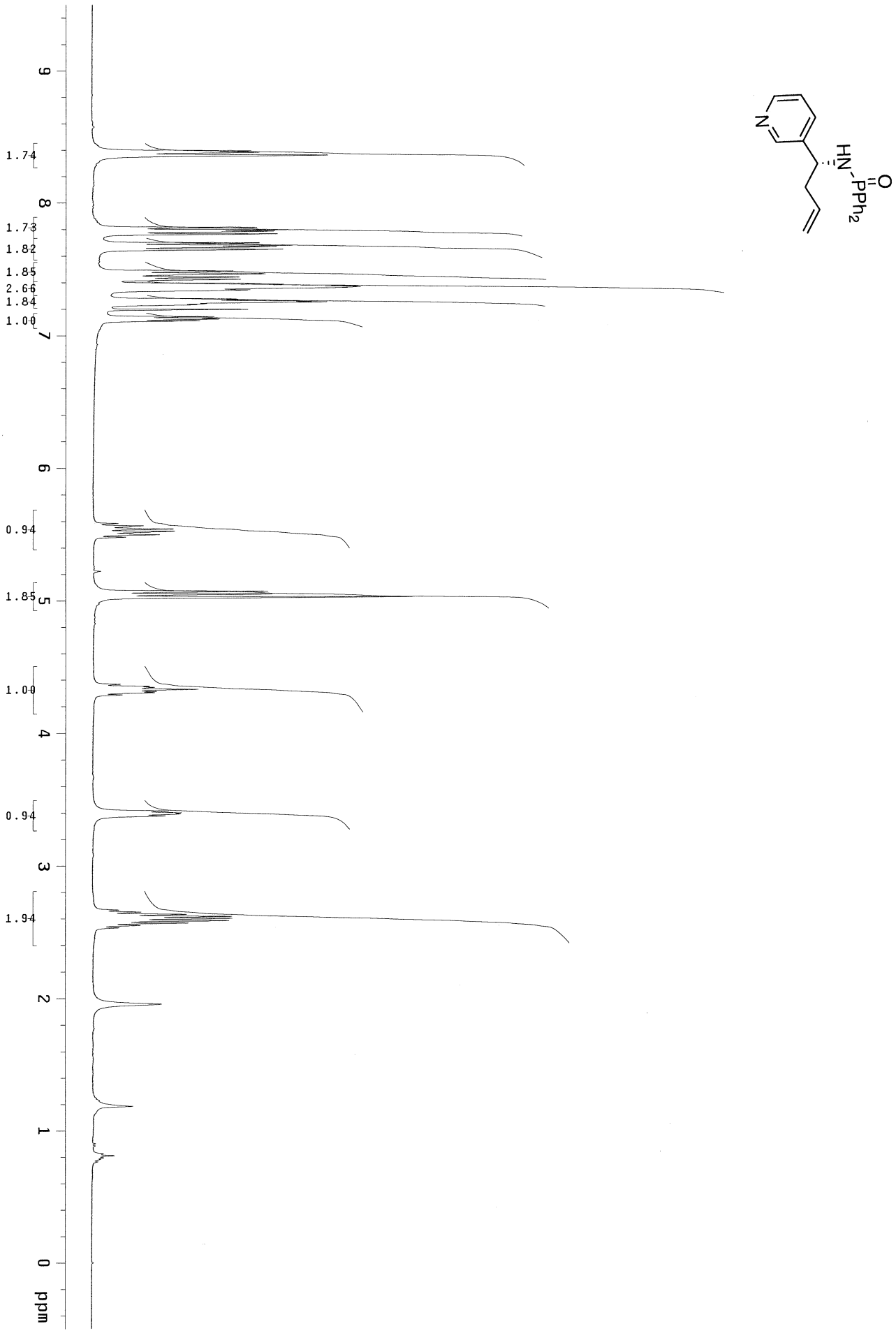
2.01

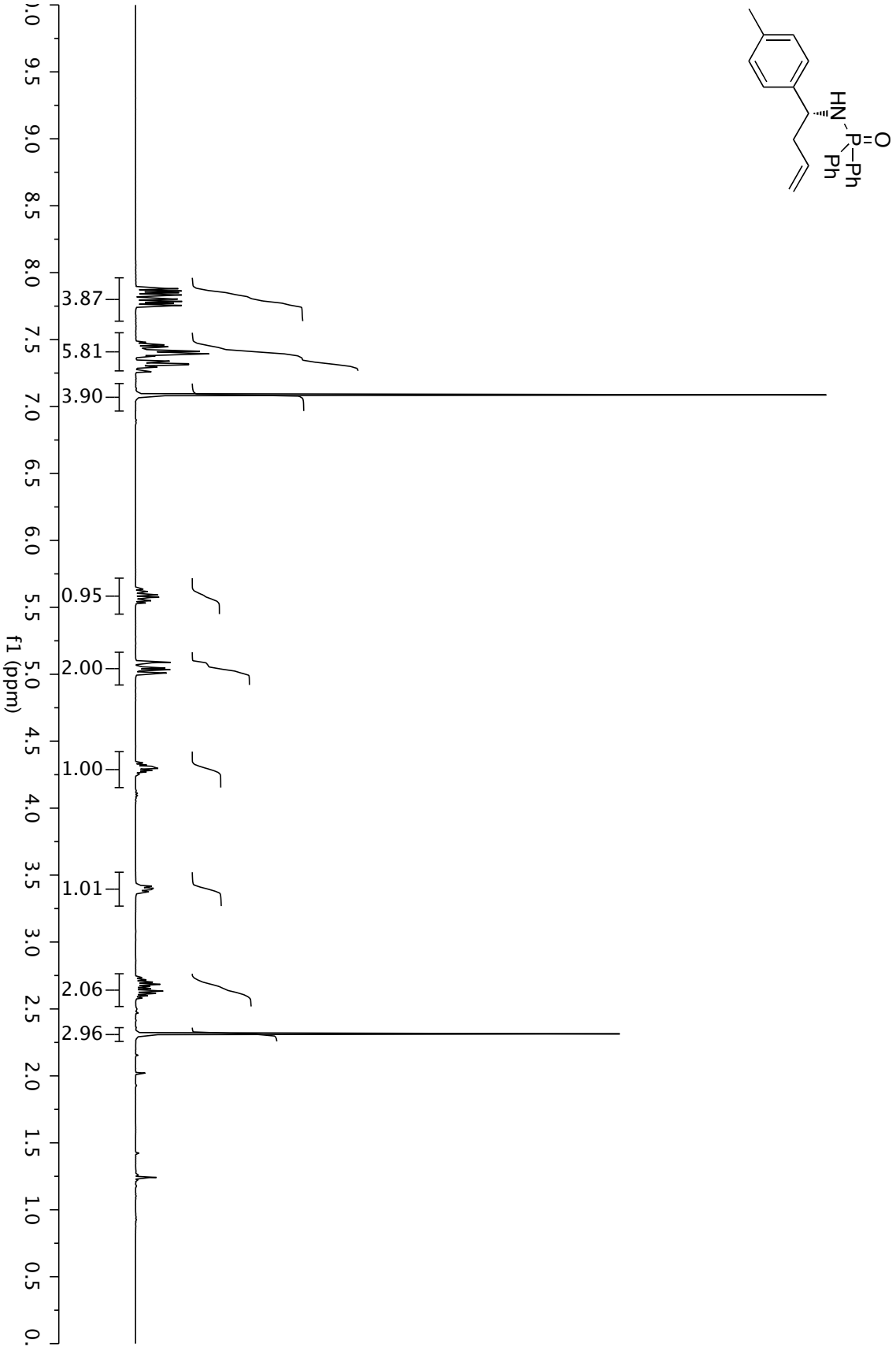

MeO2C
HN
O
P
Ph
Ph
1.87
1.89
1.90
3.77
3.98
0.97
2.03
1.01
3.00
0.98
2.05
f1 (ppm)

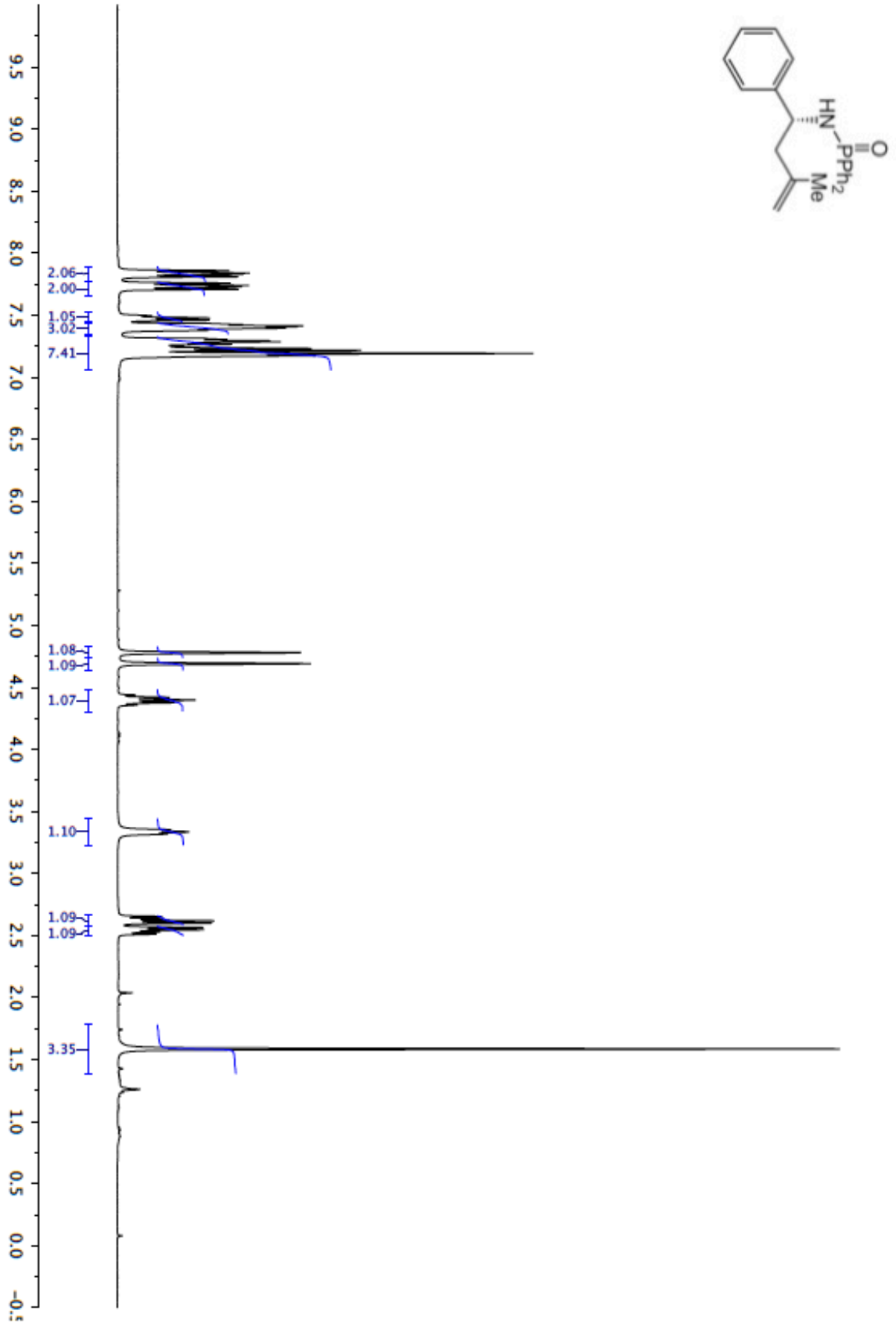

MeO
HN
O
PPh2
1.90
1.91
3.81
1.94
1.99
1.92
0.95
2.00
1.00
3.05
0.99
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

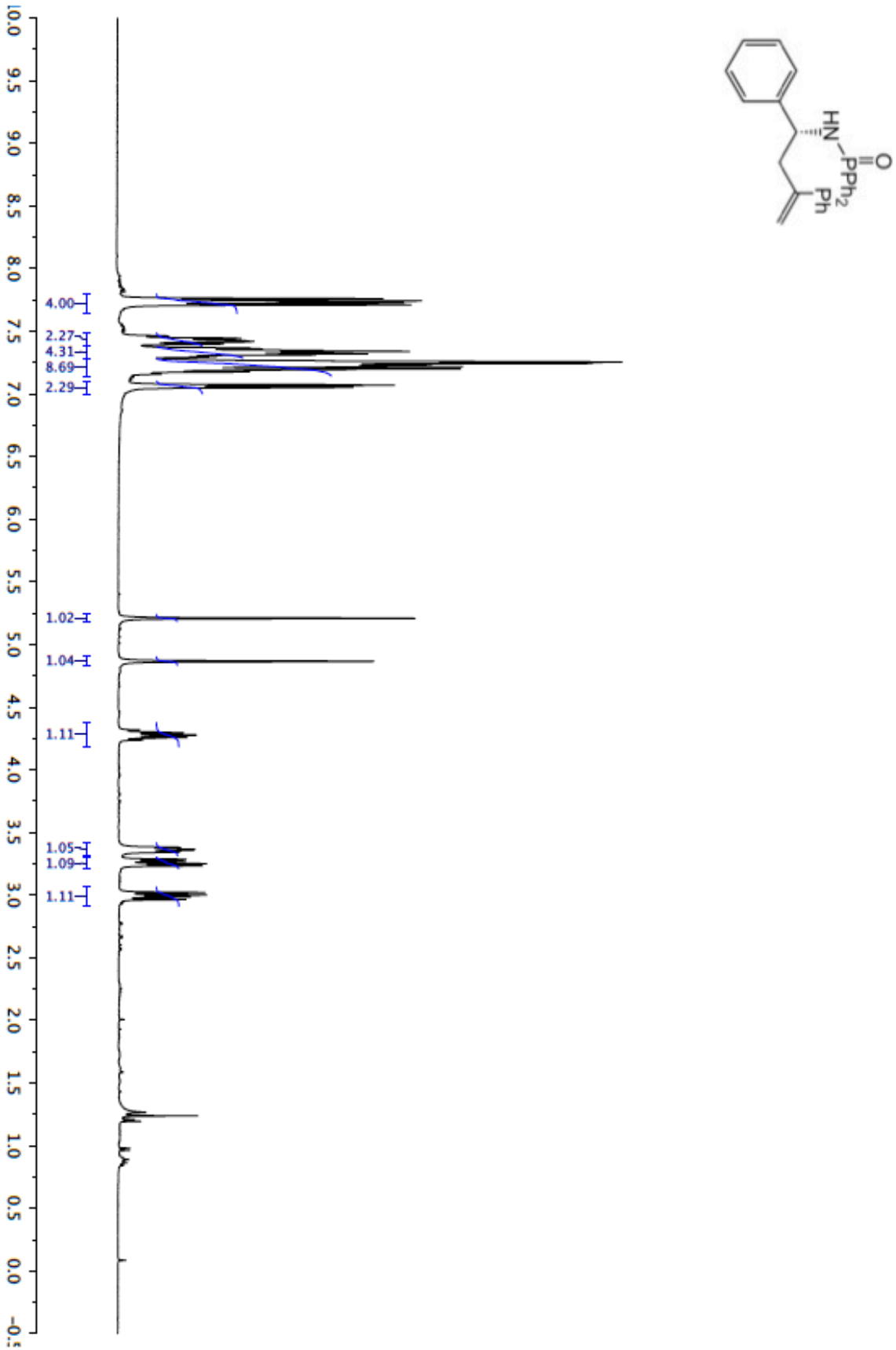

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
3.69
5.61
2.03
1.97
0.95
2.00
0.99
4.97
2.06
3.93
4.06
6.05
N
HN
P
O
Ph
Ph

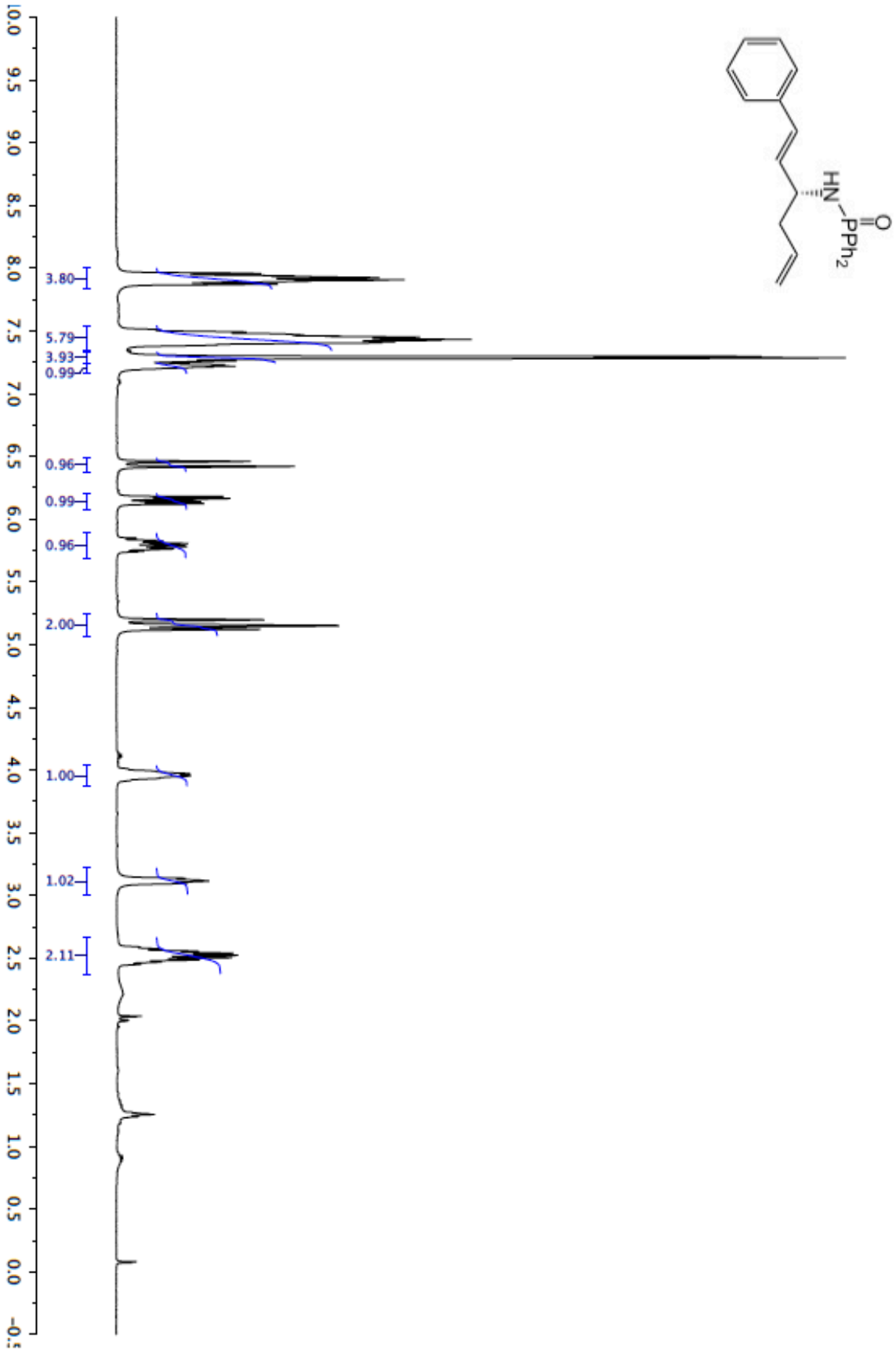

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
4.05
6.13
0.91
0.93
0.94
1.00
2.15
1.04
1.09
1.13
1.13
HN
O
PPh2

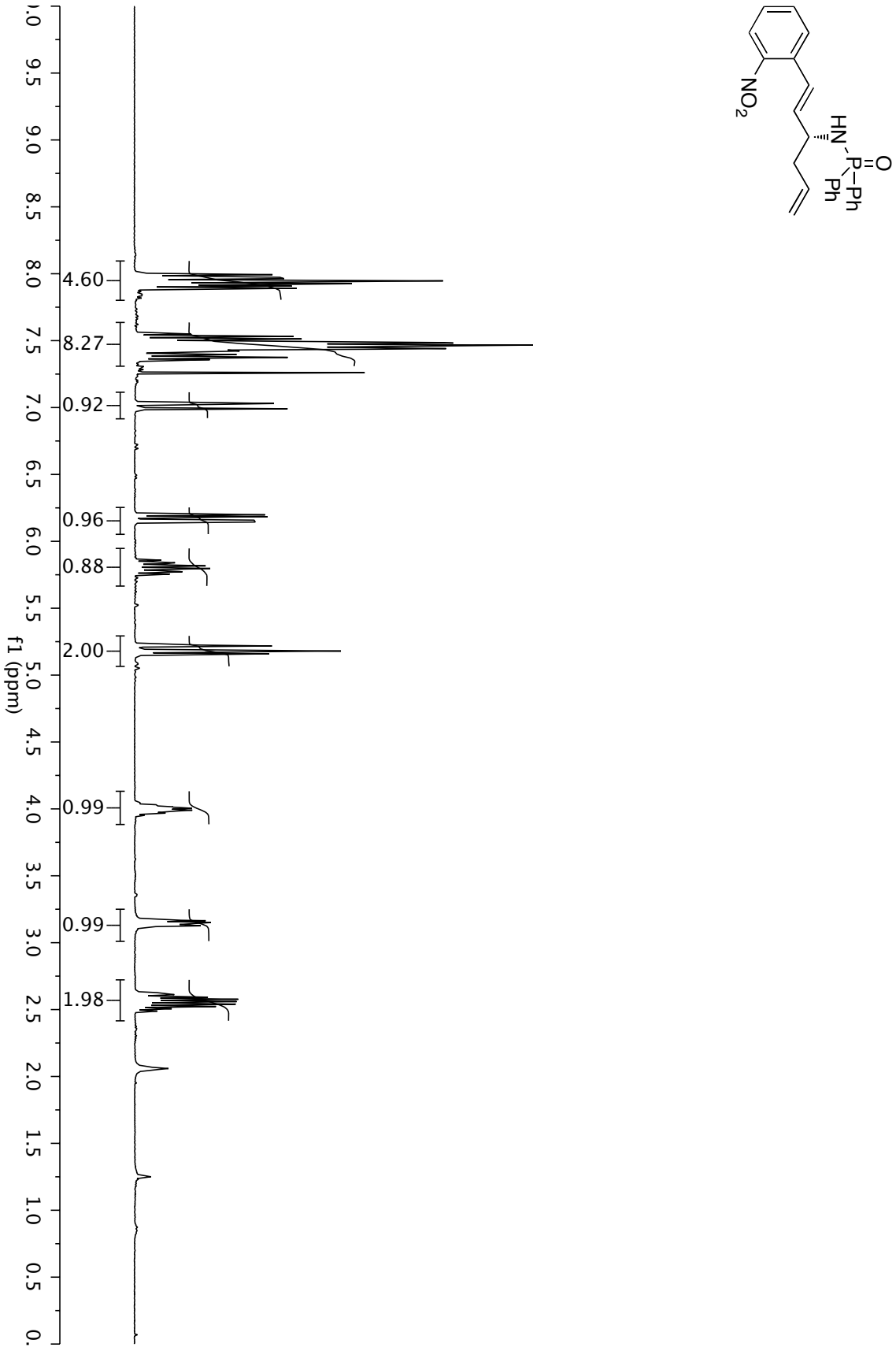

1.74
1.73
1.82
1.85
2.66
1.84
1.00
0.94
1.85
1.00
0.94
1.94
9
8
7
6
5
4
3
2
1
0
ppm
N
HN
P
O
Ph2

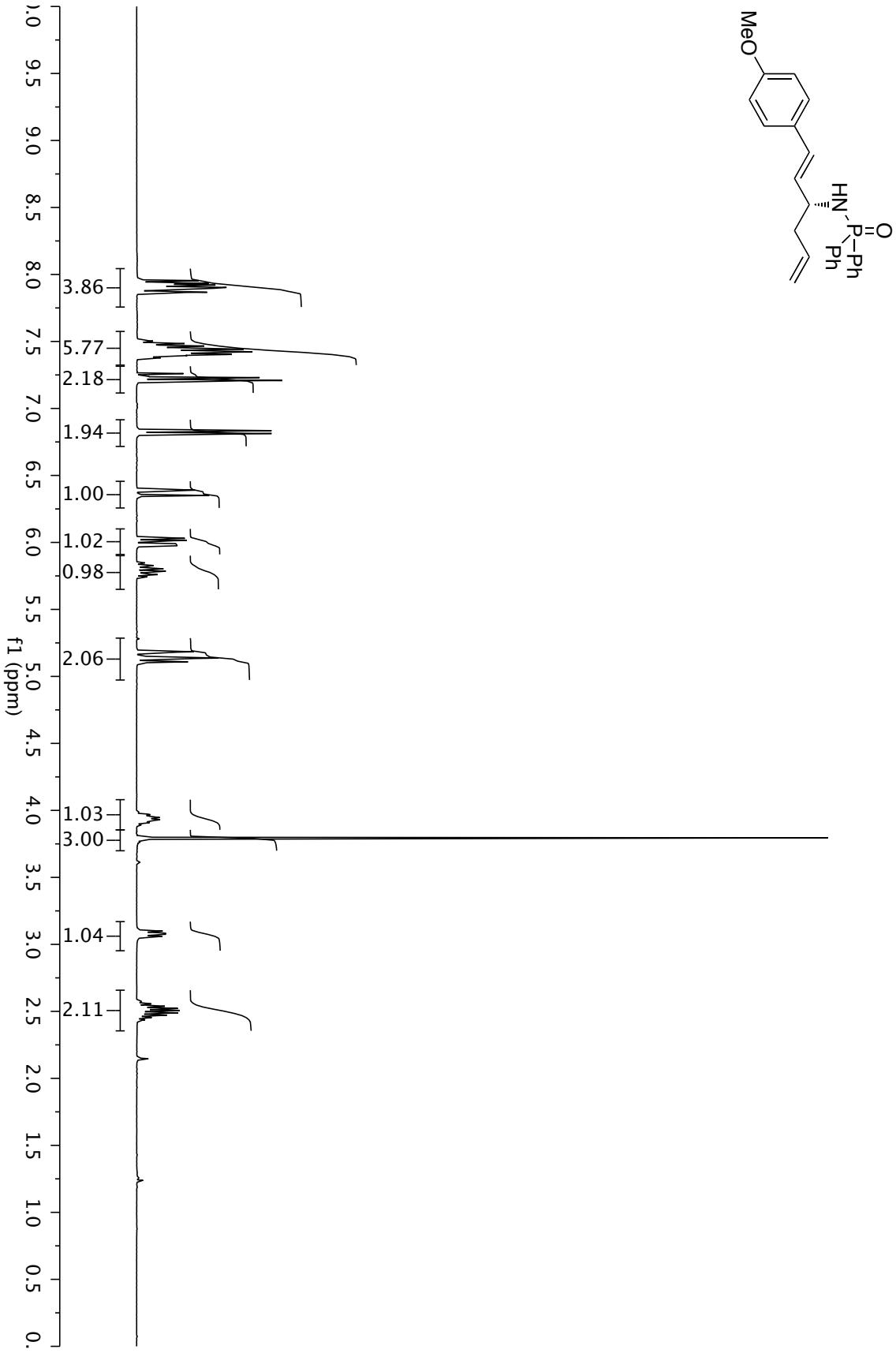

3.87
5.81
3.90
0.95
2.00
1.00
1.01
2.06
2.96
f1 (ppm)
HN
O
P
Ph
Ph

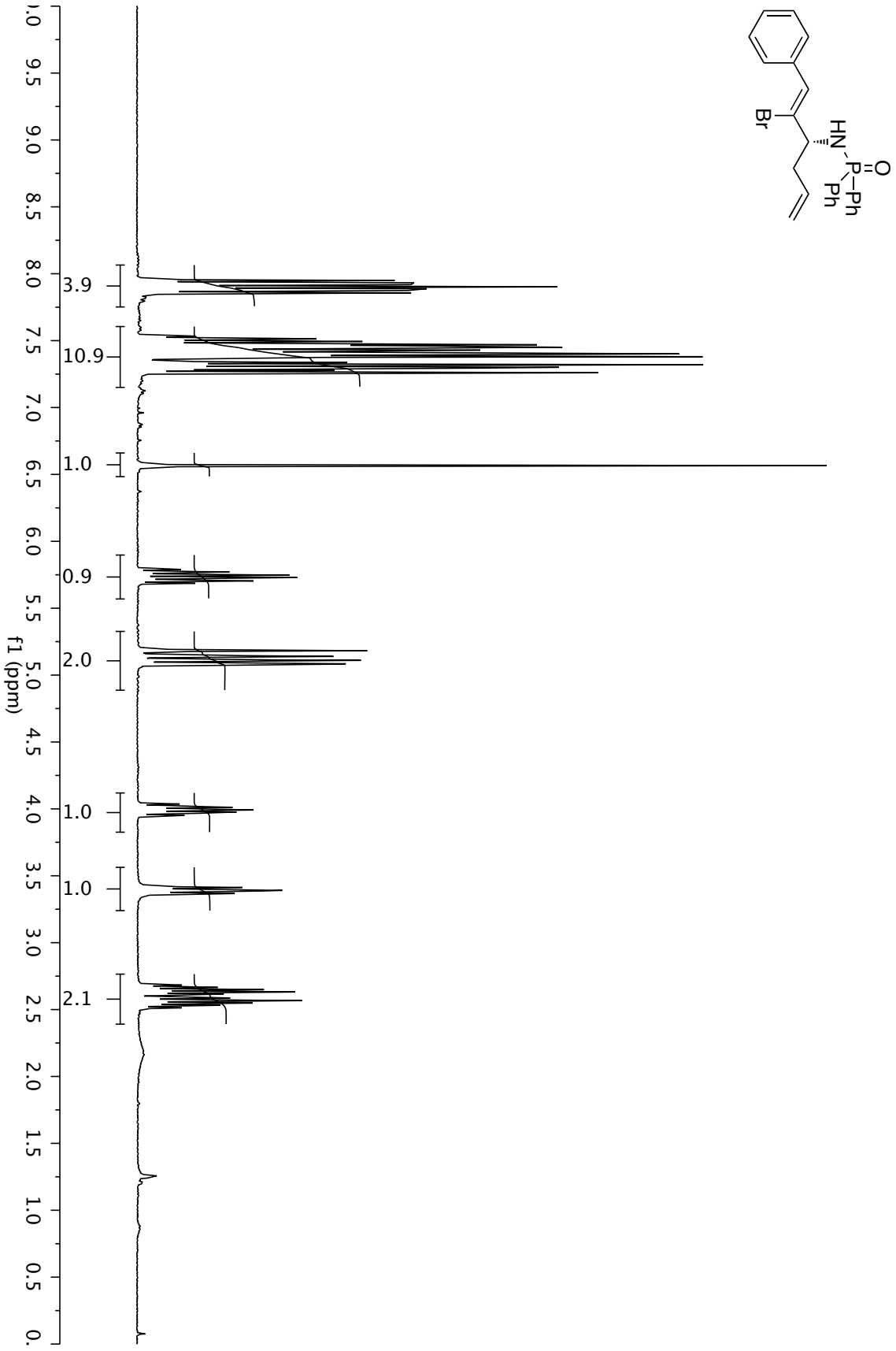

HN
O
PPh2
Me
2.06
2.00
1.05
3.02
7.41
1.08
1.09
1.07
1.10
1.09
1.09
3.35
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

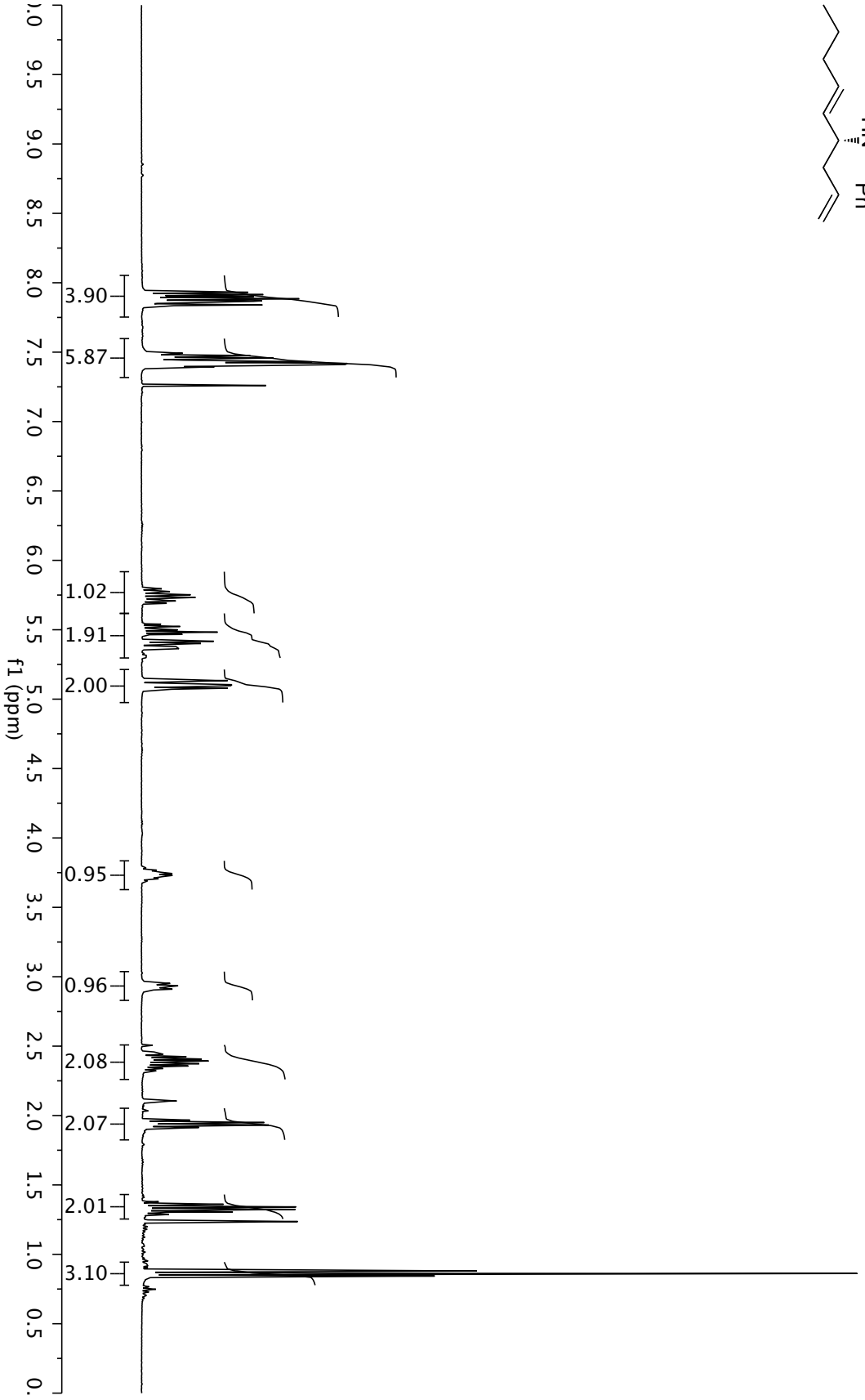

HN
O
PPh2
Ph
4.00
2.27
4.31
8.69
2.29
1.02
1.04
1.11
1.05
1.09
1.11

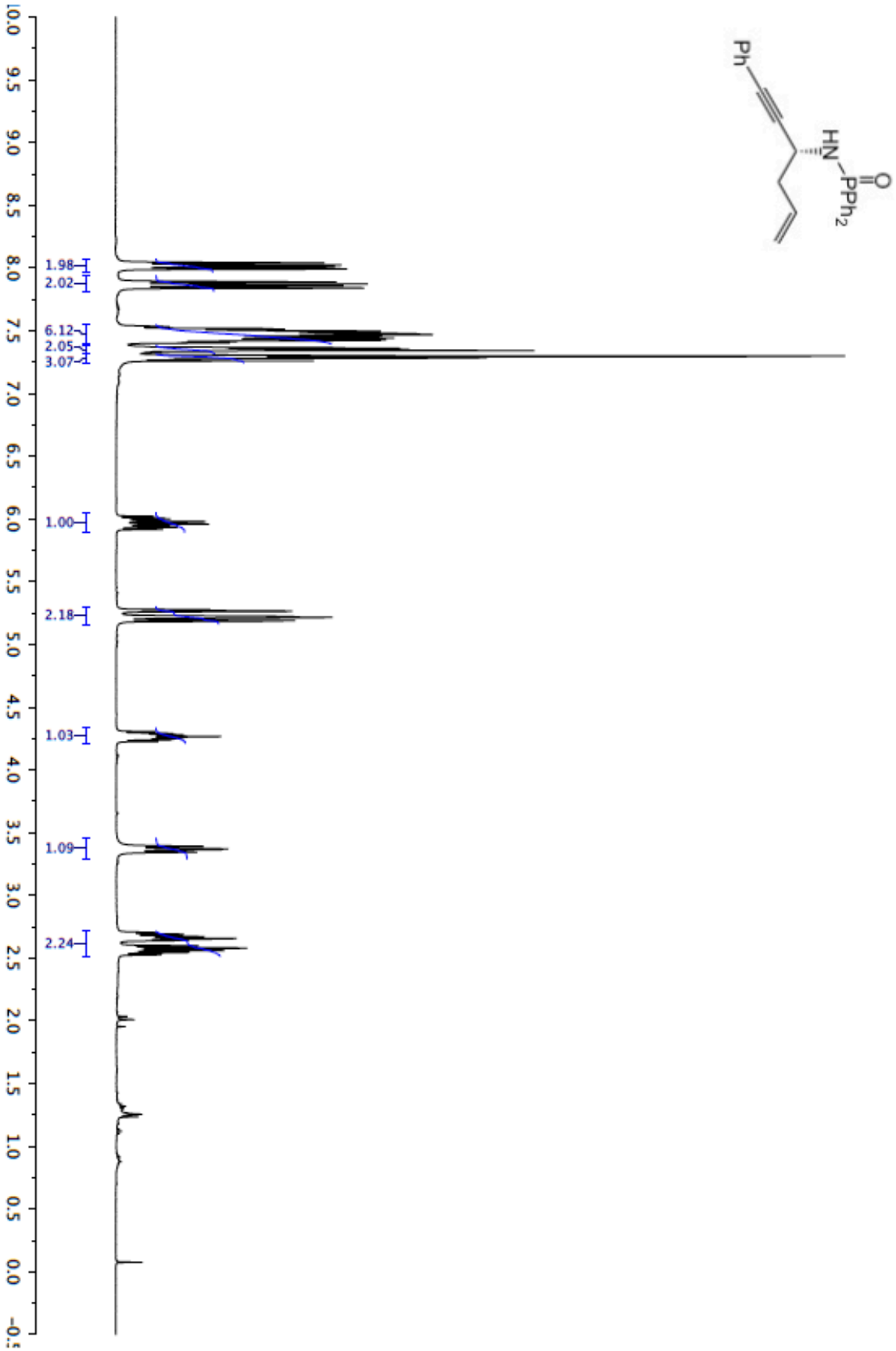

3.80
5.79
3.93
0.99
0.96
0.99
0.96
2.00
1.00
1.02
2.11
HN
O
PPh2

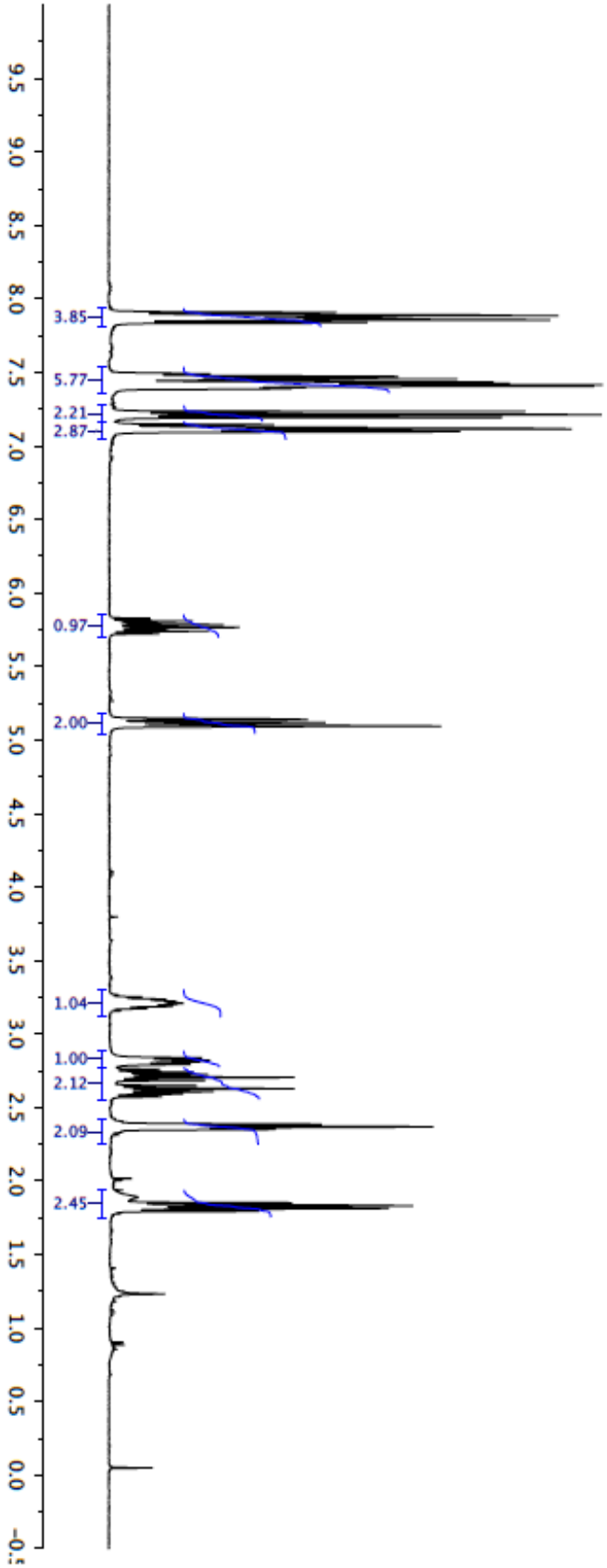

4.60
8.27
0.92
0.96
0.88
2.00
0.99
0.99
1.98
f1 (ppm)
NO2
HN
O
P
Ph
Ph

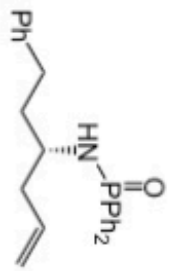

MeO
HN
O
P
Ph
Ph
3.86
5.77
2.18
1.94
1.00
1.02
0.98
2.06
1.03
3.00
1.04
2.11
f1 (ppm)

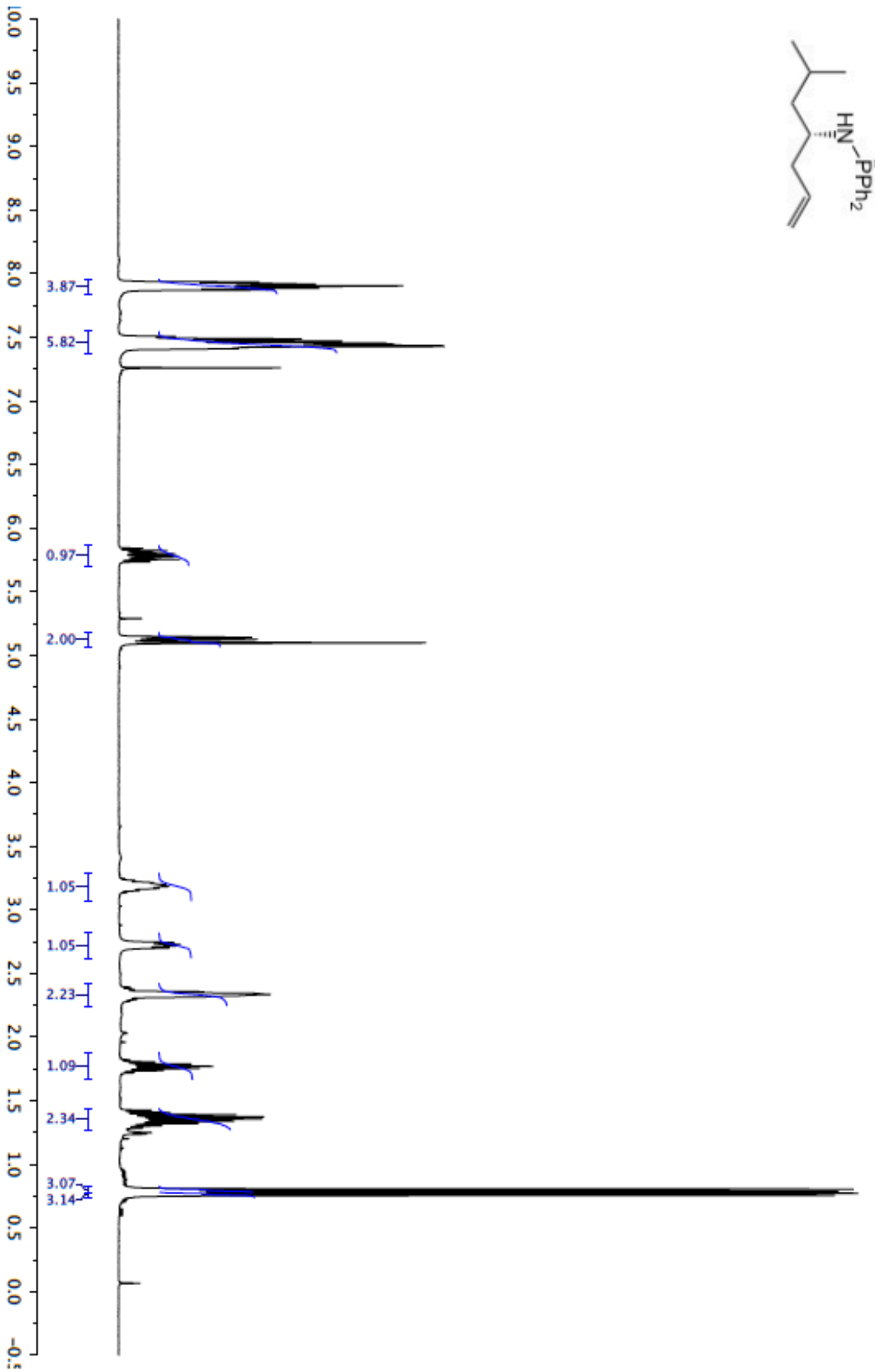

Br
HN
O
P
Ph
Ph
3.9
10.9
1.0
0.9
2.0
1.0
1.0
2.1
f1 (ppm)

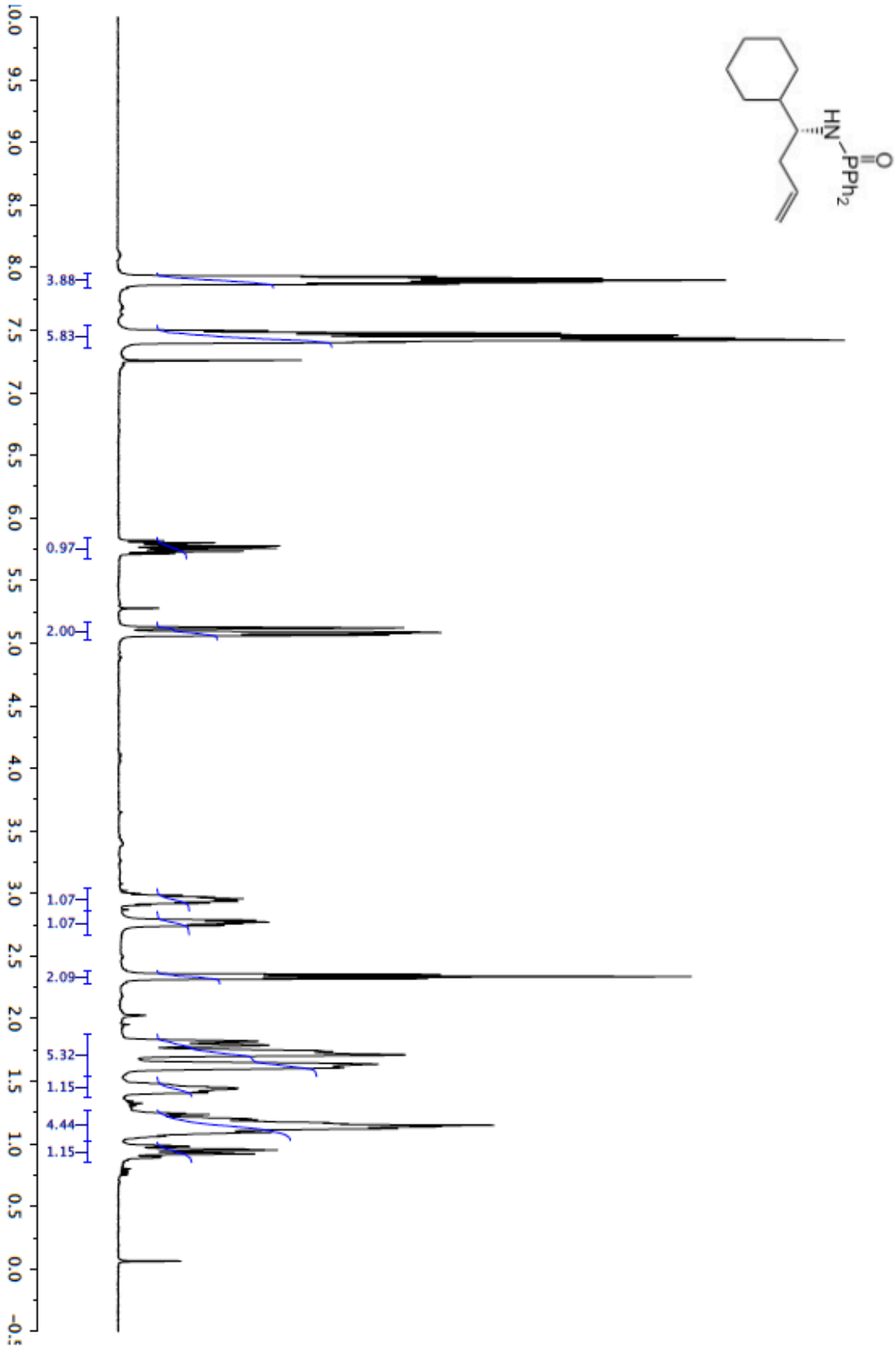

HN
P
O
Ph
Ph
3.90
5.87
1.02
1.91
2.00
0.95
0.96
2.08
2.07
2.01
3.10
f1 (ppm)

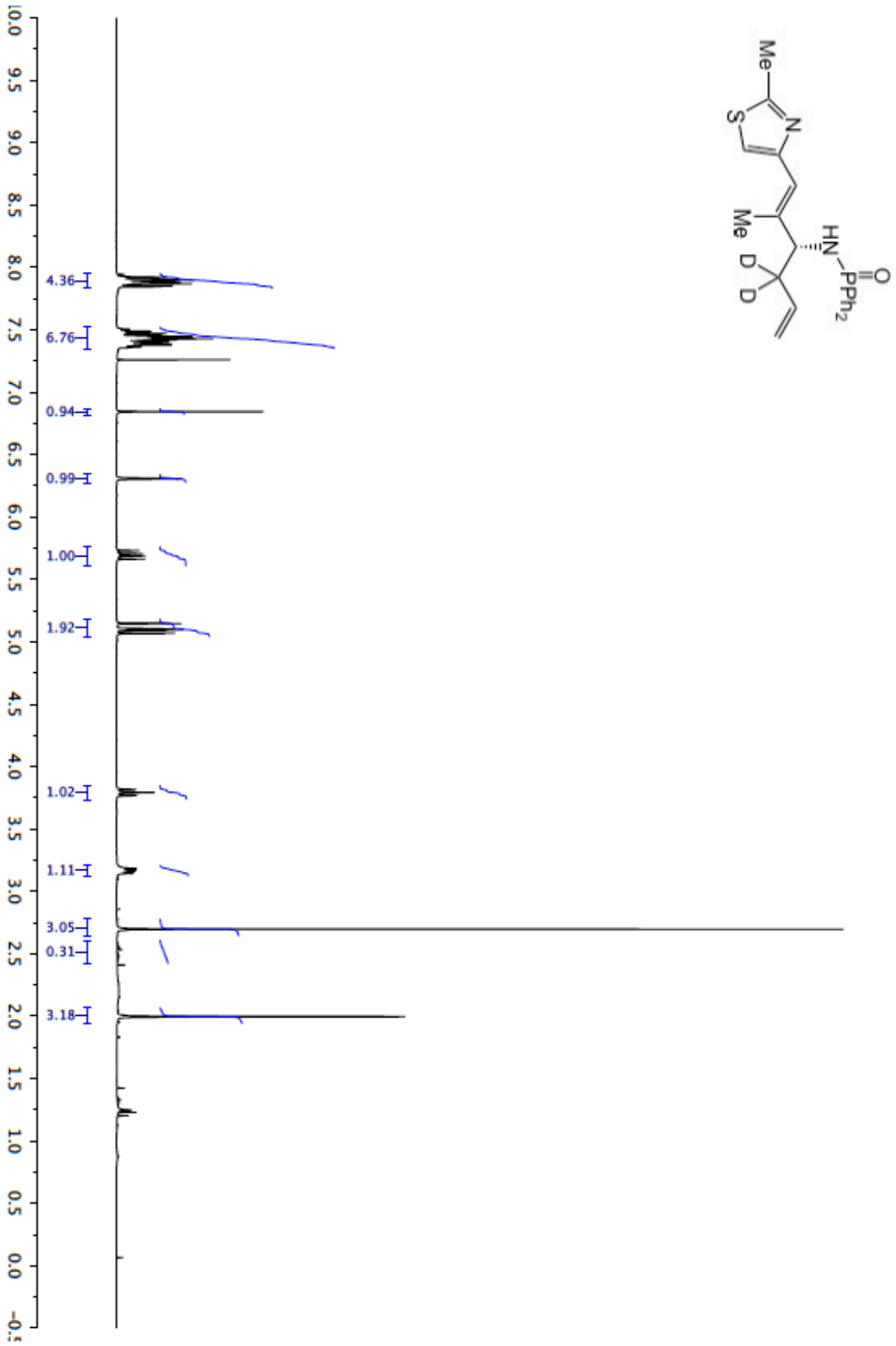

Ph
HN
O
PPh2
1.98
2.02
6.12
2.05
3.07
1.00
2.18
1.03
1.09
2.24
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

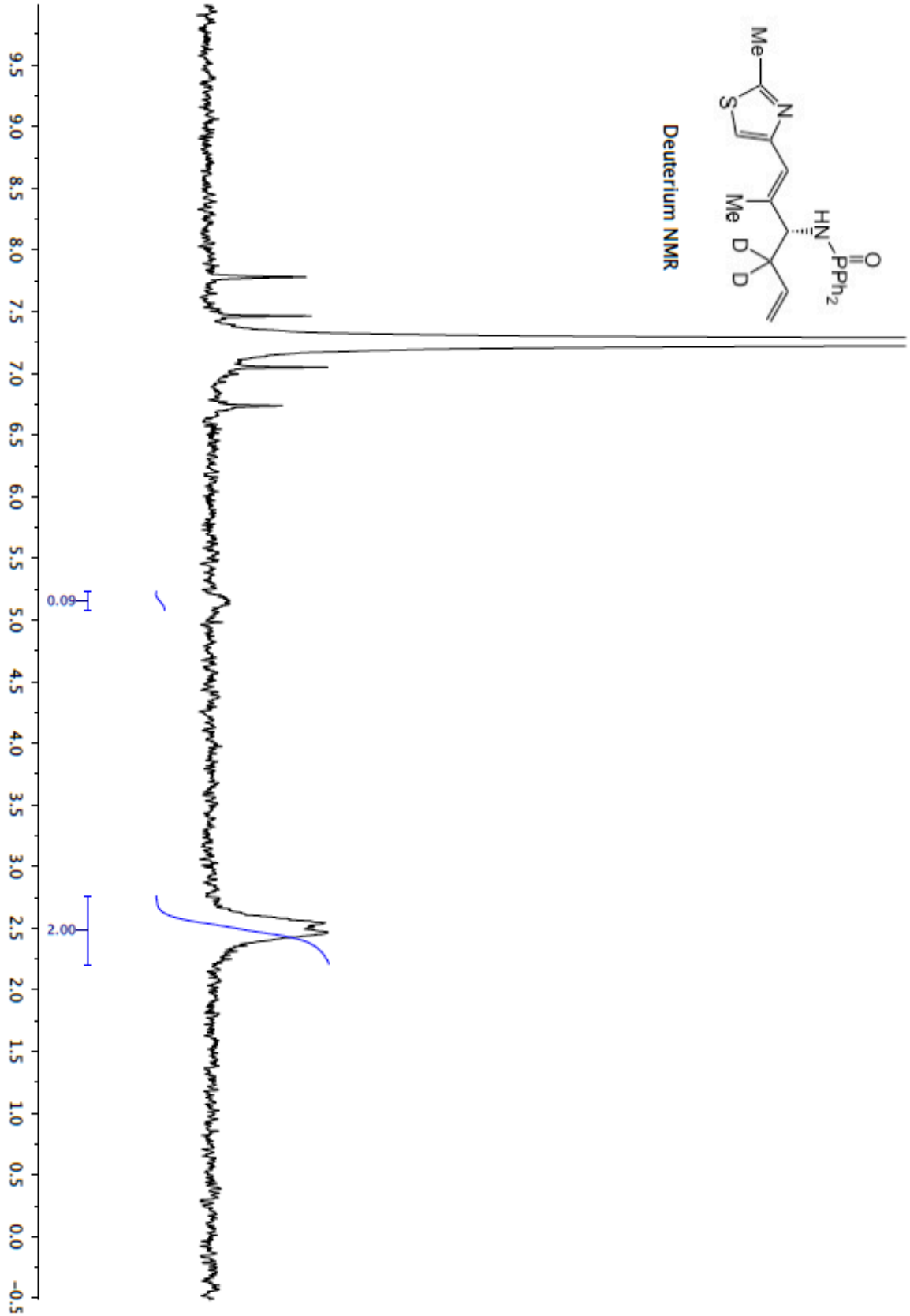

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
3.85
5.77
2.21
2.87
0.97
2.00
1.04
1.00
2.12
2.09
2.45

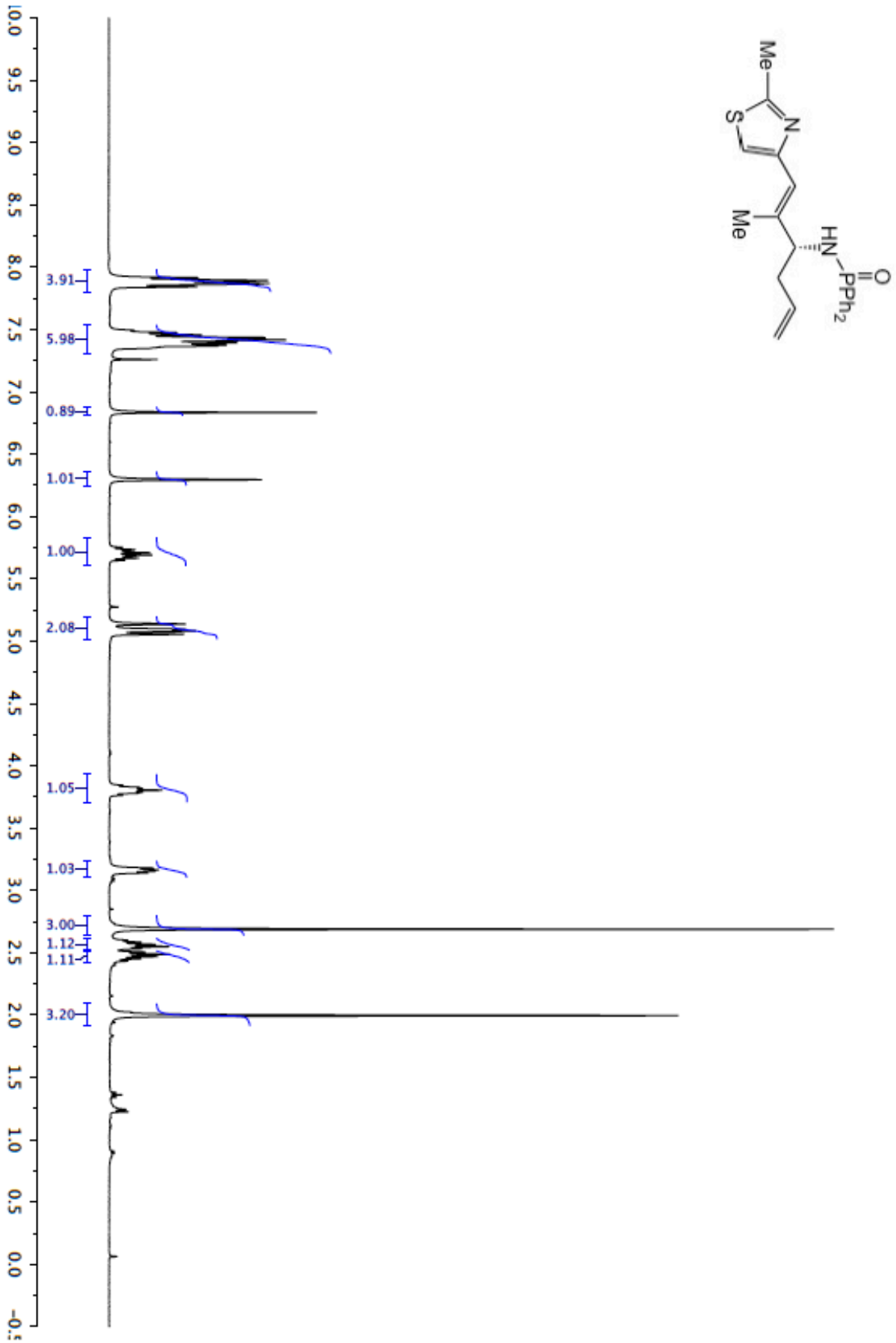

Ph
HN
O
PPh2

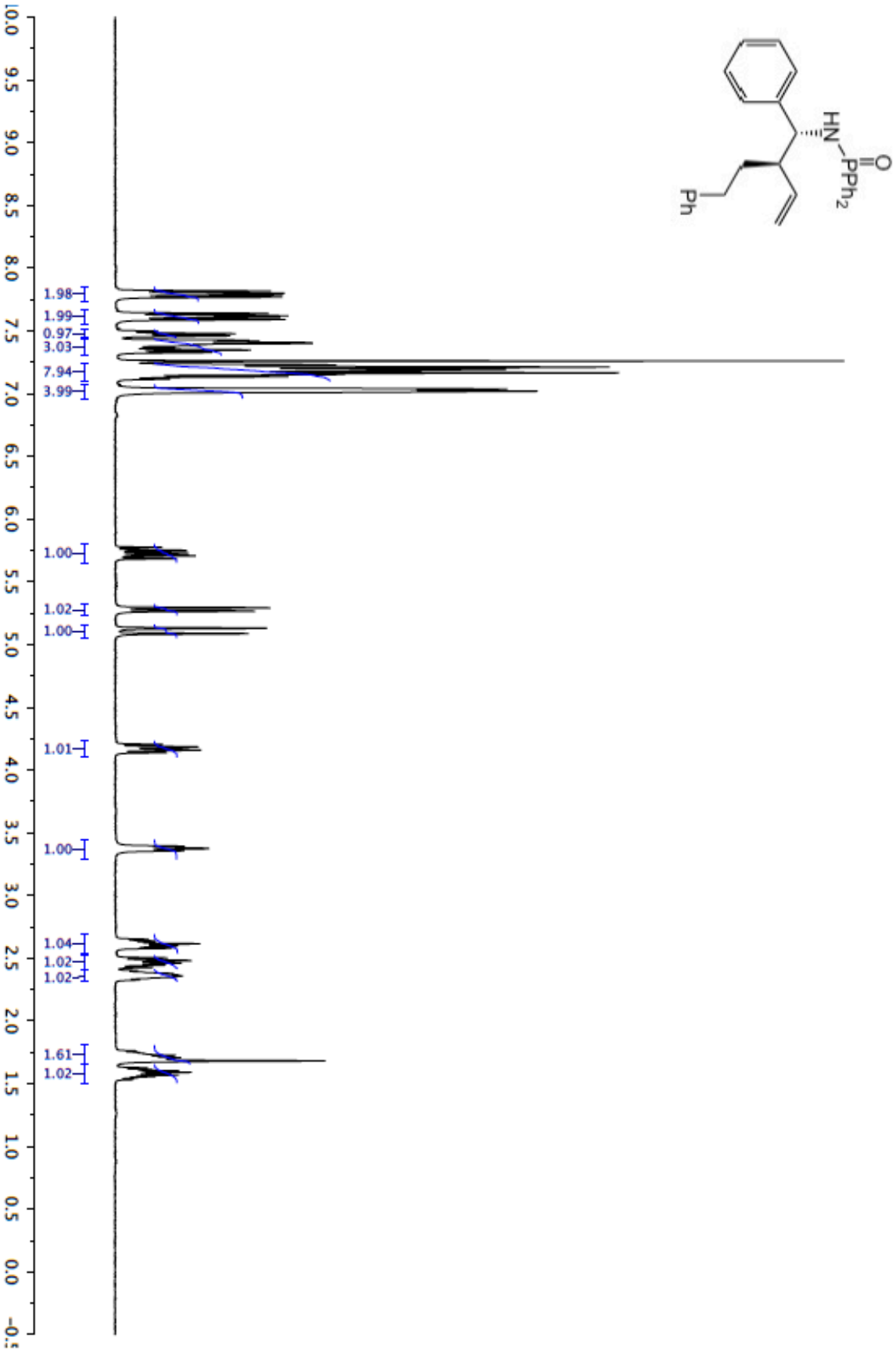

HN
O
PPh2
3.87
5.82
0.97
2.00
1.05
1.05
2.23
1.09
2.34
3.07
3.14

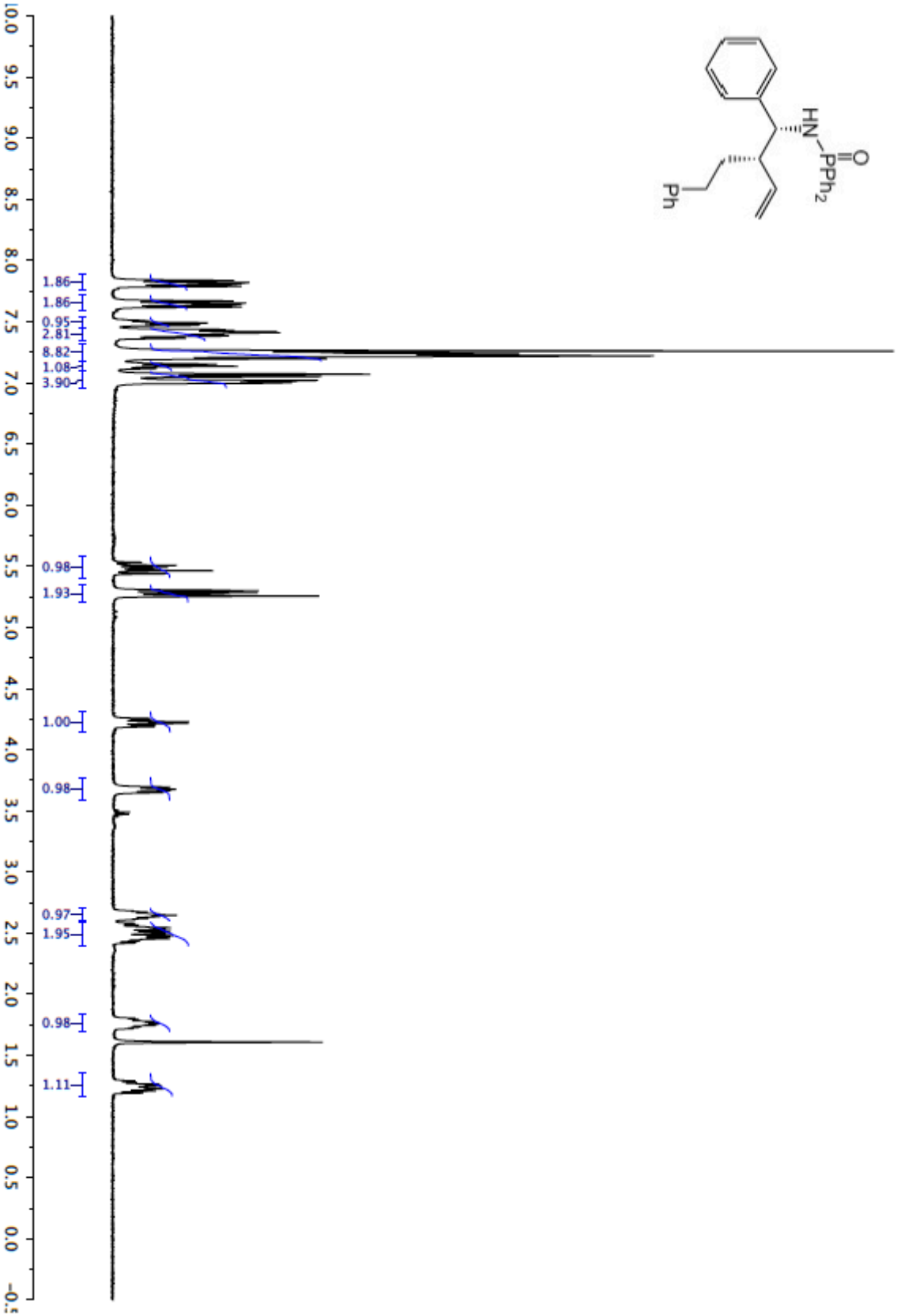

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3.88
5.83
0.97
2.00
1.07
1.07
2.09
5.32
1.15
4.44
1.15
HN
O
PPh2

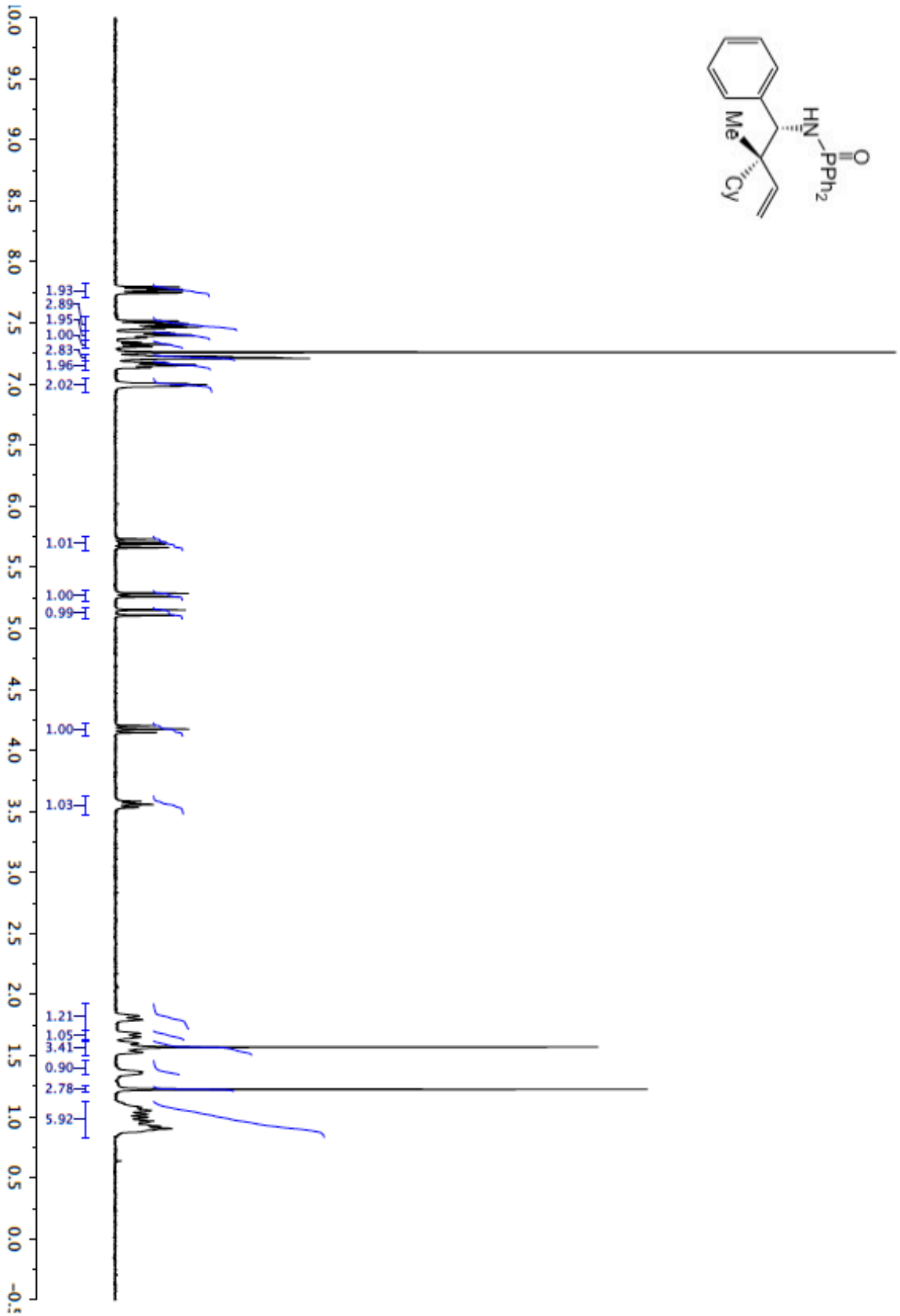

Me
S
N
Me
D
D
HN
O
PPh2
4.36
6.76
0.94
0.99
1.00
1.92
1.02
1.11
3.05
0.31
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

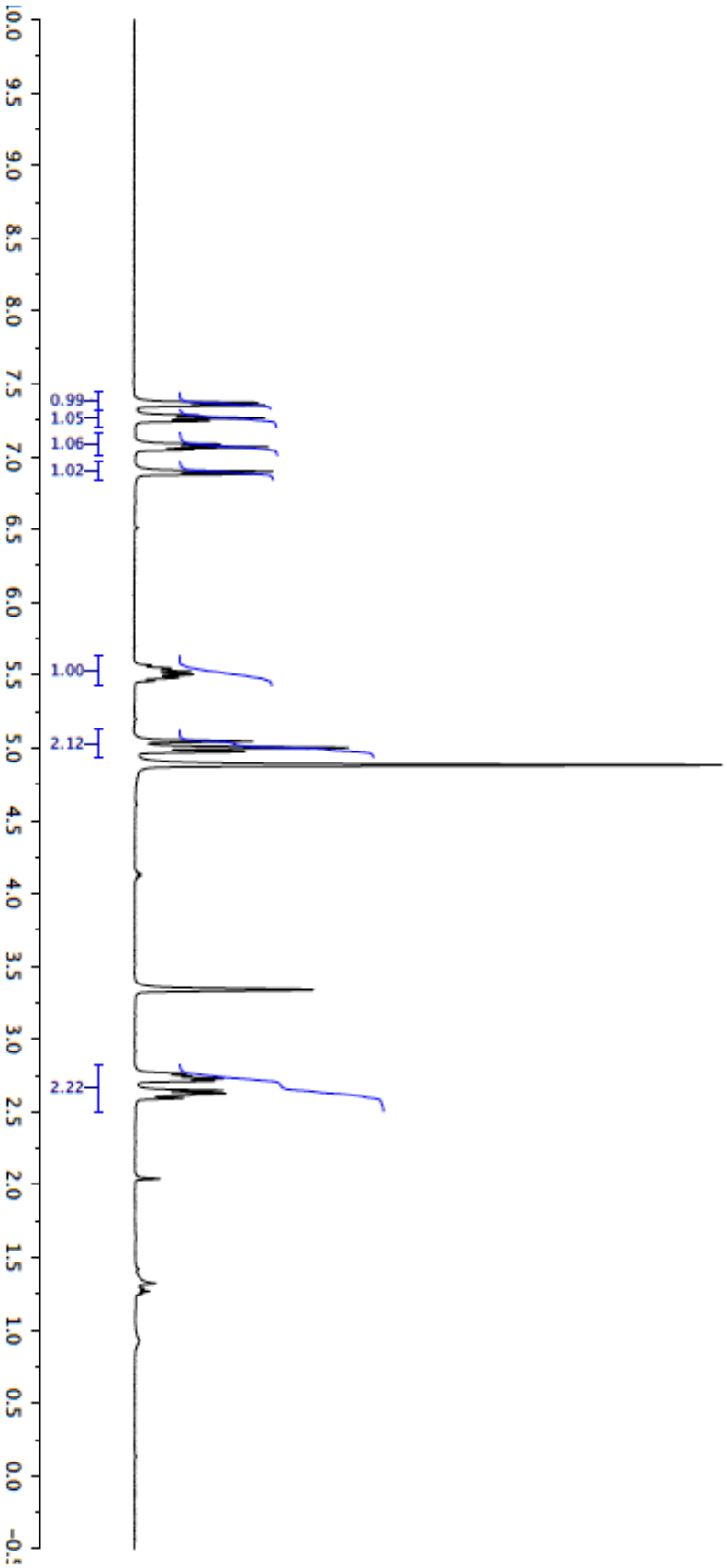

Deuterium NMR
Me
N
S
Me
D
D
HN
O
PPh2
0.09
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

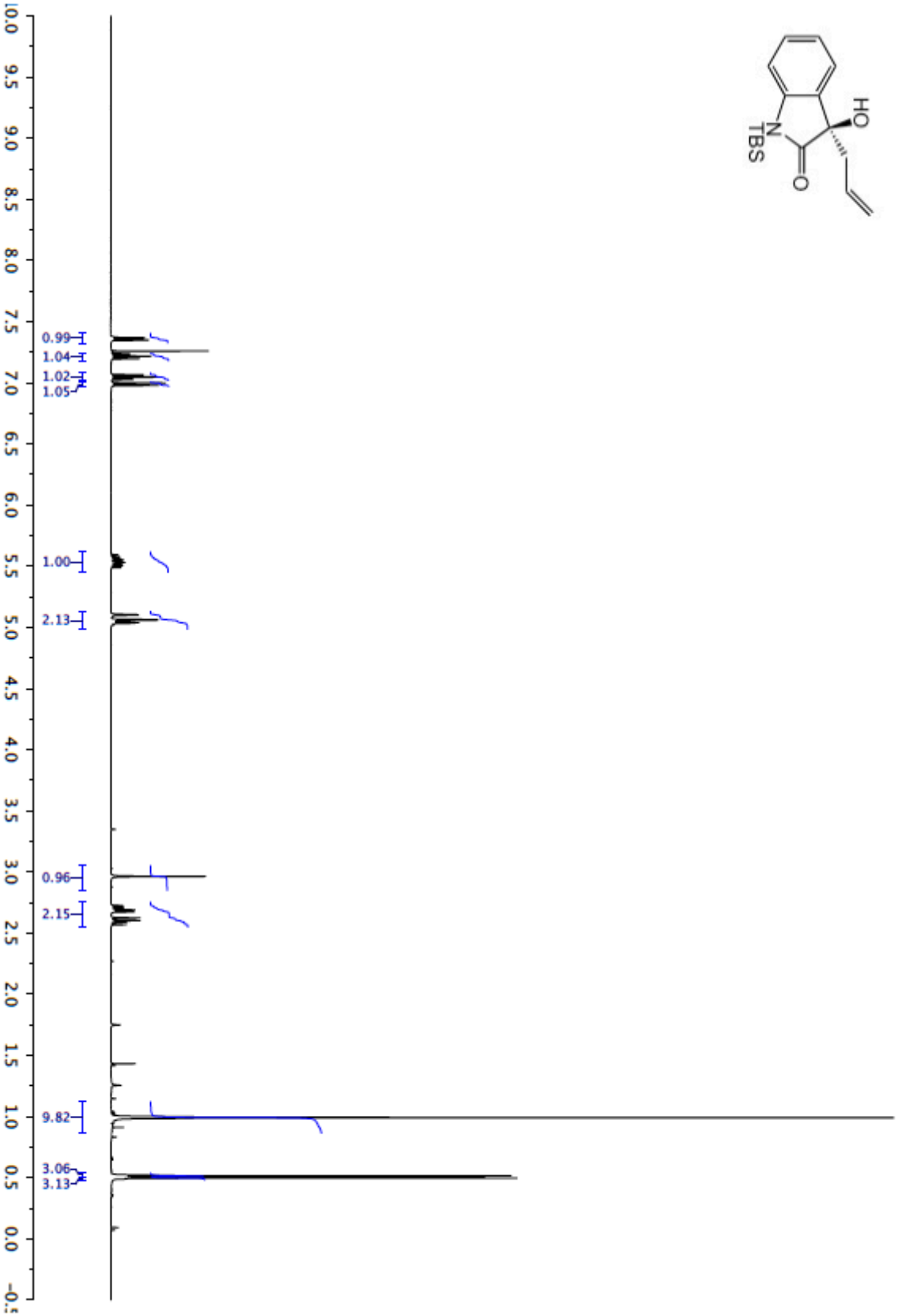

Me
S
N
Me
HN
O
PPh2
3.91
5.98
0.89
1.01
1.00
2.08
1.05
1.03
3.00
1.12
1.11
3.20

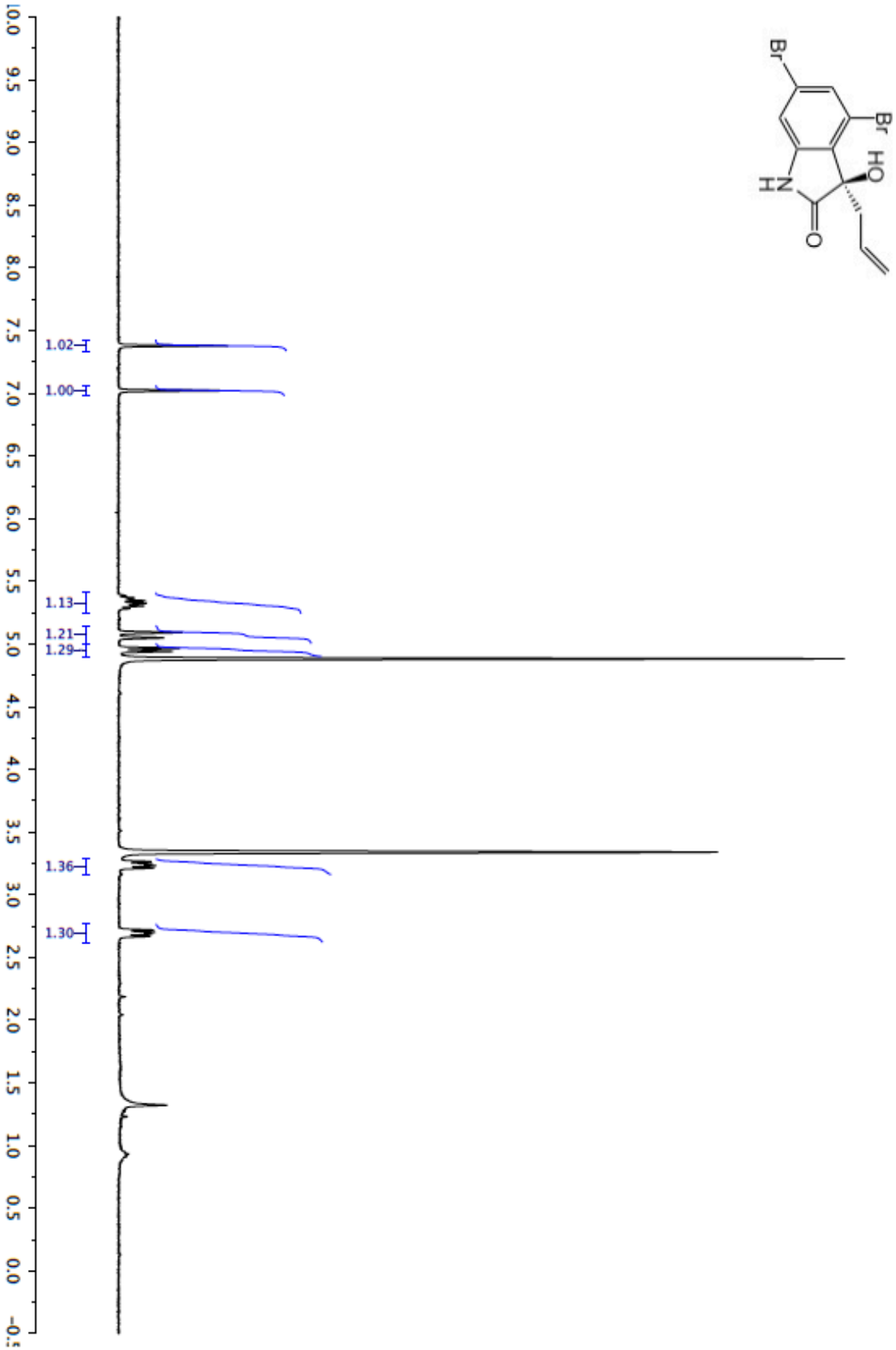

HN
O
PPh2
Ph
1.98
1.99
0.97
3.03
7.94
3.99
1.00
1.02
1.00
1.01
1.00
1.04
1.02
1.02
1.61
1.02

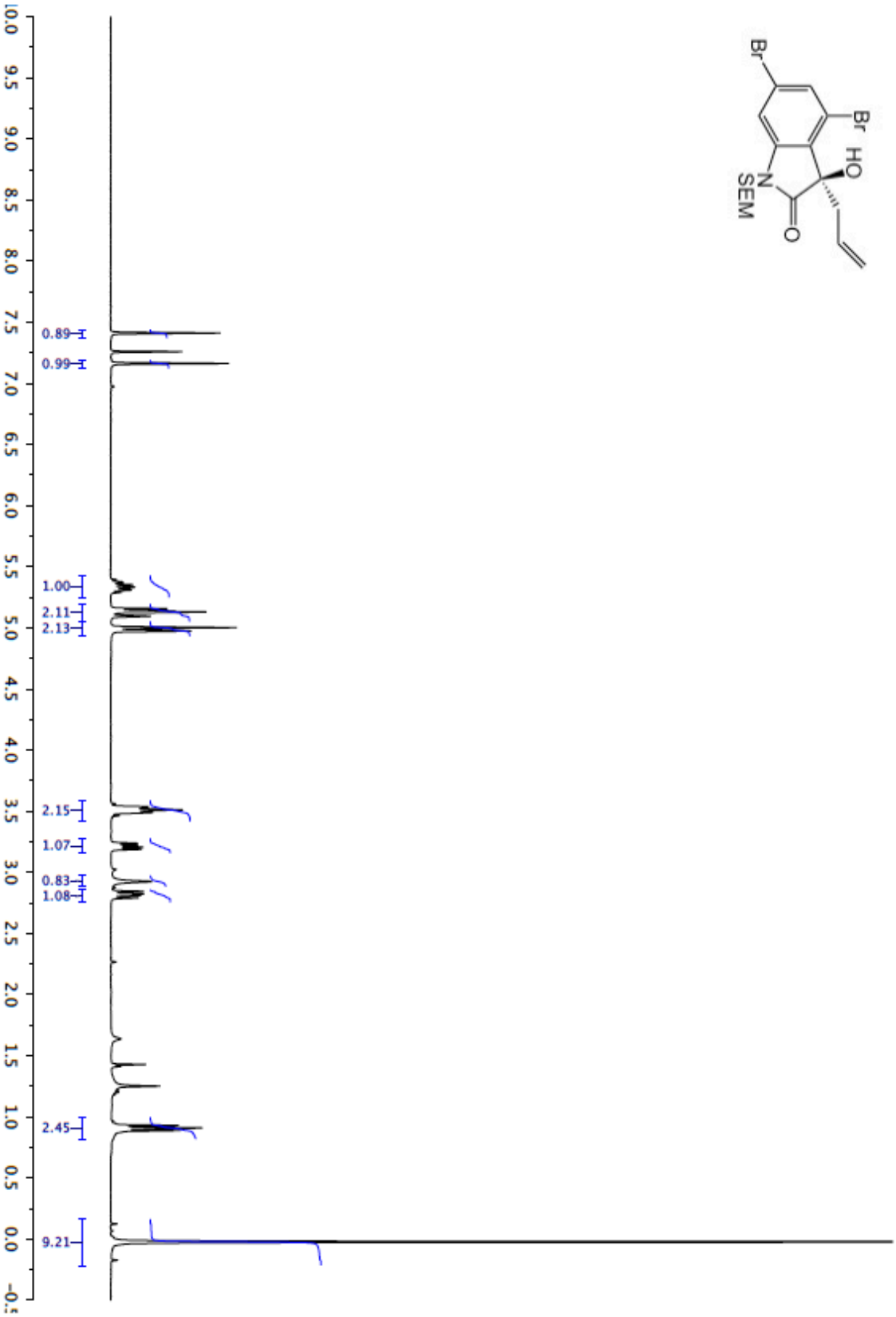

HN
O
PPh2
Ph
1.86
1.86
0.95
2.81
8.82
1.08
3.90
0.98
1.93
1.00
0.98
0.97
1.95
0.98
1.11

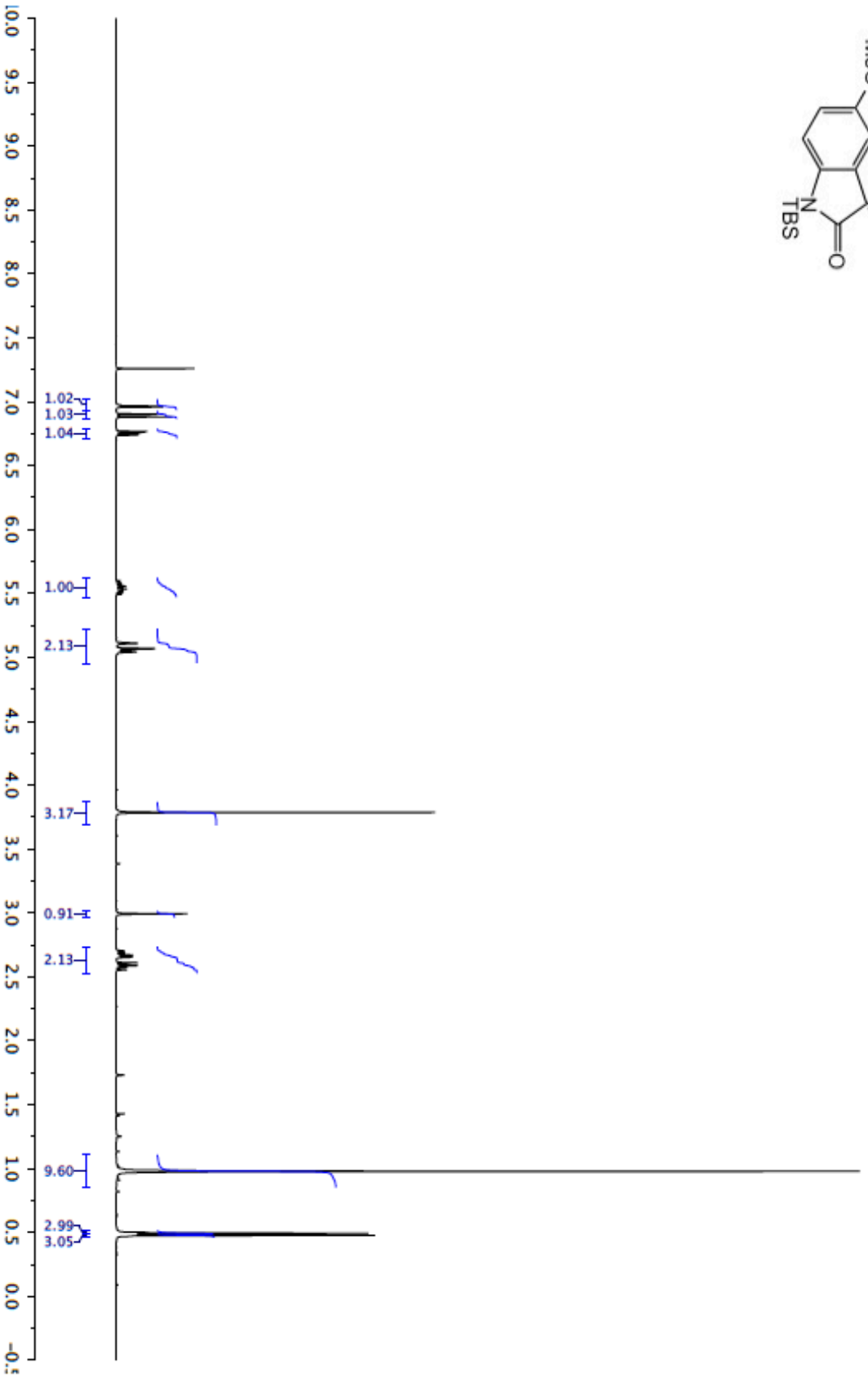

Me
Cy
HN
O
PPh2
1.93
2.89
1.95
1.00
2.83
1.96
2.02
1.01
1.00
0.99
1.00
1.03
1.21
1.05
3.41
0.90
2.78
5.92

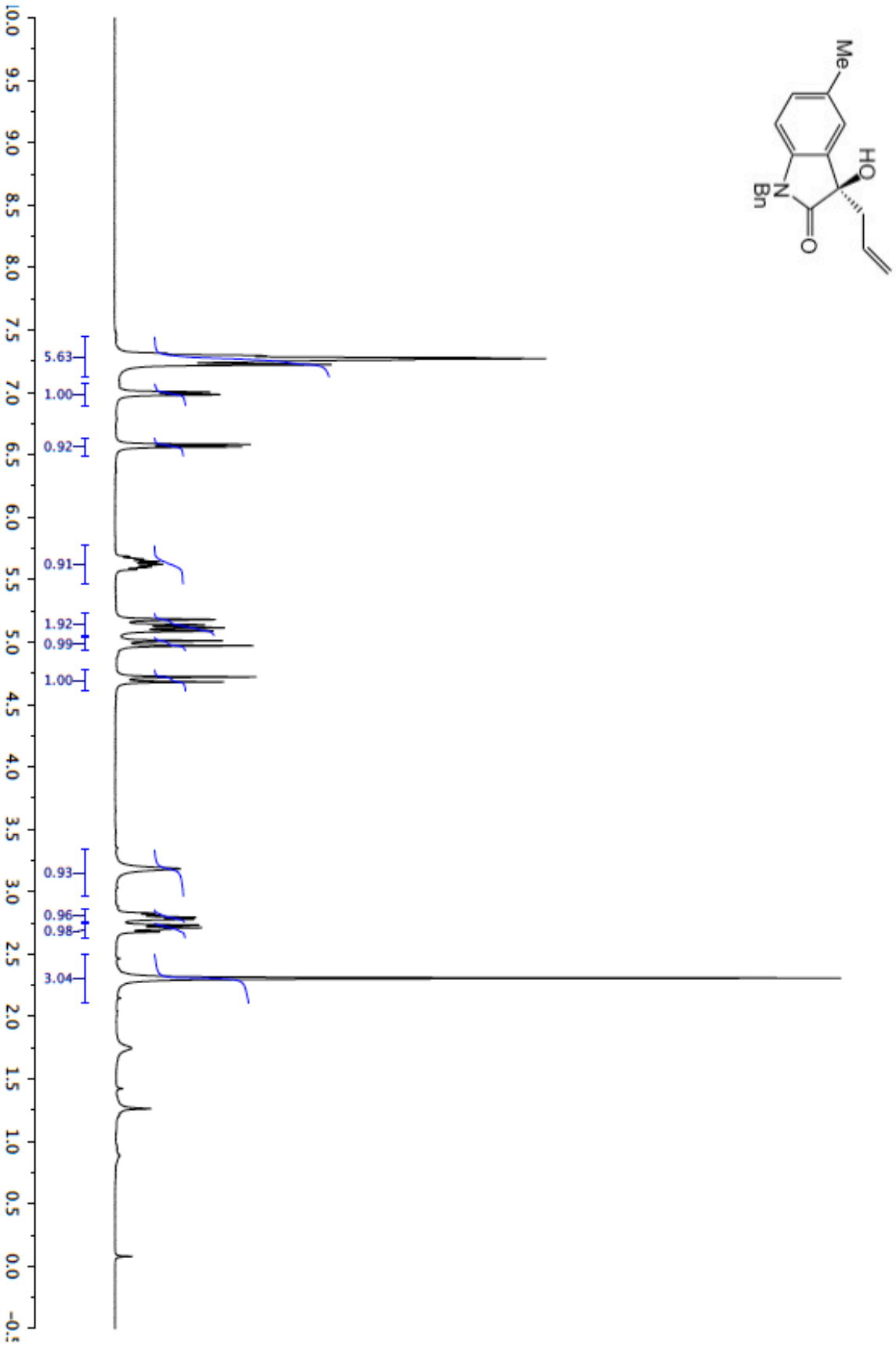

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.99
1.05
1.06
1.02
1.00
2.12
2.22
HO
HN
O

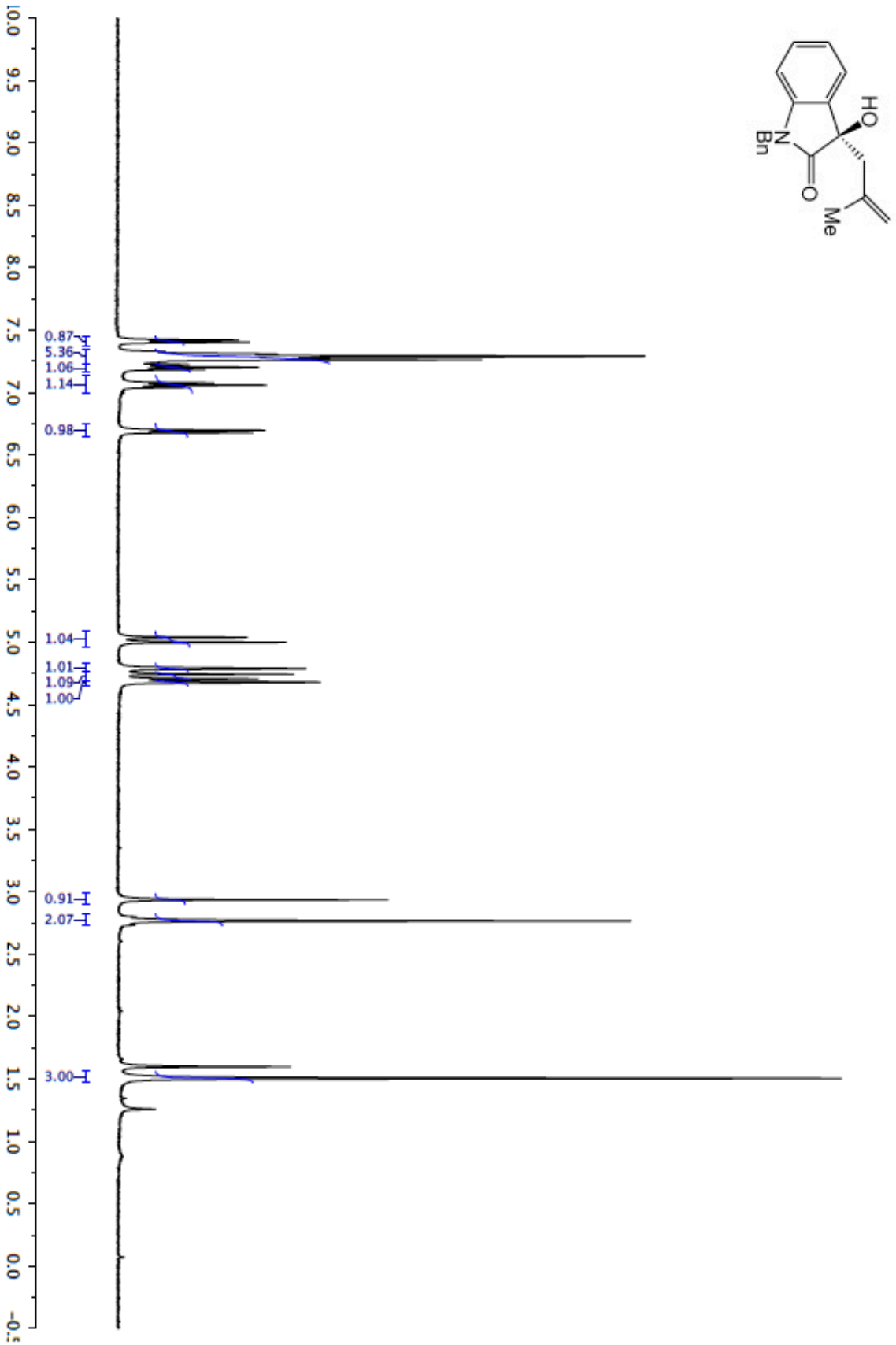

HO
N
TBS
O
0.99
1.04
1.02
1.05
1.00
2.13
0.96
2.15
9.82
3.06
3.13


Br
Br
HO
N
H
O
1.02
1.00
1.13
1.21
1.29
1.36
1.30
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


Br
Br
HO
N
SEM
O
0.89
0.99
1.00
2.11
2.13
2.15
1.07
0.83
1.08
2.45
9.21


MeO
HO
N
TBS
O
1.02
1.03
1.04
1.00
2.13
3.17
0.91
2.13
9.60
2.99
3.05


Me
HO
N
Bn
O
5.63
1.00
0.92
0.91
1.92
0.99
1.00
0.93
0.96
0.98
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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O
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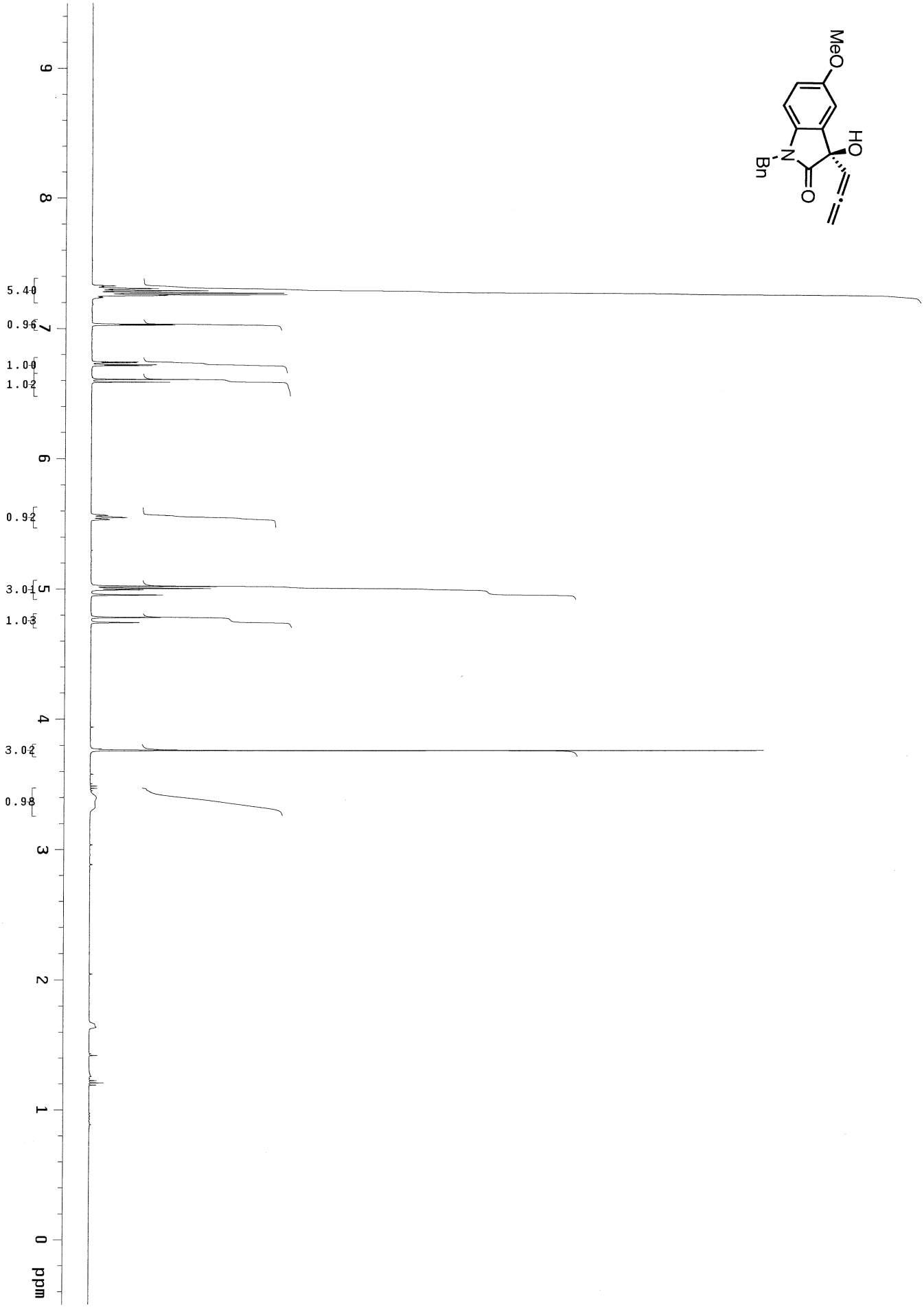
3.00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6
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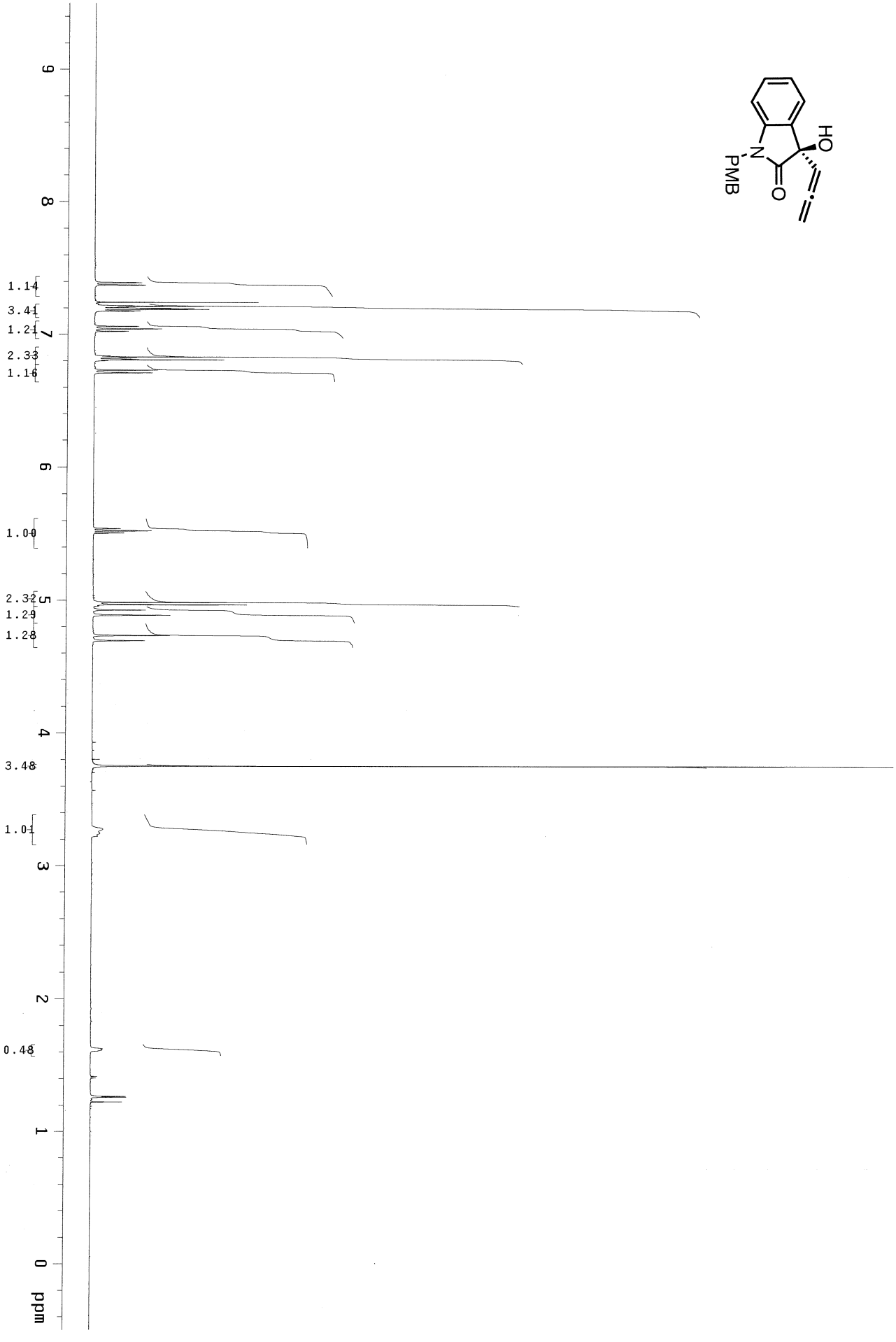
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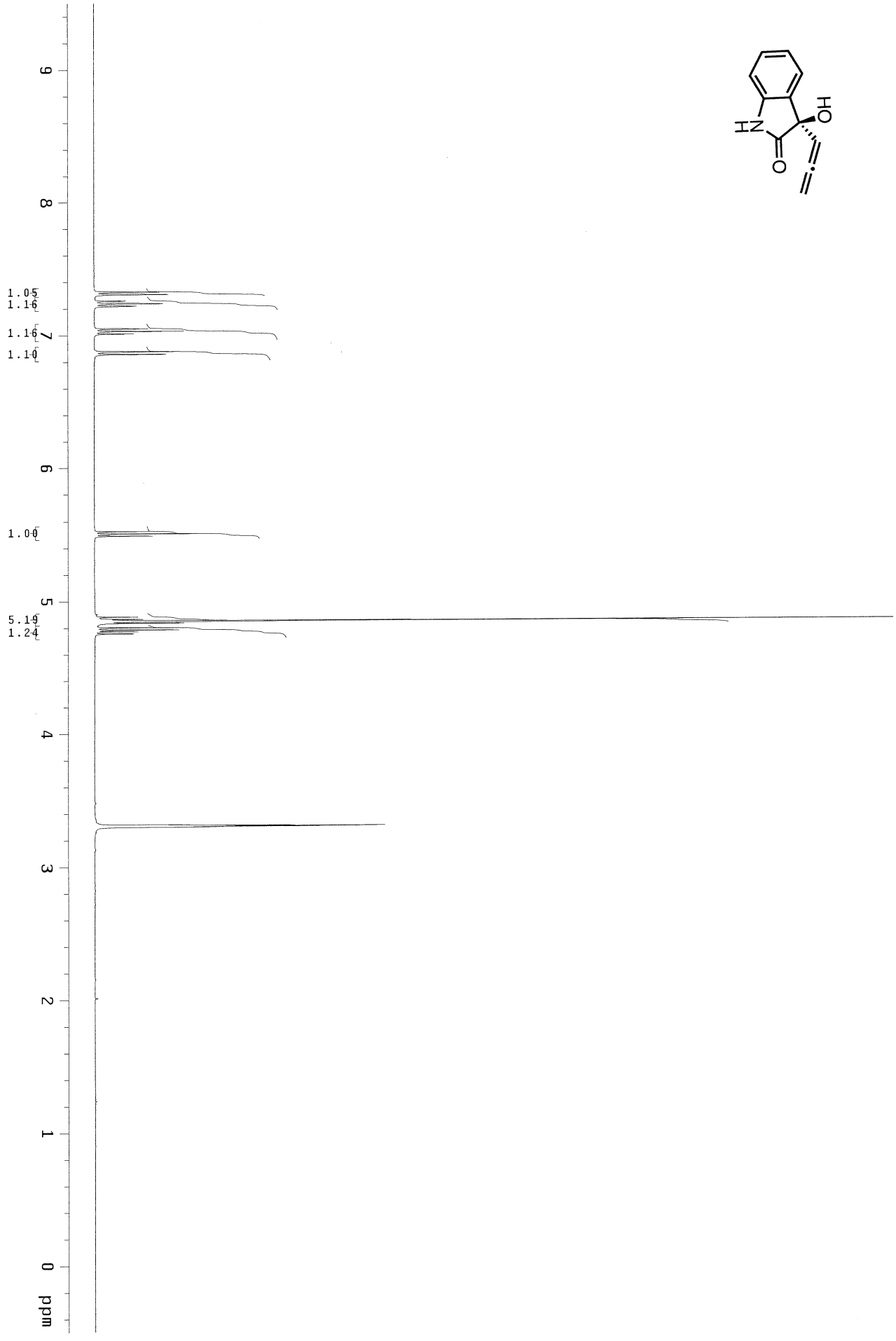
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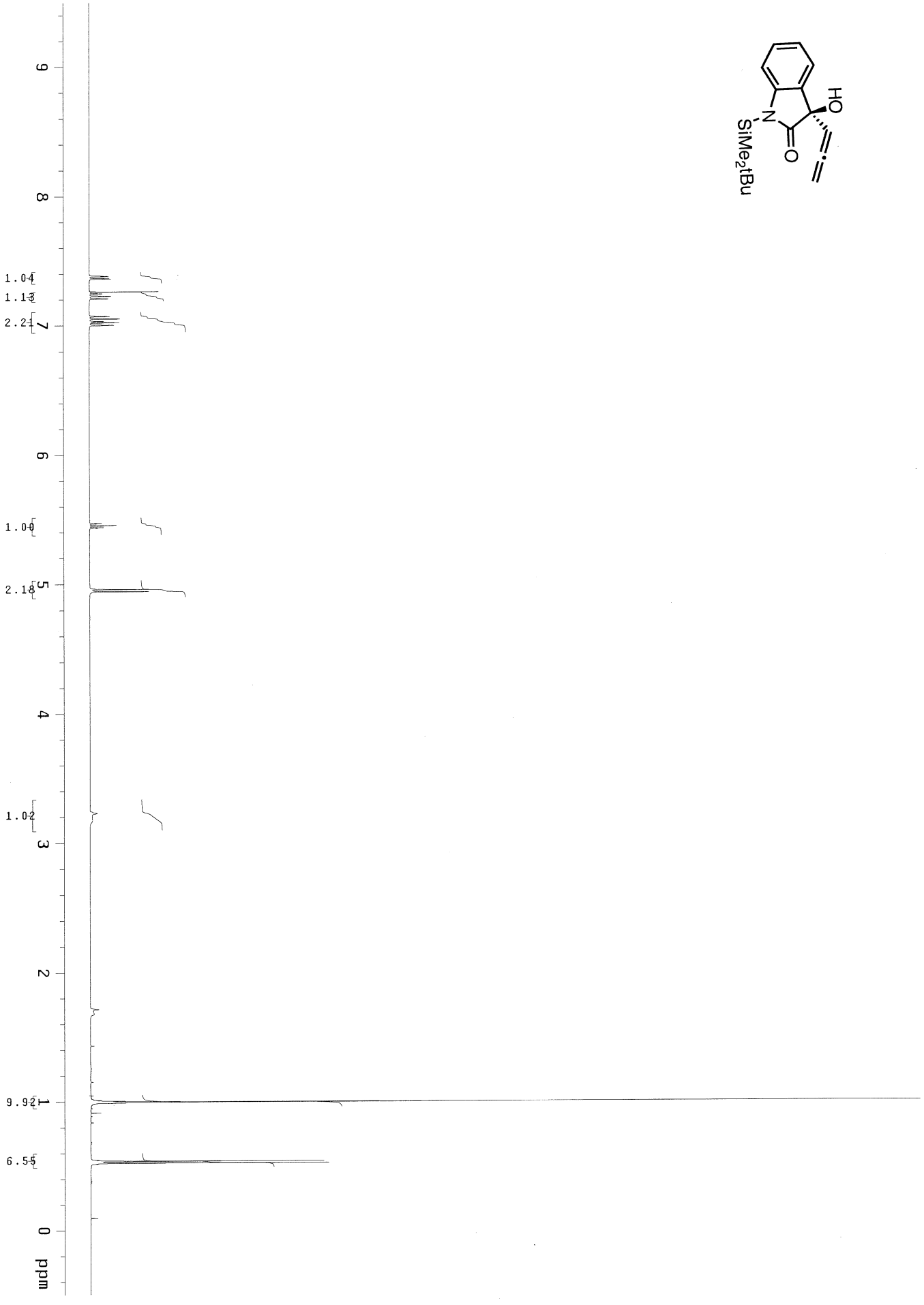
HO
HN
O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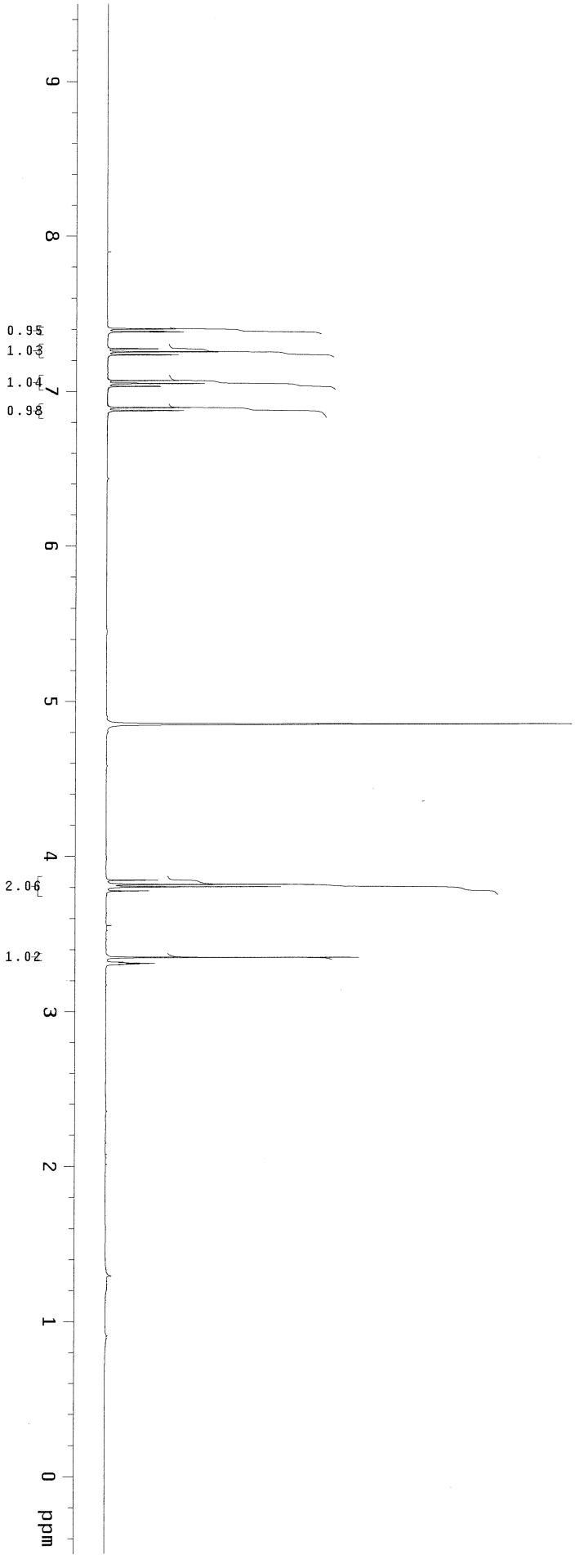
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1.04
0.98
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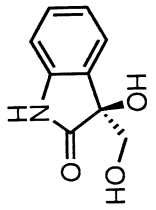
1.02


HO
H
N
O
OH

Simple Organic Molecules as Catalysts for Enantioselective Synthesis of Amines and Alcohols

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Marc L. Snapper, Fredrik Haeffner & Amir H. Hoveyda*

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SUPPLEMENTARY INFORMATION; PART D

Table of Contents ***Page***

X-ray Crystal Structure of 2g•HCl (Not shown in manuscript; see Scheme S1 in Part A of the Supplementary Information)

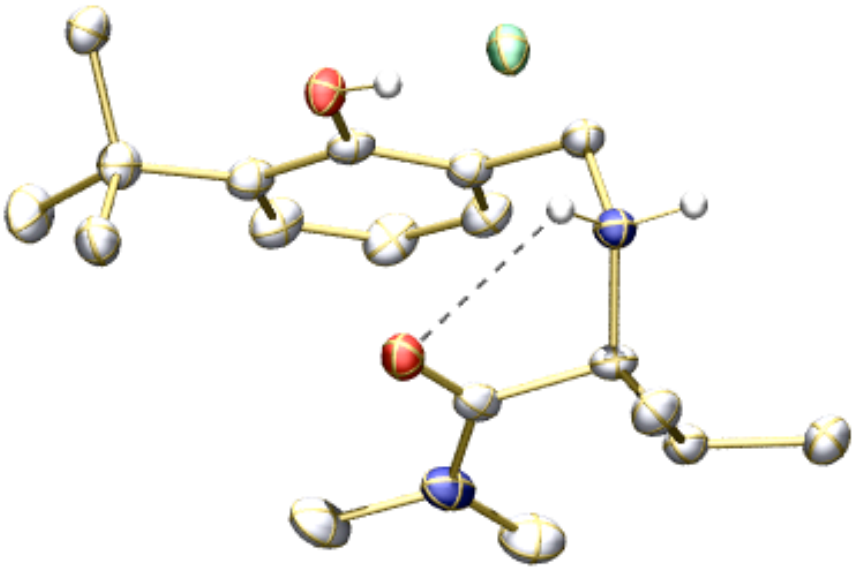

Table 1. Crystal data and structure refinement for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl)

Identification code	$C_{18}H_{31}N_2O_2Cl$	
Empirical formula	$C_{18}H_{31}N_2O_2Cl$	
Formula weight	342.90	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.1015(4) Å	α= 90°
	b = 21.8686(12) Å	β= 91.738(3)°
	c = 16.8521(9) Å	γ = 90°
Volume	2984.3(3) $Å^3$	
Z	6	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	1.776 mm^{-1}	
F(000)	1116	
Crystal size	0.15 x 0.09 x 0.03 mm^3	
Theta range for data collection	2.62 to 67.29°	
Index ranges	-6<=h<=9, -25<=k<=26, -20<=l<=20	
Reflections collected	25872	

Independent reflections	9770 [R(int) = 0.0418]
Completeness to theta = 67.29°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9487 and 0.7765
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9770 / 10 / 655
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0921
R indices (all data)	R1 = 0.0440, wR2 = 0.0956
Absolute structure parameter	0.012(9)
Extinction coefficient	na
Largest diff. peak and hole	0.280 and -0.175 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	5873(1)	4279(1)	5833(1)	26(1)
O(1)	4388(2)	5077(1)	7714(1)	26(1)
O(2)	7895(2)	4751(1)	7289(1)	24(1)
N(1)	3799(3)	5997(1)	8272(1)	31(1)
N(2)	4854(3)	5570(1)	6282(1)	22(1)
C(1)	4023(3)	5617(1)	7649(1)	24(1)
C(2)	3712(3)	5890(1)	6820(1)	22(1)
C(3)	6638(3)	5780(1)	6310(1)	23(1)
C(4)	7424(3)	5837(1)	7132(1)	23(1)
C(5)	7982(3)	5329(1)	7574(2)	23(1)
C(6)	8680(3)	5404(1)	8351(2)	26(1)
C(7)	8891(3)	6001(1)	8622(2)	32(1)
C(8)	8415(3)	6508(1)	8179(2)	33(1)
C(9)	7665(3)	6425(1)	7438(2)	29(1)
C(10)	4175(4)	5763(2)	9066(2)	43(1)

C(11)	3392(4)	6643(1)	8206(2)	41(1)
C(12)	1882(3)	5784(1)	6565(1)	25(1)
C(13)	1519(3)	5118(1)	6347(2)	29(1)
C(14)	1342(3)	6214(1)	5893(2)	31(1)
C(15)	9156(3)	4852(1)	8865(1)	27(1)
C(16)	10572(3)	4495(1)	8491(2)	29(1)
C(17)	9771(4)	5044(1)	9704(2)	38(1)
C(18)	7638(3)	4443(1)	8984(2)	30(1)
Cl(2)	5017(1)	2369(1)	3817(1)	29(1)
O(3)	3822(2)	1891(1)	6973(1)	30(1)
O(4)	7517(2)	1357(1)	7073(1)	28(1)
N(3)	3668(3)	2844(1)	7484(1)	29(1)
N(4)	5179(3)	2204(1)	5653(1)	23(1)
C(19)	3894(3)	2444(1)	6886(2)	26(1)
C(20)	4168(3)	2690(1)	6045(1)	23(1)
C(21)	7028(3)	2253(1)	5787(1)	24(1)
C(22)	7548(3)	2410(1)	6627(1)	23(1)
C(23)	7721(3)	1966(1)	7228(2)	24(1)
C(24)	8175(3)	2141(1)	8009(2)	28(1)
C(25)	8439(4)	2760(1)	8151(2)	33(1)
C(26)	8292(4)	3195(1)	7560(2)	34(1)
C(27)	7851(3)	3019(1)	6800(2)	28(1)
C(28)	3285(4)	2597(1)	8261(2)	40(1)
C(29)	3913(4)	3504(1)	7467(2)	33(1)
C(30)	2535(3)	2771(1)	5562(2)	30(1)
C(31)	1605(4)	3334(1)	5836(2)	37(1)
C(32)	1460(4)	2199(2)	5555(2)	40(1)
C(33)	8339(4)	1666(1)	8684(2)	34(1)
C(34)	6708(4)	1328(1)	8784(2)	39(1)
C(35)	8804(5)	1966(2)	9481(2)	50(1)
C(36)	9749(4)	1218(1)	8496(2)	34(1)
Cl(3)	4499(1)	5738(1)	4422(1)	26(1)
O(5)	8331(3)	3526(1)	4414(1)	41(1)
O(6)	5415(2)	3236(1)	2436(1)	30(1)
N(5)	9467(3)	3444(1)	3206(2)	38(1)
N(6)	6261(3)	4407(1)	4024(1)	26(1)

C(37)	8504(4)	3720(1)	3741(2)	32(1)
C(38)	7667(3)	4322(1)	3490(2)	29(1)
C(39)	4789(3)	4001(1)	3827(1)	23(1)
C(40)	4129(3)	4130(1)	2995(1)	24(1)
C(41)	4489(3)	3754(1)	2345(2)	24(1)
C(42)	3970(3)	3922(1)	1566(1)	25(1)
C(43)	3100(3)	4465(1)	1478(2)	30(1)
C(44)	2711(4)	4832(1)	2115(2)	34(1)
C(45)	3234(3)	4661(1)	2870(2)	28(1)
C(46)	10336(5)	2882(2)	3432(2)	53(1)
C(47)	9623(4)	3616(2)	2381(2)	39(1)
C(48)	8878(4)	4867(1)	3540(2)	39(1)
C(49)	9494(5)	4992(2)	4386(2)	61(1)
C(50)	8131(5)	5432(2)	3151(2)	57(1)
C(51)	4327(4)	3517(1)	846(2)	30(1)
C(52)	6180(4)	3407(2)	764(2)	41(1)
C(53)	3426(4)	2900(1)	933(2)	40(1)
C(54)	3689(4)	3812(2)	66(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl)

O(1)-C(1)	1.221(3)
O(2)-C(5)	1.354(3)
O(2)-H(2O)	0.857(18)
N(1)-C(1)	1.354(3)
N(1)-C(11)	1.454(4)
N(1)-C(10)	1.456(4)
N(2)-C(2)	1.491(3)
N(2)-C(3)	1.517(3)
N(2)-H(1N)	0.937(17)
N(2)-H(2N)	0.915(17)
C(1)-C(2)	1.533(3)
C(2)-C(12)	1.548(3)
C(2)-H(2B)	1.0000

C(3)-C(4)	1.512(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.398(4)
C(4)-C(5)	1.405(3)
C(5)-C(6)	1.420(3)
C(6)-C(7)	1.390(4)
C(6)-C(15)	1.528(3)
C(7)-C(8)	1.386(4)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.383(4)
C(8)-H(8A)	0.9500
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(14)	1.526(3)
C(12)-C(13)	1.528(3)
C(12)-H(12A)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.539(4)
C(15)-C(18)	1.540(4)
C(15)-C(17)	1.542(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
O(3)-C(19)	1.222(3)
O(4)-C(23)	1.367(3)
O(4)-H(4O)	0.855(18)
N(3)-C(19)	1.350(3)
N(3)-C(29)	1.457(3)
N(3)-C(28)	1.458(3)
N(4)-C(20)	1.507(3)
N(4)-C(21)	1.512(3)
N(4)-H(3N)	0.914(17)
N(4)-H(4N)	0.914(17)
C(19)-C(20)	1.538(3)
C(20)-C(30)	1.542(3)
C(20)-H(20A)	1.0000
C(21)-C(22)	1.505(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(27)	1.383(4)
C(22)-C(23)	1.407(3)
C(23)-C(24)	1.409(4)
C(24)-C(25)	1.389(4)
C(24)-C(33)	1.543(4)
C(25)-C(26)	1.379(4)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.375(4)
C(26)-H(26A)	0.9500
C(27)-H(27A)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800

C(30)-C(31)	1.524(4)
C(30)-C(32)	1.524(4)
C(30)-H(30A)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.528(4)
C(33)-C(35)	1.531(4)
C(33)-C(36)	1.545(4)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
O(5)-C(37)	1.223(4)
O(6)-C(41)	1.363(3)
O(6)-H(6O)	0.851(18)
N(5)-C(37)	1.353(4)
N(5)-C(47)	1.449(4)
N(5)-C(46)	1.460(4)
N(6)-C(38)	1.485(4)
N(6)-C(39)	1.516(3)
N(6)-H(5N)	0.909(17)
N(6)-H(6N)	0.925(17)
C(37)-C(38)	1.533(4)
C(38)-C(48)	1.544(4)
C(38)-H(38A)	1.0000
C(39)-C(40)	1.512(3)
C(39)-H(39A)	0.9900

C(39)-H(39B)	0.9900
C(40)-C(45)	1.380(3)
C(40)-C(41)	1.408(4)
C(41)-C(42)	1.416(3)
C(42)-C(43)	1.386(4)
C(42)-C(51)	1.536(3)
C(43)-C(44)	1.384(4)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.381(4)
C(44)-H(44A)	0.9500
C(45)-H(45A)	0.9500
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-C(50)	1.518(5)
C(48)-C(49)	1.521(4)
C(48)-H(48A)	1.0000
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.530(4)
C(51)-C(54)	1.538(4)
C(51)-C(53)	1.545(4)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-H(54A)	0.9800

C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800

C(5)-O(2)-H(2O)	116(2)
C(1)-N(1)-C(11)	124.9(2)
C(1)-N(1)-C(10)	117.9(2)
C(11)-N(1)-C(10)	116.9(2)
C(2)-N(2)-C(3)	116.52(19)
C(2)-N(2)-H(1N)	111.0(18)
C(3)-N(2)-H(1N)	106.0(18)
C(2)-N(2)-H(2N)	113.3(18)
C(3)-N(2)-H(2N)	104.4(19)
H(1N)-N(2)-H(2N)	105(2)
O(1)-C(1)-N(1)	124.1(2)
O(1)-C(1)-C(2)	119.4(2)
N(1)-C(1)-C(2)	116.4(2)
N(2)-C(2)-C(1)	106.47(19)
N(2)-C(2)-C(12)	111.52(19)
C(1)-C(2)-C(12)	108.9(2)
N(2)-C(2)-H(2B)	110.0
C(1)-C(2)-H(2B)	110.0
C(12)-C(2)-H(2B)	110.0
C(4)-C(3)-N(2)	115.37(19)
C(4)-C(3)-H(3A)	108.4
N(2)-C(3)-H(3A)	108.4
C(4)-C(3)-H(3B)	108.4
N(2)-C(3)-H(3B)	108.4
H(3A)-C(3)-H(3B)	107.5
C(9)-C(4)-C(5)	119.5(2)
C(9)-C(4)-C(3)	117.6(2)
C(5)-C(4)-C(3)	122.7(2)
O(2)-C(5)-C(4)	122.5(2)
O(2)-C(5)-C(6)	116.8(2)
C(4)-C(5)-C(6)	120.6(2)
C(7)-C(6)-C(5)	117.0(2)
C(7)-C(6)-C(15)	121.9(2)

C(5)-C(6)-C(15)	121.1(2)
C(8)-C(7)-C(6)	123.0(2)
C(8)-C(7)-H(7A)	118.5
C(6)-C(7)-H(7A)	118.5
C(9)-C(8)-C(7)	119.2(2)
C(9)-C(8)-H(8A)	120.4
C(7)-C(8)-H(8A)	120.4
C(8)-C(9)-C(4)	120.5(2)
C(8)-C(9)-H(9A)	119.8
C(4)-C(9)-H(9A)	119.8
N(1)-C(10)-H(10A)	109.5
N(1)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
N(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(1)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-C(13)	111.1(2)
C(14)-C(12)-C(2)	111.4(2)
C(13)-C(12)-C(2)	112.7(2)
C(14)-C(12)-H(12A)	107.1
C(13)-C(12)-H(12A)	107.1
C(2)-C(12)-H(12A)	107.1
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(6)-C(15)-C(16)	110.3(2)
C(6)-C(15)-C(18)	110.2(2)
C(16)-C(15)-C(18)	111.4(2)
C(6)-C(15)-C(17)	111.9(2)
C(16)-C(15)-C(17)	106.8(2)
C(18)-C(15)-C(17)	106.1(2)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(23)-O(4)-H(4O)	113(2)
C(19)-N(3)-C(29)	127.2(2)
C(19)-N(3)-C(28)	117.9(2)
C(29)-N(3)-C(28)	114.7(2)
C(20)-N(4)-C(21)	115.74(18)
C(20)-N(4)-H(3N)	107.2(18)
C(21)-N(4)-H(3N)	111.7(19)
C(20)-N(4)-H(4N)	112.2(18)

C(21)-N(4)-H(4N)	102.1(19)
H(3N)-N(4)-H(4N)	108(2)
O(3)-C(19)-N(3)	122.9(2)
O(3)-C(19)-C(20)	117.8(2)
N(3)-C(19)-C(20)	119.3(2)
N(4)-C(20)-C(19)	104.64(19)
N(4)-C(20)-C(30)	108.55(19)
C(19)-C(20)-C(30)	112.4(2)
N(4)-C(20)-H(20A)	110.4
C(19)-C(20)-H(20A)	110.4
C(30)-C(20)-H(20A)	110.4
C(22)-C(21)-N(4)	113.9(2)
C(22)-C(21)-H(21A)	108.8
N(4)-C(21)-H(21A)	108.8
C(22)-C(21)-H(21B)	108.8
N(4)-C(21)-H(21B)	108.8
H(21A)-C(21)-H(21B)	107.7
C(27)-C(22)-C(23)	119.9(2)
C(27)-C(22)-C(21)	117.5(2)
C(23)-C(22)-C(21)	122.6(2)
O(4)-C(23)-C(22)	121.7(2)
O(4)-C(23)-C(24)	118.0(2)
C(22)-C(23)-C(24)	120.2(2)
C(25)-C(24)-C(23)	117.3(2)
C(25)-C(24)-C(33)	121.3(2)
C(23)-C(24)-C(33)	121.3(2)
C(26)-C(25)-C(24)	122.6(2)
C(26)-C(25)-H(25A)	118.7
C(24)-C(25)-H(25A)	118.7
C(27)-C(26)-C(25)	119.6(3)
C(27)-C(26)-H(26A)	120.2
C(25)-C(26)-H(26A)	120.2
C(26)-C(27)-C(22)	120.3(2)
C(26)-C(27)-H(27A)	119.8
C(22)-C(27)-H(27A)	119.8
N(3)-C(28)-H(28A)	109.5

N(3)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(3)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
N(3)-C(29)-H(29A)	109.5
N(3)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
N(3)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-C(32)	112.2(2)
C(31)-C(30)-C(20)	110.9(2)
C(32)-C(30)-C(20)	113.0(2)
C(31)-C(30)-H(30A)	106.8
C(32)-C(30)-H(30A)	106.8
C(20)-C(30)-H(30A)	106.8
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(35)	107.6(3)
C(34)-C(33)-C(24)	110.6(2)
C(35)-C(33)-C(24)	111.8(2)
C(34)-C(33)-C(36)	111.2(2)
C(35)-C(33)-C(36)	106.7(2)
C(24)-C(33)-C(36)	108.9(2)
C(33)-C(34)-H(34A)	109.5

C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(41)-O(6)-H(6O)	110(2)
C(37)-N(5)-C(47)	126.3(2)
C(37)-N(5)-C(46)	119.0(3)
C(47)-N(5)-C(46)	114.5(3)
C(38)-N(6)-C(39)	113.96(19)
C(38)-N(6)-H(5N)	112.0(19)
C(39)-N(6)-H(5N)	102.8(19)
C(38)-N(6)-H(6N)	110.3(19)
C(39)-N(6)-H(6N)	104.8(19)
H(5N)-N(6)-H(6N)	113(3)
O(5)-C(37)-N(5)	123.2(3)
O(5)-C(37)-C(38)	119.4(3)
N(5)-C(37)-C(38)	117.3(2)
N(6)-C(38)-C(37)	106.3(2)
N(6)-C(38)-C(48)	111.6(2)
C(37)-C(38)-C(48)	111.8(2)
N(6)-C(38)-H(38A)	109.0
C(37)-C(38)-H(38A)	109.0
C(48)-C(38)-H(38A)	109.0

C(40)-C(39)-N(6)	110.31(19)
C(40)-C(39)-H(39A)	109.6
N(6)-C(39)-H(39A)	109.6
C(40)-C(39)-H(39B)	109.6
N(6)-C(39)-H(39B)	109.6
H(39A)-C(39)-H(39B)	108.1
C(45)-C(40)-C(41)	119.6(2)
C(45)-C(40)-C(39)	117.9(2)
C(41)-C(40)-C(39)	122.3(2)
O(6)-C(41)-C(40)	121.7(2)
O(6)-C(41)-C(42)	117.8(2)
C(40)-C(41)-C(42)	120.4(2)
C(43)-C(42)-C(41)	117.2(2)
C(43)-C(42)-C(51)	121.1(2)
C(41)-C(42)-C(51)	121.7(2)
C(44)-C(43)-C(42)	122.8(2)
C(44)-C(43)-H(43A)	118.6
C(42)-C(43)-H(43A)	118.6
C(45)-C(44)-C(43)	119.1(2)
C(45)-C(44)-H(44A)	120.4
C(43)-C(44)-H(44A)	120.4
C(40)-C(45)-C(44)	120.9(2)
C(40)-C(45)-H(45A)	119.6
C(44)-C(45)-H(45A)	119.6
N(5)-C(46)-H(46A)	109.5
N(5)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
N(5)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
N(5)-C(47)-H(47A)	109.5
N(5)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
N(5)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5

C(50)-C(48)-C(49)	111.8(3)
C(50)-C(48)-C(38)	111.2(3)
C(49)-C(48)-C(38)	112.3(3)
C(50)-C(48)-H(48A)	107.0
C(49)-C(48)-H(48A)	107.0
C(38)-C(48)-H(48A)	107.0
C(48)-C(49)-H(49A)	109.5
C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-C(42)	111.8(2)
C(52)-C(51)-C(54)	107.1(2)
C(42)-C(51)-C(54)	111.5(2)
C(52)-C(51)-C(53)	109.8(2)
C(42)-C(51)-C(53)	109.1(2)
C(54)-C(51)-C(53)	107.5(2)
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5

C(51)-C(54)-H(54A)	109.5
C(51)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(51)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	34(1)	25(1)	21(1)	0(1)	-3(1)	2(1)
O(1)	23(1)	31(1)	24(1)	4(1)	-1(1)	-1(1)
O(2)	26(1)	24(1)	21(1)	-2(1)	-5(1)	0(1)
N(1)	25(1)	44(1)	25(1)	-8(1)	1(1)	-3(1)
N(2)	20(1)	23(1)	22(1)	-1(1)	1(1)	0(1)
C(1)	13(1)	36(1)	23(1)	-2(1)	0(1)	-5(1)
C(2)	17(1)	24(1)	25(1)	-4(1)	4(1)	1(1)
C(3)	16(1)	28(1)	26(1)	4(1)	3(1)	0(1)
C(4)	15(1)	28(1)	27(1)	-1(1)	2(1)	-3(1)
C(5)	13(1)	28(1)	28(1)	-3(1)	2(1)	-1(1)
C(6)	18(1)	30(1)	29(1)	-3(1)	-1(1)	-1(1)
C(7)	24(2)	36(1)	37(2)	-8(1)	-6(1)	-3(1)
C(8)	29(2)	27(1)	42(2)	-9(1)	-5(1)	-2(1)
C(9)	21(1)	27(1)	38(1)	-2(1)	0(1)	-3(1)
C(10)	35(2)	72(2)	22(1)	-9(1)	0(1)	-5(2)
C(11)	39(2)	45(2)	40(2)	-14(1)	6(1)	-4(1)
C(12)	18(1)	34(1)	22(1)	-1(1)	2(1)	1(1)
C(13)	18(1)	38(2)	31(1)	1(1)	-2(1)	-2(1)
C(14)	23(2)	38(1)	32(1)	3(1)	-3(1)	3(1)

C(15)	25(2)	34(1)	22(1)	-3(1)	-5(1)	-1(1)
C(16)	22(1)	36(1)	28(1)	0(1)	-5(1)	1(1)
C(17)	40(2)	46(2)	27(2)	-6(1)	-12(1)	3(1)
C(18)	28(2)	37(2)	26(1)	4(1)	-1(1)	-1(1)
Cl(2)	40(1)	24(1)	24(1)	0(1)	-2(1)	2(1)
O(3)	32(1)	31(1)	29(1)	1(1)	2(1)	-4(1)
O(4)	32(1)	25(1)	26(1)	-1(1)	-6(1)	-1(1)
N(3)	27(1)	33(1)	27(1)	-2(1)	2(1)	-2(1)
N(4)	20(1)	25(1)	24(1)	0(1)	-1(1)	0(1)
C(19)	16(1)	33(1)	29(1)	0(1)	-2(1)	-3(1)
C(20)	20(1)	25(1)	25(1)	-3(1)	0(1)	2(1)
C(21)	19(1)	27(1)	26(1)	1(1)	0(1)	2(1)
C(22)	17(1)	28(1)	24(1)	2(1)	-1(1)	2(1)
C(23)	19(1)	25(1)	30(1)	-1(1)	1(1)	1(1)
C(24)	24(2)	31(1)	29(1)	-1(1)	-4(1)	4(1)
C(25)	33(2)	34(1)	31(1)	-7(1)	-10(1)	4(1)
C(26)	34(2)	25(1)	42(2)	-5(1)	-8(1)	-2(1)
C(27)	23(2)	27(1)	34(1)	4(1)	-3(1)	1(1)
C(28)	48(2)	43(2)	28(2)	-2(1)	10(1)	-1(1)
C(29)	33(2)	34(1)	31(1)	-4(1)	4(1)	4(1)
C(30)	21(2)	42(2)	27(1)	-2(1)	-2(1)	1(1)
C(31)	26(2)	48(2)	37(1)	2(1)	-4(1)	9(1)
C(32)	25(2)	52(2)	41(2)	-7(1)	-6(1)	-2(1)
C(33)	38(2)	34(1)	29(1)	-2(1)	-7(1)	6(1)
C(34)	46(2)	41(2)	30(1)	7(1)	6(1)	7(1)
C(35)	77(3)	42(2)	31(2)	-3(1)	-17(2)	14(2)
C(36)	39(2)	31(1)	32(1)	4(1)	-10(1)	3(1)
Cl(3)	32(1)	25(1)	21(1)	0(1)	-1(1)	1(1)
O(5)	39(1)	48(1)	36(1)	3(1)	-6(1)	10(1)
O(6)	37(1)	32(1)	22(1)	3(1)	2(1)	11(1)
N(5)	29(1)	43(1)	43(1)	-9(1)	-4(1)	9(1)
N(6)	26(1)	32(1)	21(1)	-3(1)	0(1)	0(1)
C(37)	27(2)	39(2)	31(2)	-5(1)	-7(1)	1(1)
C(38)	25(2)	37(1)	25(1)	-1(1)	-1(1)	2(1)
C(39)	23(1)	24(1)	23(1)	-2(1)	2(1)	-2(1)
C(40)	18(1)	28(1)	26(1)	-2(1)	-1(1)	-4(1)

C(41)	18(1)	25(1)	28(1)	1(1)	0(1)	0(1)
C(42)	22(2)	29(1)	26(1)	-1(1)	0(1)	-5(1)
C(43)	27(2)	32(1)	30(1)	6(1)	-8(1)	-1(1)
C(44)	34(2)	28(1)	38(2)	1(1)	-8(1)	6(1)
C(45)	24(2)	24(1)	35(1)	-6(1)	-3(1)	0(1)
C(46)	54(2)	50(2)	56(2)	0(2)	2(2)	20(2)
C(47)	31(2)	49(2)	38(2)	-11(1)	2(1)	1(1)
C(48)	34(2)	42(2)	41(2)	-9(1)	12(1)	-4(1)
C(49)	64(3)	71(2)	48(2)	-23(2)	3(2)	-30(2)
C(50)	60(3)	39(2)	75(3)	6(2)	32(2)	-2(2)
C(51)	35(2)	33(1)	23(1)	0(1)	-3(1)	0(1)
C(52)	44(2)	55(2)	25(1)	0(1)	5(1)	4(2)
C(53)	47(2)	34(2)	36(2)	-7(1)	-8(1)	-1(1)
C(54)	56(2)	46(2)	25(1)	-1(1)	-4(1)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl).

	x	y	z	U(eq)
H(2O)	7320(30)	4705(14)	6859(13)	36
H(1N)	4490(30)	5606(12)	5751(11)	26
H(2N)	4910(40)	5157(8)	6370(16)	26
H(2B)	3960	6338	6829	26
H(3A)	7297	5488	6001	28
H(3B)	6699	6183	6044	28
H(7A)	9384	6063	9134	39
H(8A)	8602	6909	8381	39
H(9A)	7312	6770	7136	34
H(10A)	4262	5317	9047	65
H(10B)	3292	5880	9421	65
H(10C)	5224	5936	9264	65
H(11A)	4405	6880	8139	62
H(11B)	2851	6777	8688	62

H(11C)	2645	6707	7745	62
H(12A)	1201	5886	7032	30
H(13A)	348	5075	6194	43
H(13B)	1777	4856	6805	43
H(13C)	2197	4997	5902	43
H(14A)	180	6139	5748	47
H(14B)	2023	6141	5432	47
H(14C)	1477	6639	6069	47
H(16A)	11517	4767	8423	43
H(16B)	10200	4335	7973	43
H(16C)	10900	4154	8840	43
H(17A)	10743	5308	9662	57
H(17B)	10068	4679	10013	57
H(17C)	8895	5268	9968	57
H(18A)	7195	4307	8466	45
H(18B)	6791	4675	9257	45
H(18C)	7962	4086	9304	45
H(4O)	6910(40)	1290(15)	6658(14)	42
H(3N)	4790(40)	1834(9)	5814(16)	28
H(4N)	5070(40)	2218(13)	5112(10)	28
H(20A)	4790	3085	6071	28
H(21A)	7539	1858	5643	29
H(21B)	7456	2569	5427	29
H(25A)	8732	2888	8675	39
H(26A)	8494	3613	7678	40
H(27A)	7753	3317	6391	34
H(28A)	3041	2159	8211	59
H(28B)	2323	2810	8465	59
H(28C)	4234	2655	8627	59
H(29A)	4293	3625	6944	49
H(29B)	4743	3620	7875	49
H(29C)	2868	3710	7571	49
H(30A)	2838	2848	4999	36
H(31A)	570	3375	5523	55
H(31B)	2286	3699	5761	55
H(31C)	1359	3292	6399	55

H(32A)	440	2277	5244	60
H(32B)	1188	2092	6100	60
H(32C)	2061	1859	5316	60
H(34A)	5839	1622	8905	58
H(34B)	6830	1033	9219	58
H(34C)	6409	1111	8291	58
H(35A)	7940	2256	9623	76
H(35B)	9855	2184	9438	76
H(35C)	8915	1651	9892	76
H(36A)	9865	915	8923	51
H(36B)	10785	1445	8454	51
H(36C)	9490	1009	7993	51
H(6O)	5220(40)	3068(14)	2878(13)	45
H(5N)	6530(40)	4301(14)	4533(11)	32
H(6N)	5860(40)	4802(9)	3982(17)	32
H(38A)	7230	4281	2931	35
H(39A)	5124	3566	3869	28
H(39B)	3912	4075	4212	28
H(43A)	2757	4591	959	36
H(44A)	2093	5197	2033	41
H(45A)	2974	4911	3310	33
H(46A)	10179	2800	3997	80
H(46B)	11516	2930	3338	80
H(46C)	9894	2541	3115	80
H(47A)	8932	3975	2265	59
H(47B)	9264	3276	2039	59
H(47C)	10778	3714	2281	59
H(48A)	9863	4752	3229	47
H(49A)	10255	5341	4388	91
H(49B)	10070	4630	4597	91
H(49C)	8553	5087	4717	91
H(50A)	8924	5770	3191	86
H(50B)	7121	5546	3422	86
H(50C)	7865	5347	2591	86
H(52A)	6360	3147	301	61
H(52B)	6624	3204	1243	61

H(52C)	6742	3800	695	61
H(53A)	3646	2640	474	59
H(53B)	2236	2971	962	59
H(53C)	3826	2695	1420	59
H(54A)	3927	3542	-380	63
H(54B)	4239	4206	-6	63
H(54C)	2494	3876	89	63

Table 6. Torsion angles [°] for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl)

C(11)-N(1)-C(1)-O(1)	178.9(3)
C(10)-N(1)-C(1)-O(1)	6.3(4)
C(11)-N(1)-C(1)-C(2)	-3.9(4)
C(10)-N(1)-C(1)-C(2)	-176.6(2)
C(3)-N(2)-C(2)-C(1)	-78.7(2)
C(3)-N(2)-C(2)-C(12)	162.57(19)
O(1)-C(1)-C(2)-N(2)	-34.0(3)
N(1)-C(1)-C(2)-N(2)	148.7(2)
O(1)-C(1)-C(2)-C(12)	86.4(3)
N(1)-C(1)-C(2)-C(12)	-90.9(3)
C(2)-N(2)-C(3)-C(4)	48.5(3)
N(2)-C(3)-C(4)-C(9)	-105.6(3)
N(2)-C(3)-C(4)-C(5)	77.6(3)
C(9)-C(4)-C(5)-O(2)	-175.1(2)
C(3)-C(4)-C(5)-O(2)	1.7(4)
C(9)-C(4)-C(5)-C(6)	4.5(4)
C(3)-C(4)-C(5)-C(6)	-178.7(2)
O(2)-C(5)-C(6)-C(7)	175.1(2)
C(4)-C(5)-C(6)-C(7)	-4.6(4)
O(2)-C(5)-C(6)-C(15)	-5.6(4)
C(4)-C(5)-C(6)-C(15)	174.7(2)
C(5)-C(6)-C(7)-C(8)	1.7(4)
C(15)-C(6)-C(7)-C(8)	-177.6(3)
C(6)-C(7)-C(8)-C(9)	1.3(5)

C(7)-C(8)-C(9)-C(4)	-1.5(4)
C(5)-C(4)-C(9)-C(8)	-1.4(4)
C(3)-C(4)-C(9)-C(8)	-178.4(2)
N(2)-C(2)-C(12)-C(14)	-81.6(3)
C(1)-C(2)-C(12)-C(14)	161.2(2)
N(2)-C(2)-C(12)-C(13)	44.0(3)
C(1)-C(2)-C(12)-C(13)	-73.2(2)
C(7)-C(6)-C(15)-C(16)	-115.4(3)
C(5)-C(6)-C(15)-C(16)	65.3(3)
C(7)-C(6)-C(15)-C(18)	121.1(3)
C(5)-C(6)-C(15)-C(18)	-58.2(3)
C(7)-C(6)-C(15)-C(17)	3.4(4)
C(5)-C(6)-C(15)-C(17)	-175.9(3)
C(29)-N(3)-C(19)-O(3)	172.3(3)
C(28)-N(3)-C(19)-O(3)	-1.5(4)
C(29)-N(3)-C(19)-C(20)	-10.9(4)
C(28)-N(3)-C(19)-C(20)	175.4(2)
C(21)-N(4)-C(20)-C(19)	-86.5(2)
C(21)-N(4)-C(20)-C(30)	153.2(2)
O(3)-C(19)-C(20)-N(4)	-30.7(3)
N(3)-C(19)-C(20)-N(4)	152.3(2)
O(3)-C(19)-C(20)-C(30)	86.9(3)
N(3)-C(19)-C(20)-C(30)	-90.1(3)
C(20)-N(4)-C(21)-C(22)	42.3(3)
N(4)-C(21)-C(22)-C(27)	-95.7(3)
N(4)-C(21)-C(22)-C(23)	83.8(3)
C(27)-C(22)-C(23)-O(4)	-176.5(2)
C(21)-C(22)-C(23)-O(4)	3.9(4)
C(27)-C(22)-C(23)-C(24)	1.0(4)
C(21)-C(22)-C(23)-C(24)	-178.5(2)
O(4)-C(23)-C(24)-C(25)	177.6(3)
C(22)-C(23)-C(24)-C(25)	-0.1(4)
O(4)-C(23)-C(24)-C(33)	-3.6(4)
C(22)-C(23)-C(24)-C(33)	178.7(3)
C(23)-C(24)-C(25)-C(26)	-0.8(5)
C(33)-C(24)-C(25)-C(26)	-179.6(3)

C(24)-C(25)-C(26)-C(27)	0.7(5)
C(25)-C(26)-C(27)-C(22)	0.3(4)
C(23)-C(22)-C(27)-C(26)	-1.2(4)
C(21)-C(22)-C(27)-C(26)	178.4(3)
N(4)-C(20)-C(30)-C(31)	-169.4(2)
C(19)-C(20)-C(30)-C(31)	75.3(3)
N(4)-C(20)-C(30)-C(32)	63.5(3)
C(19)-C(20)-C(30)-C(32)	-51.7(3)
C(25)-C(24)-C(33)-C(34)	120.0(3)
C(23)-C(24)-C(33)-C(34)	-58.8(4)
C(25)-C(24)-C(33)-C(35)	0.1(4)
C(23)-C(24)-C(33)-C(35)	-178.6(3)
C(25)-C(24)-C(33)-C(36)	-117.6(3)
C(23)-C(24)-C(33)-C(36)	63.7(3)
C(47)-N(5)-C(37)-O(5)	174.4(3)
C(46)-N(5)-C(37)-O(5)	0.6(4)
C(47)-N(5)-C(37)-C(38)	-8.5(4)
C(46)-N(5)-C(37)-C(38)	177.7(3)
C(39)-N(6)-C(38)-C(37)	-75.6(2)
C(39)-N(6)-C(38)-C(48)	162.2(2)
O(5)-C(37)-C(38)-N(6)	-23.1(3)
N(5)-C(37)-C(38)-N(6)	159.7(2)
O(5)-C(37)-C(38)-C(48)	98.9(3)
N(5)-C(37)-C(38)-C(48)	-78.3(3)
C(38)-N(6)-C(39)-C(40)	-60.4(3)
N(6)-C(39)-C(40)-C(45)	-74.9(3)
N(6)-C(39)-C(40)-C(41)	100.7(3)
C(45)-C(40)-C(41)-O(6)	177.8(2)
C(39)-C(40)-C(41)-O(6)	2.2(4)
C(45)-C(40)-C(41)-C(42)	1.3(4)
C(39)-C(40)-C(41)-C(42)	-174.3(2)
O(6)-C(41)-C(42)-C(43)	-176.9(2)
C(40)-C(41)-C(42)-C(43)	-0.2(4)
O(6)-C(41)-C(42)-C(51)	4.1(4)
C(40)-C(41)-C(42)-C(51)	-179.3(2)
C(41)-C(42)-C(43)-C(44)	-1.1(4)

C(51)-C(42)-C(43)-C(44)	178.0(3)
C(42)-C(43)-C(44)-C(45)	1.3(4)
C(41)-C(40)-C(45)-C(44)	-1.1(4)
C(39)-C(40)-C(45)-C(44)	174.6(2)
C(43)-C(44)-C(45)-C(40)	-0.2(4)
N(6)-C(38)-C(48)-C(50)	-71.3(3)
C(37)-C(38)-C(48)-C(50)	169.7(2)
N(6)-C(38)-C(48)-C(49)	54.9(3)
C(37)-C(38)-C(48)-C(49)	-64.1(3)
C(43)-C(42)-C(51)-C(52)	122.7(3)
C(41)-C(42)-C(51)-C(52)	-58.2(3)
C(43)-C(42)-C(51)-C(54)	2.9(4)
C(41)-C(42)-C(51)-C(54)	-178.0(3)
C(43)-C(42)-C(51)-C(53)	-115.6(3)
C(41)-C(42)-C(51)-C(53)	63.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{18}H_{31}N_2O_2Cl$ (2g•HCl) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...Cl(1)	0.857(18)	2.26(2)	3.0861(17)	162(3)
N(2)-H(2N)...Cl(1)	0.915(17)	2.27(2)	3.042(2)	142(2)
N(2)-H(1N)...Cl(3)	0.937(17)	2.259(19)	3.161(2)	161(2)
O(4)-H(4O)...Cl(3)#1	0.855(18)	2.44(2)	3.2538(18)	160(3)
N(4)-H(3N)...O(3)	0.914(17)	2.13(3)	2.603(3)	111(2)
N(4)-H(3N)...Cl(3)#1	0.914(17)	2.50(2)	3.218(2)	136(2)
N(4)-H(4N)...Cl(2)	0.914(17)	2.205(18)	3.113(2)	172(3)
O(6)-H(6O)...Cl(2)	0.851(18)	2.21(2)	3.0290(19)	161(3)
N(6)-H(5N)...Cl(1)	0.909(17)	2.27(2)	3.087(2)	149(3)
N(6)-H(6N)...Cl(3)	0.925(17)	2.45(2)	3.320(2)	157(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+1

X-ray Crystal Structure of 2g (Table 1)

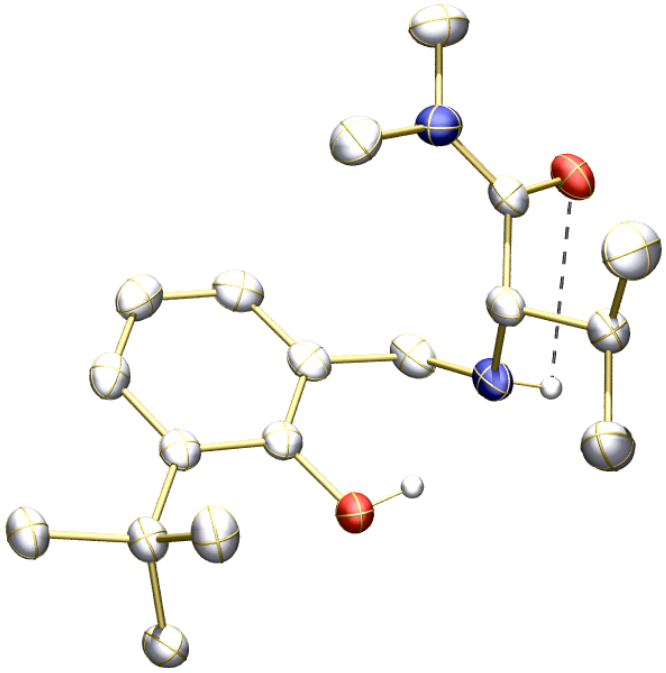

Table 1. Crystal data and structure refinement for $C_{18}H_{30}N_2O_2$ (2g).

Identification code	$C_{18}H_{30}N_2O_2$	
Empirical formula	$C_{18}H_{30}N_2O_2$	
Formula weight	306.44	
Temperature	143(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.4590(6) Å	α= 90°
	b = 14.9795(12) Å	β= 90°
	c = 16.2770(13) Å	γ = 90°
Volume	1818.7(3) $Å^3$	
Z	4	
Density (calculated)	1.119 Mg/m^3	
Absorption coefficient	0.570 mm^{-1}	
F(000)	672	
Crystal size	0.17 x 0.10 x 0.05 mm^3	

Theta range for data collection	4.01 to 67.94°
Index ranges	-8<=h<=3, -18<=k<=17, -19<=l<=19
Reflections collected	13923
Independent reflections	3190 [R(int) = 0.0179]
Completeness to theta = 67.94°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9721 and 0.9093
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3190 / 3 / 210
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0292, wR2 = 0.0780
R indices (all data)	R1 = 0.0293, wR2 = 0.0781
Absolute structure parameter	0.09(19)
Extinction coefficient	na
Largest diff. peak and hole	0.144 and -0.103 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{18}H_{30}N_2O_2$ (2g). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-318(1)	6477(1)	2399(1)	34(1)
O(2)	4304(1)	8137(1)	390(1)	39(1)
N(1)	1412(2)	7118(1)	1121(1)	33(1)
N(2)	5199(2)	8362(1)	1699(1)	36(1)
C(1)	-51(2)	7283(1)	2771(1)	28(1)
C(2)	-223(2)	7349(1)	3633(1)	28(1)
C(3)	18(2)	8194(1)	3976(1)	33(1)
C(4)	456(2)	8934(1)	3510(1)	37(1)
C(5)	650(2)	8851(1)	2667(1)	36(1)
C(6)	380(2)	8032(1)	2291(1)	31(1)
C(7)	503(2)	7944(1)	1367(1)	36(1)
C(8)	3309(2)	7046(1)	1351(1)	29(1)
C(9)	4330(2)	7894(1)	1115(1)	31(1)

C(10)	5325(2)	8115(1)	2566(1)	44(1)
C(11)	6055(2)	9200(1)	1471(1)	48(1)
C(12)	-610(2)	6519(1)	4160(1)	31(1)
C(13)	882(2)	5825(1)	4040(1)	40(1)
C(14)	-2426(2)	6110(1)	3925(1)	40(1)
C(15)	-673(2)	6747(1)	5081(1)	38(1)
C(16)	4143(2)	6228(1)	933(1)	35(1)
C(17)	6119(2)	6137(1)	1134(1)	54(1)
C(18)	3107(3)	5387(1)	1155(1)	56(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{18}H_{30}N_2O_2$ (2g)

O(1)-C(1)	1.3656(15)
O(1)-H(1O)	0.839(13)
O(2)-C(9)	1.2351(15)
N(1)-C(7)	1.4659(19)
N(1)-C(8)	1.4678(17)
N(1)-H(1N)	0.898(13)
N(2)-C(9)	1.3472(17)
N(2)-C(11)	1.4563(18)
N(2)-C(10)	1.4629(18)
C(1)-C(6)	1.4043(17)
C(1)-C(2)	1.4111(17)
C(2)-C(3)	1.3956(18)
C(2)-C(12)	1.5382(17)
C(3)-C(4)	1.382(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.385(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3858(19)
C(5)-H(5)	0.9500
C(6)-C(7)	1.5127(17)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900

C(8)-C(9)	1.5297(17)
C(8)-C(16)	1.5332(19)
C(8)-H(8)	0.991(12)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(14)	1.535(2)
C(12)-C(13)	1.5355(19)
C(12)-C(15)	1.5385(17)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.516(2)
C(16)-C(18)	1.522(2)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(1)-O(1)-H(1O)	106.8(11)
C(7)-N(1)-C(8)	115.97(11)
C(7)-N(1)-H(1N)	109.7(10)
C(8)-N(1)-H(1N)	110.8(11)
C(9)-N(2)-C(11)	118.70(12)
C(9)-N(2)-C(10)	125.46(11)

C(11)-N(2)-C(10)	115.81(12)
O(1)-C(1)-C(6)	119.55(11)
O(1)-C(1)-C(2)	119.25(11)
C(6)-C(1)-C(2)	121.20(11)
C(3)-C(2)-C(1)	116.73(11)
C(3)-C(2)-C(12)	122.22(11)
C(1)-C(2)-C(12)	121.03(11)
C(4)-C(3)-C(2)	122.53(12)
C(4)-C(3)-H(3)	118.7
C(2)-C(3)-H(3)	118.7
C(3)-C(4)-C(5)	119.78(12)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	120.08(12)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	119.65(12)
C(5)-C(6)-C(7)	120.53(12)
C(1)-C(6)-C(7)	119.80(12)
N(1)-C(7)-C(6)	111.95(10)
N(1)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
N(1)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
N(1)-C(8)-C(9)	110.81(10)
N(1)-C(8)-C(16)	109.65(11)
C(9)-C(8)-C(16)	110.53(10)
N(1)-C(8)-H(8)	107.6(9)
C(9)-C(8)-H(8)	110.4(9)
C(16)-C(8)-H(8)	107.7(9)
O(2)-C(9)-N(2)	121.89(12)
O(2)-C(9)-C(8)	118.46(11)
N(2)-C(9)-C(8)	119.64(11)
N(2)-C(10)-H(10A)	109.5
N(2)-C(10)-H(10B)	109.5

H(10A)-C(10)-H(10B)	109.5
N(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-H(11A)	109.5
N(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-C(13)	109.77(11)
C(14)-C(12)-C(2)	110.44(11)
C(13)-C(12)-C(2)	109.86(11)
C(14)-C(12)-C(15)	107.73(11)
C(13)-C(12)-C(15)	107.23(11)
C(2)-C(12)-C(15)	111.73(11)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(18)	111.58(14)
C(17)-C(16)-C(8)	111.74(12)

C(18)-C(16)-C(8)	110.55(11)
C(17)-C(16)-H(16)	107.6
C(18)-C(16)-H(16)	107.6
C(8)-C(16)-H(16)	107.6
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{18}H_{30}N_2O_2$ (2g). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	36(1)	38(1)	26(1)	-3(1)	4(1)	-7(1)
O(2)	41(1)	46(1)	31(1)	8(1)	8(1)	-2(1)
N(1)	28(1)	46(1)	23(1)	2(1)	-2(1)	-3(1)
N(2)	32(1)	36(1)	40(1)	0(1)	0(1)	-4(1)
C(1)	20(1)	33(1)	30(1)	-1(1)	-1(1)	1(1)
C(2)	20(1)	34(1)	31(1)	0(1)	-1(1)	4(1)
C(3)	27(1)	38(1)	34(1)	-6(1)	-2(1)	8(1)
C(4)	33(1)	31(1)	48(1)	-6(1)	-4(1)	6(1)
C(5)	27(1)	33(1)	48(1)	8(1)	-1(1)	4(1)
C(6)	19(1)	38(1)	34(1)	5(1)	0(1)	4(1)

C(7)	28(1)	47(1)	32(1)	11(1)	-1(1)	1(1)
C(8)	27(1)	38(1)	22(1)	2(1)	0(1)	-3(1)
C(9)	25(1)	35(1)	31(1)	2(1)	5(1)	2(1)
C(10)	39(1)	54(1)	40(1)	-3(1)	-11(1)	-4(1)
C(11)	41(1)	36(1)	68(1)	1(1)	-3(1)	-6(1)
C(12)	31(1)	35(1)	28(1)	1(1)	3(1)	2(1)
C(13)	47(1)	38(1)	36(1)	4(1)	4(1)	10(1)
C(14)	39(1)	46(1)	35(1)	2(1)	4(1)	-9(1)
C(15)	39(1)	46(1)	29(1)	1(1)	3(1)	3(1)
C(16)	35(1)	38(1)	32(1)	-1(1)	4(1)	-3(1)
C(17)	41(1)	48(1)	73(1)	-7(1)	0(1)	10(1)
C(18)	64(1)	38(1)	65(1)	-4(1)	22(1)	-8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{18}H_{30}N_2O_2$ (2g)

	x	y	z	U(eq)
H(1O)	120(20)	6516(10)	1925(9)	40
H(1N)	1270(20)	7029(10)	580(8)	39
H(3)	-124	8263	4553	40
H(4)	624	9497	3768	45
H(5)	968	9357	2347	43
H(7A)	-720	7951	1131	43
H(7B)	1166	8461	1142	43
H(8)	3360(20)	6950(10)	1952(8)	35
H(10A)	4172	8227	2836	67
H(10B)	6260	8473	2832	67
H(10C)	5627	7481	2612	67
H(11A)	6098	9250	871	72
H(11B)	7277	9215	1692	72
H(11C)	5365	9700	1697	72
H(13A)	2038	6088	4194	60
H(13B)	919	5640	3463	60

H(13C)	642	5304	4388	60
H(14A)	-2422	5956	3340	60
H(14B)	-3382	6543	4034	60
H(14C)	-2634	5570	4252	60
H(15A)	476	7006	5249	57
H(15B)	-899	6202	5398	57
H(15C)	-1637	7178	5183	57
H(16)	4036	6315	326	42
H(17A)	6744	6690	987	81
H(17B)	6628	5639	821	81
H(17C)	6263	6024	1723	81
H(18A)	1839	5468	1017	84
H(18B)	3226	5271	1745	84
H(18C)	3590	4880	845	84

Table 6. Torsion angles [°] for $C_{18}H_{30}N_2O_2$ (2g)

O(1)-C(1)-C(2)-C(3)	-178.35(11)
C(6)-C(1)-C(2)-C(3)	1.33(17)
O(1)-C(1)-C(2)-C(12)	3.12(18)
C(6)-C(1)-C(2)-C(12)	-177.20(11)
C(1)-C(2)-C(3)-C(4)	-1.86(19)
C(12)-C(2)-C(3)-C(4)	176.65(12)
C(2)-C(3)-C(4)-C(5)	0.8(2)
C(3)-C(4)-C(5)-C(6)	0.9(2)
C(4)-C(5)-C(6)-C(1)	-1.42(19)
C(4)-C(5)-C(6)-C(7)	177.15(12)
O(1)-C(1)-C(6)-C(5)	179.94(11)
C(2)-C(1)-C(6)-C(5)	0.27(18)
O(1)-C(1)-C(6)-C(7)	1.36(17)
C(2)-C(1)-C(6)-C(7)	-178.31(12)
C(8)-N(1)-C(7)-C(6)	-65.06(14)
C(5)-C(6)-C(7)-N(1)	139.83(12)
C(1)-C(6)-C(7)-N(1)	-41.61(16)

C(7)-N(1)-C(8)-C(9)	-48.44(13)
C(7)-N(1)-C(8)-C(16)	-170.73(10)
C(11)-N(2)-C(9)-O(2)	3.13(19)
C(10)-N(2)-C(9)-O(2)	-178.84(13)
C(11)-N(2)-C(9)-C(8)	-175.71(12)
C(10)-N(2)-C(9)-C(8)	2.32(19)
N(1)-C(8)-C(9)-O(2)	-56.90(15)
C(16)-C(8)-C(9)-O(2)	64.87(15)
N(1)-C(8)-C(9)-N(2)	121.98(12)
C(16)-C(8)-C(9)-N(2)	-116.25(13)
C(3)-C(2)-C(12)-C(14)	119.40(13)
C(1)-C(2)-C(12)-C(14)	-62.15(15)
C(3)-C(2)-C(12)-C(13)	-119.37(13)
C(1)-C(2)-C(12)-C(13)	59.08(16)
C(3)-C(2)-C(12)-C(15)	-0.49(17)
C(1)-C(2)-C(12)-C(15)	177.96(12)
N(1)-C(8)-C(16)-C(17)	178.59(12)
C(9)-C(8)-C(16)-C(17)	56.14(15)
N(1)-C(8)-C(16)-C(18)	-56.50(15)
C(9)-C(8)-C(16)-C(18)	-178.95(13)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{18}H_{30}N_2O_2$ (2g) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...N(1)	0.839(13)	1.860(14)	2.6297(14)	151.9(15)
N(1)-H(1N)...O(2)#1	0.898(13)	2.167(14)	2.9439(14)	144.4(14)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+3/2,-z

X-ray Crystal Structure of S7 (Not shown in manuscript; see Chart S1 in Part A of the Supplementary Information)

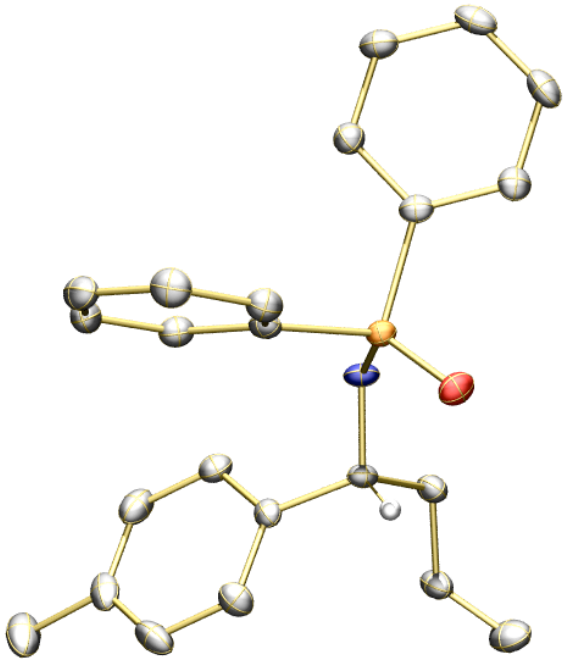

Table 1. Crystal data and structure refinement for $C_{23}H_{24}NOP$ (S7)

Identification code	$C_{23}H_{24}NOP$	
Empirical formula	$C_{23}H_{24}NOP$	
Formula weight	361.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)	
Unit cell dimensions	a = 9.9115(7) Å	α= 90°
	b = 19.7080(12) Å	β= 101.997(4)°
	c = 10.2367(7) Å	γ = 90°
Volume	1955.9(2) $Å^3$	
Z	4	
Density (calculated)	1.227 Mg/m^3	
Absorption coefficient	0.152 mm^{-1}	
F(000)	768	
Crystal size	0.14 x 0.08 x 0.05 mm^3	

Theta range for data collection	2.03 to 28.43°
Index ranges	-12<=h<=13, -26<=k<=26, -13<=l<=13
Reflections collected	42680
Independent reflections	9807 [R(int) = 0.0707]
Completeness to theta = 28.43°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9925 and 0.9791
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9807 / 5 / 483
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.0796
R indices (all data)	R1 = 0.0613, wR2 = 0.0867
Absolute structure parameter	0.04(6)
Extinction coefficient	na
Largest diff. peak and hole	0.360 and -0.247 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for XXX. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	9053(1)	7653(1)	1992(1)	17(1)
O(1)	8854(2)	7958(1)	634(1)	23(1)
N(1)	8318(2)	8098(1)	2991(2)	20(1)
C(1)	9941(3)	10334(1)	4205(3)	45(1)
C(2)	8899(3)	9939(1)	4126(2)	32(1)
C(3)	8960(2)	9179(1)	4177(2)	25(1)
C(4)	8168(2)	8840(1)	2881(2)	19(1)
C(5)	6664(2)	9044(1)	2560(2)	20(1)
C(6)	5698(2)	8734(1)	3176(2)	23(1)
C(7)	4332(2)	8937(1)	2895(2)	26(1)
C(8)	3876(2)	9459(1)	1984(2)	29(1)
C(9)	4839(3)	9758(1)	1368(2)	30(1)
C(10)	6201(2)	9557(1)	1641(2)	25(1)
C(11)	2404(3)	9694(1)	1729(3)	45(1)

C(12)	10858(2)	7526(1)	2686(2)	19(1)
C(13)	11354(2)	7499(1)	4063(2)	24(1)
C(14)	12722(2)	7348(1)	4577(2)	28(1)
C(15)	13616(2)	7227(1)	3721(2)	27(1)
C(16)	13136(2)	7261(1)	2359(2)	26(1)
C(17)	11762(2)	7410(1)	1837(2)	22(1)
C(18)	8271(2)	6825(1)	2005(2)	18(1)
C(19)	9019(2)	6240(1)	2433(2)	23(1)
C(20)	8367(2)	5614(1)	2356(2)	26(1)
C(21)	6966(2)	5564(1)	1842(2)	27(1)
C(22)	6217(2)	6140(1)	1423(2)	31(1)
C(23)	6856(2)	6769(1)	1504(2)	26(1)
P(2)	1823(1)	2359(1)	3130(1)	15(1)
O(2)	1432(1)	2673(1)	4319(1)	22(1)
N(2)	2302(2)	2892(1)	2097(2)	18(1)
C(24)	2526(3)	5298(1)	2712(2)	34(1)
C(25)	3013(2)	4794(1)	2109(2)	24(1)
C(26)	2293(2)	4125(1)	1794(2)	22(1)
C(27)	3094(2)	3516(1)	2530(2)	16(1)
C(28)	4549(2)	3499(1)	2299(2)	17(1)
C(29)	4824(2)	3329(1)	1062(2)	22(1)
C(30)	6148(2)	3380(1)	828(2)	28(1)
C(31)	7240(2)	3607(1)	1811(2)	27(1)
C(32)	6966(2)	3764(1)	3047(2)	28(1)
C(33)	5642(2)	3713(1)	3291(2)	24(1)
C(34)	8661(3)	3702(1)	1536(3)	40(1)
C(35)	409(2)	1896(1)	2116(2)	18(1)
C(36)	-925(2)	2044(1)	2252(2)	21(1)
C(37)	-2044(2)	1693(1)	1503(2)	25(1)
C(38)	-1821(2)	1187(1)	644(2)	25(1)
C(39)	-496(2)	1032(1)	503(2)	24(1)
C(40)	622(2)	1388(1)	1234(2)	21(1)
C(41)	3159(2)	1734(1)	3632(2)	18(1)
C(42)	3063(2)	1295(1)	4685(2)	21(1)
C(43)	3994(2)	766(1)	5009(2)	24(1)
C(44)	5029(2)	671(1)	4313(2)	24(1)

C(45)	5157(2)	1112(1)	3295(2)	24(1)
C(46)	4218(2)	1640(1)	2943(2)	20(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{23}H_{24}NOP$ (S7)

P(1)-O(1)	1.4889(14)
P(1)-N(1)	1.6299(18)
P(1)-C(12)	1.800(2)
P(1)-C(18)	1.806(2)
N(1)-C(4)	1.472(2)
N(1)-H(1N)	0.855(15)
C(1)-C(2)	1.283(3)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(3)	1.499(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.546(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.512(3)
C(4)-H(4)	0.987(16)
C(5)-C(6)	1.393(3)
C(5)-C(10)	1.393(3)
C(6)-C(7)	1.384(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.398(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.381(4)
C(8)-C(11)	1.501(3)
C(9)-C(10)	1.378(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800

C(11)-H(11C)	0.9800
C(12)-C(17)	1.391(3)
C(12)-C(13)	1.393(3)
C(13)-C(14)	1.382(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.390(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.378(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.386(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.393(3)
C(18)-C(23)	1.393(3)
C(19)-C(20)	1.386(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.383(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.377(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.387(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
P(2)-O(2)	1.4868(14)
P(2)-N(2)	1.6297(18)
P(2)-C(41)	1.803(2)
P(2)-C(35)	1.807(2)
N(2)-C(27)	1.476(2)
N(2)-H(2N)	0.841(15)
C(24)-C(25)	1.313(3)
C(24)-H(24A)	0.9500
C(24)-H(24B)	0.9500
C(25)-C(26)	1.501(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.546(3)
C(26)-H(26A)	0.9900

C(26)-H(26B)	0.9900
C(27)-C(28)	1.509(3)
C(27)-H(27)	1.005(15)
C(28)-C(33)	1.388(3)
C(28)-C(29)	1.390(3)
C(29)-C(30)	1.385(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.390(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.383(3)
C(31)-C(34)	1.503(3)
C(32)-C(33)	1.390(3)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.389(3)
C(35)-C(40)	1.393(3)
C(36)-C(37)	1.394(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.378(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.385(3)
C(38)-H(38)	0.9500
C(39)-C(40)	1.390(3)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
C(41)-C(46)	1.393(3)
C(41)-C(42)	1.401(3)
C(42)-C(43)	1.387(3)
C(42)-H(42)	0.9500
C(43)-C(44)	1.378(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.381(3)
C(44)-H(44)	0.9500

C(45)-C(46)	1.393(3)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
O(1)-P(1)-N(1)	112.21(9)
O(1)-P(1)-C(12)	110.65(9)
N(1)-P(1)-C(12)	111.32(9)
O(1)-P(1)-C(18)	113.47(9)
N(1)-P(1)-C(18)	103.48(9)
C(12)-P(1)-C(18)	105.33(9)
C(4)-N(1)-P(1)	122.62(15)
C(4)-N(1)-H(1N)	116.6(15)
P(1)-N(1)-H(1N)	116.4(15)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(3)	125.4(2)
C(1)-C(2)-H(2)	117.3
C(3)-C(2)-H(2)	117.3
C(2)-C(3)-C(4)	113.09(17)
C(2)-C(3)-H(3A)	109.0
C(4)-C(3)-H(3A)	109.0
C(2)-C(3)-H(3B)	109.0
C(4)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
N(1)-C(4)-C(5)	111.13(17)
N(1)-C(4)-C(3)	109.79(16)
C(5)-C(4)-C(3)	111.93(17)
N(1)-C(4)-H(4)	107.0(13)
C(5)-C(4)-H(4)	110.2(13)
C(3)-C(4)-H(4)	106.6(13)
C(6)-C(5)-C(10)	117.6(2)
C(6)-C(5)-C(4)	121.63(18)
C(10)-C(5)-C(4)	120.8(2)
C(7)-C(6)-C(5)	121.0(2)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5

C(6)-C(7)-C(8)	121.2(2)
C(6)-C(7)-H(7)	119.4
C(8)-C(7)-H(7)	119.4
C(9)-C(8)-C(7)	117.5(2)
C(9)-C(8)-C(11)	121.8(2)
C(7)-C(8)-C(11)	120.7(2)
C(10)-C(9)-C(8)	121.6(2)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(9)-C(10)-C(5)	121.2(2)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	119.24(18)
C(17)-C(12)-P(1)	119.50(15)
C(13)-C(12)-P(1)	121.14(16)
C(14)-C(13)-C(12)	120.3(2)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	120.0(2)
C(13)-C(14)-H(14)	120.0
C(15)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	119.9(2)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(17)	120.3(2)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(16)-C(17)-C(12)	120.15(19)
C(16)-C(17)-H(17)	119.9
C(12)-C(17)-H(17)	119.9

C(19)-C(18)-C(23)	118.62(19)
C(19)-C(18)-P(1)	123.33(16)
C(23)-C(18)-P(1)	117.98(15)
C(20)-C(19)-C(18)	120.6(2)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(21)-C(20)-C(19)	120.3(2)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	119.6(2)
C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	120.6(2)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(22)-C(23)-C(18)	120.3(2)
C(22)-C(23)-H(23)	119.8
C(18)-C(23)-H(23)	119.8
O(2)-P(2)-N(2)	115.09(9)
O(2)-P(2)-C(41)	110.59(9)
N(2)-P(2)-C(41)	109.20(10)
O(2)-P(2)-C(35)	112.16(9)
N(2)-P(2)-C(35)	104.38(9)
C(41)-P(2)-C(35)	104.77(9)
C(27)-N(2)-P(2)	123.38(13)
C(27)-N(2)-H(2N)	117.9(15)
P(2)-N(2)-H(2N)	117.0(15)
C(25)-C(24)-H(24A)	120.0
C(25)-C(24)-H(24B)	120.0
H(24A)-C(24)-H(24B)	120.0
C(24)-C(25)-C(26)	124.1(2)
C(24)-C(25)-H(25)	117.9
C(26)-C(25)-H(25)	117.9
C(25)-C(26)-C(27)	113.86(16)
C(25)-C(26)-H(26A)	108.8
C(27)-C(26)-H(26A)	108.8

C(25)-C(26)-H(26B)	108.8
C(27)-C(26)-H(26B)	108.8
H(26A)-C(26)-H(26B)	107.7
N(2)-C(27)-C(28)	113.55(16)
N(2)-C(27)-C(26)	108.28(15)
C(28)-C(27)-C(26)	110.55(16)
N(2)-C(27)-H(27)	104.8(12)
C(28)-C(27)-H(27)	112.6(12)
C(26)-C(27)-H(27)	106.6(12)
C(33)-C(28)-C(29)	117.90(19)
C(33)-C(28)-C(27)	120.33(18)
C(29)-C(28)-C(27)	121.52(18)
C(30)-C(29)-C(28)	120.8(2)
C(30)-C(29)-H(29)	119.6
C(28)-C(29)-H(29)	119.6
C(29)-C(30)-C(31)	121.5(2)
C(29)-C(30)-H(30)	119.3
C(31)-C(30)-H(30)	119.3
C(32)-C(31)-C(30)	117.5(2)
C(32)-C(31)-C(34)	120.9(2)
C(30)-C(31)-C(34)	121.6(2)
C(31)-C(32)-C(33)	121.4(2)
C(31)-C(32)-H(32)	119.3
C(33)-C(32)-H(32)	119.3
C(28)-C(33)-C(32)	120.9(2)
C(28)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-C(40)	119.42(19)
C(36)-C(35)-P(2)	118.47(15)
C(40)-C(35)-P(2)	122.09(16)

C(35)-C(36)-C(37)	120.3(2)
C(35)-C(36)-H(36)	119.8
C(37)-C(36)-H(36)	119.8
C(38)-C(37)-C(36)	119.7(2)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.5(2)
C(37)-C(38)-H(38)	119.8
C(39)-C(38)-H(38)	119.8
C(38)-C(39)-C(40)	120.0(2)
C(38)-C(39)-H(39)	120.0
C(40)-C(39)-H(39)	120.0
C(39)-C(40)-C(35)	120.0(2)
C(39)-C(40)-H(40)	120.0
C(35)-C(40)-H(40)	120.0
C(46)-C(41)-C(42)	119.07(19)
C(46)-C(41)-P(2)	122.18(15)
C(42)-C(41)-P(2)	118.55(16)
C(43)-C(42)-C(41)	120.0(2)
C(43)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	120.5(2)
C(44)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8
C(43)-C(44)-C(45)	120.0(2)
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(44)-C(45)-C(46)	120.3(2)
C(44)-C(45)-H(45)	119.9
C(46)-C(45)-H(45)	119.9
C(41)-C(46)-C(45)	120.1(2)
C(41)-C(46)-H(46)	120.0
C(45)-C(46)-H(46)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{23}H_{24}NOP$ (S7). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	19(1)	17(1)	12(1)	1(1)	1(1)	4(1)
O(1)	28(1)	26(1)	14(1)	2(1)	2(1)	3(1)
N(1)	28(1)	16(1)	15(1)	4(1)	5(1)	5(1)
C(1)	51(2)	38(1)	42(2)	5(1)	4(1)	-8(1)
C(2)	35(1)	25(1)	32(1)	-2(1)	-5(1)	1(1)
C(3)	28(1)	20(1)	23(1)	1(1)	0(1)	2(1)
C(4)	27(1)	15(1)	16(1)	2(1)	5(1)	3(1)
C(5)	29(1)	15(1)	13(1)	-4(1)	0(1)	2(1)
C(6)	30(1)	18(1)	20(1)	2(1)	2(1)	3(1)
C(7)	29(1)	24(1)	26(1)	-5(1)	4(1)	0(1)
C(8)	30(1)	27(1)	26(1)	-4(1)	-3(1)	9(1)
C(9)	41(1)	22(1)	24(1)	1(1)	-1(1)	11(1)
C(10)	36(1)	19(1)	18(1)	0(1)	3(1)	4(1)
C(11)	32(2)	49(2)	49(2)	-3(1)	-2(1)	18(1)
C(12)	22(1)	14(1)	20(1)	-1(1)	2(1)	1(1)
C(13)	25(1)	24(1)	22(1)	0(1)	1(1)	3(1)
C(14)	28(1)	25(1)	26(1)	3(1)	-4(1)	3(1)
C(15)	17(1)	19(1)	42(1)	1(1)	-2(1)	2(1)
C(16)	23(1)	22(1)	36(1)	0(1)	11(1)	0(1)
C(17)	26(1)	18(1)	21(1)	-1(1)	3(1)	-1(1)
C(18)	24(1)	18(1)	13(1)	-2(1)	5(1)	3(1)
C(19)	23(1)	22(1)	23(1)	0(1)	3(1)	3(1)
C(20)	30(1)	20(1)	26(1)	0(1)	4(1)	4(1)
C(21)	34(1)	21(1)	25(1)	-5(1)	6(1)	-7(1)
C(22)	22(1)	30(1)	37(1)	-1(1)	-2(1)	-4(1)
C(23)	24(1)	21(1)	30(1)	1(1)	-1(1)	4(1)
P(2)	18(1)	15(1)	13(1)	0(1)	2(1)	-1(1)
O(2)	28(1)	22(1)	16(1)	-2(1)	7(1)	0(1)
N(2)	23(1)	16(1)	13(1)	-1(1)	0(1)	-5(1)
C(24)	39(1)	21(1)	38(1)	-3(1)	-2(1)	1(1)

C(25)	20(1)	20(1)	31(1)	1(1)	0(1)	-2(1)
C(26)	18(1)	21(1)	26(1)	-1(1)	-1(1)	-1(1)
C(27)	18(1)	17(1)	14(1)	-2(1)	2(1)	-4(1)
C(28)	18(1)	14(1)	20(1)	3(1)	3(1)	1(1)
C(29)	27(1)	17(1)	23(1)	-1(1)	5(1)	-1(1)
C(30)	36(1)	22(1)	31(1)	-1(1)	17(1)	0(1)
C(31)	23(1)	16(1)	44(1)	8(1)	12(1)	3(1)
C(32)	20(1)	28(1)	34(1)	8(1)	-4(1)	-4(1)
C(33)	23(1)	27(1)	20(1)	4(1)	1(1)	0(1)
C(34)	29(1)	26(1)	68(2)	7(1)	21(1)	-1(1)
C(35)	23(1)	15(1)	16(1)	3(1)	3(1)	-2(1)
C(36)	23(1)	19(1)	21(1)	5(1)	8(1)	0(1)
C(37)	16(1)	29(1)	30(1)	9(1)	4(1)	-2(1)
C(38)	23(1)	24(1)	26(1)	7(1)	-3(1)	-9(1)
C(39)	28(1)	20(1)	22(1)	-1(1)	0(1)	-3(1)
C(40)	20(1)	20(1)	22(1)	1(1)	4(1)	0(1)
C(41)	17(1)	18(1)	15(1)	-2(1)	-2(1)	-2(1)
C(42)	22(1)	23(1)	19(1)	1(1)	4(1)	-1(1)
C(43)	29(1)	24(1)	19(1)	6(1)	3(1)	0(1)
C(44)	24(1)	18(1)	27(1)	0(1)	0(1)	2(1)
C(45)	19(1)	23(1)	31(1)	-4(1)	7(1)	0(1)
C(46)	24(1)	20(1)	18(1)	0(1)	5(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{23}H_{24}NOP$ (S7)

	x	y	z	U(eq)
H(1N)	8320(20)	7925(11)	3756(17)	24
H(1A)	10842	10150	4305	54
H(1B)	9812	10812	4164	54
H(2)	8017	10144	4027	39
H(3A)	8569	9020	4937	30
H(3B)	9937	9034	4341	30

H(4)	8630(20)	8986(11)	2160(19)	23
H(6)	5981	8378	3798	28
H(7)	3691	8718	3329	32
H(9)	4556	10112	740	36
H(10)	6834	9772	1194	30
H(11A)	2303	10045	2381	67
H(11B)	1802	9310	1815	67
H(11C)	2147	9882	825	67
H(13)	10747	7586	4651	29
H(14)	13053	7327	5516	33
H(15)	14556	7122	4074	33
H(16)	13749	7181	1775	32
H(17)	11438	7433	897	26
H(19)	9983	6269	2780	28
H(20)	8886	5218	2659	31
H(21)	6524	5134	1779	32
H(22)	5253	6107	1074	37
H(23)	6327	7164	1216	31
H(2N)	1920(20)	2858(11)	1287(16)	22
H(24A)	1668	5252	2977	41
H(24B)	3033	5709	2882	41
H(25)	3874	4856	1857	29
H(26A)	2142	4045	820	27
H(26B)	1377	4150	2035	27
H(27)	3060(20)	3566(10)	3500(16)	20
H(29)	4096	3176	369	27
H(30)	6312	3256	-22	34
H(32)	7698	3910	3743	34
H(33)	5484	3825	4148	29
H(34A)	8775	4174	1278	60
H(34B)	8781	3399	808	60
H(34C)	9352	3593	2342	60
H(36)	-1076	2387	2858	25
H(37)	-2956	1802	1584	30
H(38)	-2582	942	146	30
H(39)	-350	683	-92	29

H(40)	1530	1285	1131	25
H(42)	2358	1359	5176	26
H(43)	3918	466	5717	29
H(44)	5655	304	4532	29
H(45)	5887	1053	2834	29
H(46)	4301	1937	2233	25

Table 6. Torsion angles [°] for $C_{23}H_{24}NOP$ (S7)

O(1)-P(1)-N(1)-C(4)	-31.06(19)
C(12)-P(1)-N(1)-C(4)	93.57(17)
C(18)-P(1)-N(1)-C(4)	-153.76(16)
C(1)-C(2)-C(3)-C(4)	-117.7(3)
P(1)-N(1)-C(4)-C(5)	117.35(18)
P(1)-N(1)-C(4)-C(3)	-118.27(18)
C(2)-C(3)-C(4)-N(1)	177.94(19)
C(2)-C(3)-C(4)-C(5)	-58.2(3)
N(1)-C(4)-C(5)-C(6)	41.9(3)
C(3)-C(4)-C(5)-C(6)	-81.2(2)
N(1)-C(4)-C(5)-C(10)	-138.74(19)
C(3)-C(4)-C(5)-C(10)	98.1(2)
C(10)-C(5)-C(6)-C(7)	-0.9(3)
C(4)-C(5)-C(6)-C(7)	178.47(19)
C(5)-C(6)-C(7)-C(8)	0.1(3)
C(6)-C(7)-C(8)-C(9)	0.6(3)
C(6)-C(7)-C(8)-C(11)	-177.5(2)
C(7)-C(8)-C(9)-C(10)	-0.4(3)
C(11)-C(8)-C(9)-C(10)	177.6(2)
C(8)-C(9)-C(10)-C(5)	-0.4(3)
C(6)-C(5)-C(10)-C(9)	1.1(3)
C(4)-C(5)-C(10)-C(9)	-178.31(19)
O(1)-P(1)-C(12)-C(17)	-28.89(18)
N(1)-P(1)-C(12)-C(17)	-154.39(15)
C(18)-P(1)-C(12)-C(17)	94.11(17)

O(1)-P(1)-C(12)-C(13)	155.11(15)
N(1)-P(1)-C(12)-C(13)	29.61(19)
C(18)-P(1)-C(12)-C(13)	-81.89(17)
C(17)-C(12)-C(13)-C(14)	-1.1(3)
P(1)-C(12)-C(13)-C(14)	174.89(16)
C(12)-C(13)-C(14)-C(15)	0.5(3)
C(13)-C(14)-C(15)-C(16)	0.2(3)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
C(15)-C(16)-C(17)-C(12)	-0.2(3)
C(13)-C(12)-C(17)-C(16)	0.9(3)
P(1)-C(12)-C(17)-C(16)	-175.13(15)
O(1)-P(1)-C(18)-C(19)	118.70(18)
N(1)-P(1)-C(18)-C(19)	-119.45(18)
C(12)-P(1)-C(18)-C(19)	-2.5(2)
O(1)-P(1)-C(18)-C(23)	-58.24(19)
N(1)-P(1)-C(18)-C(23)	63.61(18)
C(12)-P(1)-C(18)-C(23)	-179.42(16)
C(23)-C(18)-C(19)-C(20)	0.2(3)
P(1)-C(18)-C(19)-C(20)	-176.75(17)
C(18)-C(19)-C(20)-C(21)	0.6(3)
C(19)-C(20)-C(21)-C(22)	-0.9(3)
C(20)-C(21)-C(22)-C(23)	0.4(4)
C(21)-C(22)-C(23)-C(18)	0.4(4)
C(19)-C(18)-C(23)-C(22)	-0.7(3)
P(1)-C(18)-C(23)-C(22)	176.43(18)
O(2)-P(2)-N(2)-C(27)	35.84(19)
C(41)-P(2)-N(2)-C(27)	-89.21(17)
C(35)-P(2)-N(2)-C(27)	159.20(16)
C(24)-C(25)-C(26)-C(27)	-116.1(2)
P(2)-N(2)-C(27)-C(28)	111.83(18)
P(2)-N(2)-C(27)-C(26)	-124.99(17)
C(25)-C(26)-C(27)-N(2)	-177.98(18)
C(25)-C(26)-C(27)-C(28)	-53.0(2)
N(2)-C(27)-C(28)-C(33)	-134.69(19)
C(26)-C(27)-C(28)-C(33)	103.4(2)
N(2)-C(27)-C(28)-C(29)	51.1(2)

C(26)-C(27)-C(28)-C(29)	-70.9(2)
C(33)-C(28)-C(29)-C(30)	-0.7(3)
C(27)-C(28)-C(29)-C(30)	173.62(19)
C(28)-C(29)-C(30)-C(31)	-0.6(3)
C(29)-C(30)-C(31)-C(32)	1.7(3)
C(29)-C(30)-C(31)-C(34)	-176.4(2)
C(30)-C(31)-C(32)-C(33)	-1.6(3)
C(34)-C(31)-C(32)-C(33)	176.6(2)
C(29)-C(28)-C(33)-C(32)	0.9(3)
C(27)-C(28)-C(33)-C(32)	-173.51(19)
C(31)-C(32)-C(33)-C(28)	0.2(3)
O(2)-P(2)-C(35)-C(36)	20.04(18)
N(2)-P(2)-C(35)-C(36)	-105.21(16)
C(41)-P(2)-C(35)-C(36)	140.04(16)
O(2)-P(2)-C(35)-C(40)	-158.36(15)
N(2)-P(2)-C(35)-C(40)	76.39(18)
C(41)-P(2)-C(35)-C(40)	-38.36(19)
C(40)-C(35)-C(36)-C(37)	-0.7(3)
P(2)-C(35)-C(36)-C(37)	-179.10(15)
C(35)-C(36)-C(37)-C(38)	1.4(3)
C(36)-C(37)-C(38)-C(39)	-1.1(3)
C(37)-C(38)-C(39)-C(40)	0.2(3)
C(38)-C(39)-C(40)-C(35)	0.5(3)
C(36)-C(35)-C(40)-C(39)	-0.3(3)
P(2)-C(35)-C(40)-C(39)	178.10(16)
O(2)-P(2)-C(41)-C(46)	-143.20(16)
N(2)-P(2)-C(41)-C(46)	-15.57(19)
C(35)-P(2)-C(41)-C(46)	95.76(18)
O(2)-P(2)-C(41)-C(42)	41.95(18)
N(2)-P(2)-C(41)-C(42)	169.58(15)
C(35)-P(2)-C(41)-C(42)	-79.09(17)
C(46)-C(41)-C(42)-C(43)	-1.5(3)
P(2)-C(41)-C(42)-C(43)	173.55(16)
C(41)-C(42)-C(43)-C(44)	0.7(3)
C(42)-C(43)-C(44)-C(45)	0.9(3)
C(43)-C(44)-C(45)-C(46)	-1.8(3)

C(42)-C(41)-C(46)-C(45)	0.6(3)
P(2)-C(41)-C(46)-C(45)	-174.26(15)
C(44)-C(45)-C(46)-C(41)	1.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{23}H_{24}NOP$ (S7) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(2)#1	0.855(15)	1.998(16)	2.840(2)	169(2)
N(2)-H(2N)...O(1)#2	0.841(15)	1.966(16)	2.796(2)	169(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y+1/2,-z+1 #2 -x+1,y-1/2,-z

X-ray Crystal Structure of S12 (Table 4)

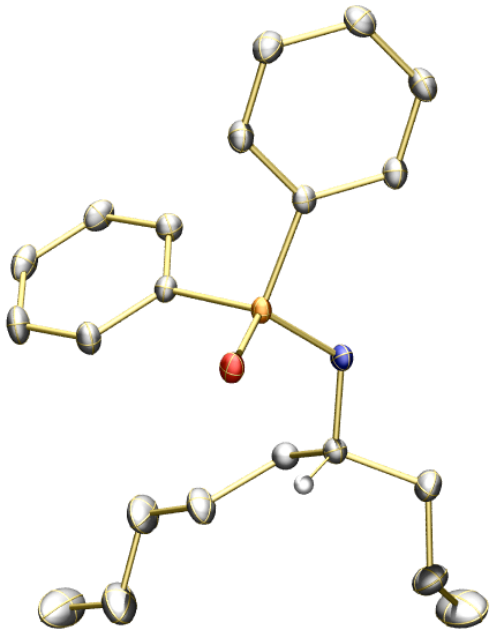

Table 1. Crystal data and structure refinement for $C_{21}H_{26}NOP$ (S12)

Identification code	$C_{21}H_{26}NOP$	
Empirical formula	$C_{21}H_{26}NOP$	
Formula weight	339.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)	
Unit cell dimensions	a = 5.3475(3) Å	α= 90°
	b = 8.4812(4) Å	β= 91.983(2)°
	c = 21.2781(10) Å	γ = 90°
Volume	964.45(8) $Å^3$	
Z	2	
Density (calculated)	1.169 Mg/m^3	
Absorption coefficient	0.149 mm^{-1}	
F(000)	364	
Crystal size	0.30 x 0.24 x 0.08 mm^3	
Theta range for data collection	1.92 to 28.48°	
Index ranges	-7<=h<=7, -11<=k<=11, -28<=l<=28	
Reflections collected	39105	
Independent reflections	4895 [R(int) = 0.0215]	
Completeness to theta = 28.48°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9882 and 0.9566	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4895 / 77 / 253	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0718	
R indices (all data)	R1 = 0.0278, wR2 = 0.0722	
Absolute structure parameter	0.00(5)	
Extinction coefficient	na	
Largest diff. peak and hole	0.404 and -0.262 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{21}H_{26}NOP$ (S12). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	520(1)	-860(1)	8324(1)	13(1)
O(1)	-1929(1)	-1644(1)	8175(1)	17(1)
N(1)	2774(2)	-1603(1)	7910(1)	16(1)
C(1)	5612(4)	-3552(4)	5942(1)	62(1)
C(2)	3843(3)	-3594(2)	6350(1)	36(1)
C(3)	4157(2)	-3166(2)	7029(1)	25(1)
C(4)	2418(2)	-1834(1)	7224(1)	17(1)
C(5)	2527(10)	-366(5)	6853(2)	25(1)
C(6)	698(7)	310(4)	6539(1)	29(1)
C(7)	855(8)	1837(4)	6190(2)	40(1)
C(8)	-89(8)	1743(5)	5514(2)	46(1)
C(9)	17(11)	3306(5)	5178(2)	63(1)
C(5X)	3096(9)	-323(6)	6874(3)	20(1)
C(6X)	1493(8)	673(5)	6602(2)	36(1)
C(7X)	2153(8)	2236(5)	6320(2)	46(1)
C(8X)	1431(9)	2386(6)	5634(2)	60(1)
C(9X)	-1310(11)	2407(8)	5500(3)	80(2)
C(10)	1615(2)	-1035(1)	9129(1)	15(1)
C(11)	3681(2)	-1934(1)	9332(1)	19(1)
C(12)	4308(2)	-2036(2)	9972(1)	22(1)
C(13)	2892(2)	-1251(1)	10408(1)	22(1)
C(14)	841(2)	-353(2)	10210(1)	23(1)
C(15)	211(2)	-247(2)	9573(1)	20(1)
C(16)	159(2)	1236(1)	8196(1)	15(1)
C(17)	1976(2)	2315(1)	8408(1)	19(1)
C(18)	1664(2)	3917(1)	8290(1)	23(1)
C(19)	-454(3)	4460(1)	7960(1)	25(1)
C(20)	-2246(2)	3391(2)	7741(1)	26(1)
C(21)	-1952(2)	1790(2)	7864(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{21}H_{26}NOP$ (S12)

P(1)-O(1)	1.4931(8)
P(1)-N(1)	1.6428(9)
P(1)-C(10)	1.7978(11)
P(1)-C(16)	1.8083(12)
N(1)-C(4)	1.4767(14)
N(1)-H(1N)	0.885(13)
C(1)-C(2)	1.307(3)
C(1)-H(1A)	0.993(17)
C(1)-H(1B)	0.986(16)
C(2)-C(3)	1.4923(19)
C(2)-H(2)	0.980(15)
C(3)-C(4)	1.5302(16)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.477(5)
C(4)-H(4)	0.989(12)
C(5)-C(6)	1.298(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.497(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.509(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.509(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(15)	1.3976(15)
C(10)-C(11)	1.3991(15)
C(11)-C(12)	1.3924(17)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3886(17)

C(12)-H(12)	0.9500
C(13)-C(14)	1.3889(17)
C(13)-H(13)	0.9500
C(14)-C(15)	1.3867(17)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.3922(15)
C(16)-C(17)	1.3979(16)
C(17)-C(18)	1.3900(17)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3914(18)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.3902(18)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500

O(1)-P(1)-N(1)	111.71(5)
O(1)-P(1)-C(10)	114.84(5)
N(1)-P(1)-C(10)	105.01(5)
O(1)-P(1)-C(16)	108.53(5)
N(1)-P(1)-C(16)	111.89(5)
C(10)-P(1)-C(16)	104.70(5)
C(4)-N(1)-P(1)	120.56(7)
C(4)-N(1)-H(1N)	115.7(10)
P(1)-N(1)-H(1N)	118.5(10)
C(2)-C(1)-H(1A)	119.6(17)
C(2)-C(1)-H(1B)	122.8(16)
H(1A)-C(1)-H(1B)	118(2)
C(1)-C(2)-C(3)	125.23(16)
C(1)-C(2)-H(2)	117.9(12)
C(3)-C(2)-H(2)	116.9(12)
C(2)-C(3)-C(4)	113.21(11)
C(2)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3A)	108.9

C(2)-C(3)-H(3B)	108.9
C(4)-C(3)-H(3B)	108.9
H(3A)-C(3)-H(3B)	107.7
C(5)-C(4)-N(1)	114.2(2)
C(5)-C(4)-C(3)	116.2(2)
N(1)-C(4)-C(3)	107.93(9)
C(5)-C(4)-H(4)	99.3(10)
N(1)-C(4)-H(4)	107.5(9)
C(3)-C(4)-H(4)	111.2(10)
C(6)-C(5)-C(4)	127.2(4)
C(6)-C(5)-H(5)	116.4
C(4)-C(5)-H(5)	116.4
C(5)-C(6)-C(7)	125.7(4)
C(5)-C(6)-H(6)	117.2
C(7)-C(6)-H(6)	117.2
C(6)-C(7)-C(8)	113.9(3)
C(6)-C(7)-H(7A)	108.8
C(8)-C(7)-H(7A)	108.8
C(6)-C(7)-H(7B)	108.8
C(8)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
C(7)-C(8)-C(9)	112.9(3)
C(7)-C(8)-H(8A)	109.0
C(9)-C(8)-H(8A)	109.0
C(7)-C(8)-H(8B)	109.0
C(9)-C(8)-H(8B)	109.0
H(8A)-C(8)-H(8B)	107.8
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(15)-C(10)-C(11)	119.24(10)
C(15)-C(10)-P(1)	116.15(8)
C(11)-C(10)-P(1)	124.57(8)

C(12)-C(11)-C(10)	119.79(11)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(13)-C(12)-C(11)	120.37(11)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(12)-C(13)-C(14)	120.16(11)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	119.70(11)
C(15)-C(14)-H(14)	120.2
C(13)-C(14)-H(14)	120.2
C(14)-C(15)-C(10)	120.75(11)
C(14)-C(15)-H(15)	119.6
C(10)-C(15)-H(15)	119.6
C(21)-C(16)-C(17)	119.01(11)
C(21)-C(16)-P(1)	119.24(9)
C(17)-C(16)-P(1)	121.73(9)
C(18)-C(17)-C(16)	120.27(11)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(17)-C(18)-C(19)	120.32(11)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(20)-C(19)-C(18)	119.57(11)
C(20)-C(19)-H(19)	120.2
C(18)-C(19)-H(19)	120.2
C(19)-C(20)-C(21)	120.21(12)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(20)-C(21)-C(16)	120.60(12)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{21}H_{26}NOP$ (S12). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	9(1)	12(1)	18(1)	0(1)	0(1)	0(1)
O(1)	10(1)	16(1)	26(1)	-3(1)	-1(1)	-1(1)
N(1)	11(1)	18(1)	18(1)	-2(1)	0(1)	2(1)
C(1)	57(1)	95(2)	33(1)	-19(1)	9(1)	12(1)
C(2)	36(1)	40(1)	31(1)	-15(1)	0(1)	8(1)
C(3)	26(1)	26(1)	24(1)	-2(1)	3(1)	9(1)
C(4)	14(1)	18(1)	18(1)	-1(1)	0(1)	2(1)
C(5)	24(2)	27(2)	26(2)	3(1)	2(2)	-1(2)
C(6)	30(2)	31(2)	24(1)	10(1)	2(1)	8(2)
C(7)	55(2)	34(2)	30(1)	9(1)	-1(1)	15(2)
C(8)	54(2)	53(2)	32(2)	9(2)	2(1)	20(2)
C(9)	116(4)	41(2)	31(2)	9(2)	-6(2)	15(2)
C(10)	13(1)	12(1)	18(1)	2(1)	1(1)	-1(1)
C(11)	15(1)	19(1)	22(1)	1(1)	2(1)	3(1)
C(12)	18(1)	26(1)	24(1)	5(1)	-1(1)	3(1)
C(13)	23(1)	24(1)	19(1)	5(1)	0(1)	-1(1)
C(14)	25(1)	23(1)	20(1)	1(1)	6(1)	4(1)
C(15)	18(1)	20(1)	22(1)	2(1)	3(1)	4(1)
C(16)	15(1)	13(1)	17(1)	1(1)	2(1)	2(1)
C(17)	18(1)	17(1)	21(1)	1(1)	0(1)	-1(1)
C(18)	28(1)	14(1)	26(1)	0(1)	4(1)	-3(1)
C(19)	30(1)	15(1)	30(1)	4(1)	9(1)	4(1)
C(20)	22(1)	22(1)	33(1)	7(1)	1(1)	7(1)
C(21)	16(1)	20(1)	28(1)	1(1)	-2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3)

for $C_{21}H_{26}NOP$ (S12)

	x	y	z	U(eq)
H(1N)	4340(20)	-1474(19)	8048(7)	19
H(1A)	7340(40)	-3260(30)	6082(13)	74
H(1B)	5330(50)	-3860(30)	5497(8)	74
H(2)	2180(30)	-3950(20)	6204(10)	43
H(3A)	5913	-2841	7116	30
H(3B)	3830	-4109	7287	30
H(4)	640(20)	-2114(19)	7140(7)	20
H(5)	4110	140	6843	31
H(6)	-877	-210	6531	34
H(7A)	2620	2190	6199	48
H(7B)	-128	2642	6410	48
H(8A)	-1840	1362	5503	56
H(8B)	928	965	5289	56
H(9A)	-656	3184	4746	94
H(9B)	1757	3666	5169	94
H(9C)	-983	4084	5399	94
H(5X)	4825	-80	6850	24
H(6X)	-220	375	6584	43
H(7XA)	1313	3082	6554	55
H(7XB)	3981	2399	6374	55
H(8XA)	2162	3370	5471	72
H(8XB)	2167	1493	5404	72
H(9XA)	-1640	2485	5045	120
H(9XB)	-2048	3317	5709	120
H(9XC)	-2053	1434	5658	120
H(11)	4654	-2474	9035	23
H(12)	5711	-2647	10110	27
H(13)	3327	-1328	10844	27
H(14)	-125	186	10508	27
H(15)	-1191	368	9438	24
H(17)	3429	1952	8633	23

H(18)	2904	4644	8437	27
H(19)	-672	5556	7883	30
H(20)	-3677	3753	7507	31
H(21)	-3204	1068	7721	26

Table 6. Torsion angles [°] for $C_{21}H_{26}NOP$ (S12)

O(1)-P(1)-N(1)-C(4)	47.67(10)
C(10)-P(1)-N(1)-C(4)	172.76(9)
C(16)-P(1)-N(1)-C(4)	-74.24(10)
C(1)-C(2)-C(3)-C(4)	121.7(2)
P(1)-N(1)-C(4)-C(5)	75.1(2)
P(1)-N(1)-C(4)-C(3)	-154.04(9)
C(2)-C(3)-C(4)-C(5)	-54.4(3)
C(2)-C(3)-C(4)-N(1)	175.89(12)
N(1)-C(4)-C(5)-C(6)	-111.9(5)
C(3)-C(4)-C(5)-C(6)	121.5(5)
C(4)-C(5)-C(6)-C(7)	177.3(4)
C(5)-C(6)-C(7)-C(8)	127.5(5)
C(6)-C(7)-C(8)-C(9)	178.3(4)
O(1)-P(1)-C(10)-C(15)	-67.14(10)
N(1)-P(1)-C(10)-C(15)	169.76(9)
C(16)-P(1)-C(10)-C(15)	51.77(10)
O(1)-P(1)-C(10)-C(11)	110.54(10)
N(1)-P(1)-C(10)-C(11)	-12.56(11)
C(16)-P(1)-C(10)-C(11)	-130.55(10)
C(15)-C(10)-C(11)-C(12)	0.16(17)
P(1)-C(10)-C(11)-C(12)	-177.45(9)
C(10)-C(11)-C(12)-C(13)	0.03(18)
C(11)-C(12)-C(13)-C(14)	-0.18(19)
C(12)-C(13)-C(14)-C(15)	0.13(19)
C(13)-C(14)-C(15)-C(10)	0.06(19)
C(11)-C(10)-C(15)-C(14)	-0.20(18)
P(1)-C(10)-C(15)-C(14)	177.61(10)

O(1)-P(1)-C(16)-C(21)	-14.04(11)
N(1)-P(1)-C(16)-C(21)	109.67(10)
C(10)-P(1)-C(16)-C(21)	-137.13(9)
O(1)-P(1)-C(16)-C(17)	167.59(9)
N(1)-P(1)-C(16)-C(17)	-68.70(10)
C(10)-P(1)-C(16)-C(17)	44.50(10)
C(21)-C(16)-C(17)-C(18)	0.30(18)
P(1)-C(16)-C(17)-C(18)	178.68(9)
C(16)-C(17)-C(18)-C(19)	-0.20(19)
C(17)-C(18)-C(19)-C(20)	-0.64(19)
C(18)-C(19)-C(20)-C(21)	1.37(19)
C(19)-C(20)-C(21)-C(16)	-1.3(2)
C(17)-C(16)-C(21)-C(20)	0.43(18)
P(1)-C(16)-C(21)-C(20)	-177.98(10)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{21}H_{26}NOP$ (S12) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(1)#1	0.885(13)	2.009(13)	2.8692(12)	163.7(14)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z

X-ray Crystal Structure of 10 (Figure 3a)

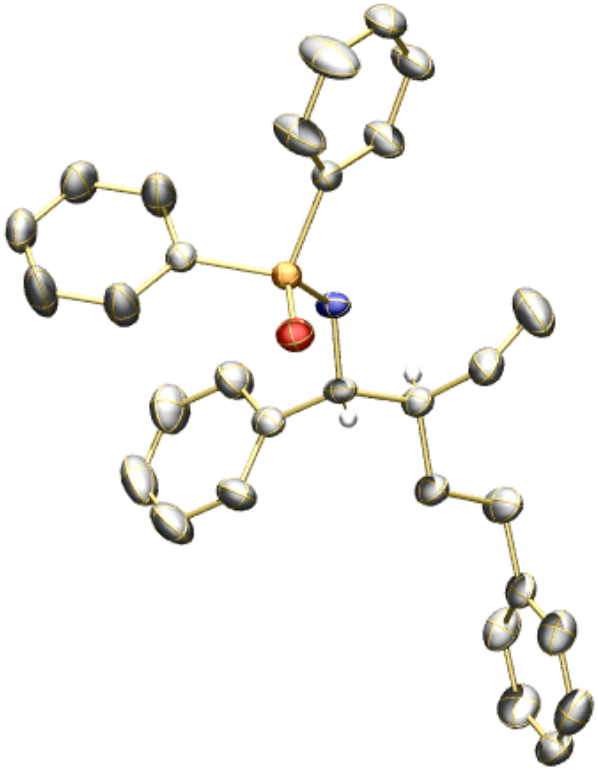

Table 1. Crystal data and structure refinement for $C_{30}H_{30}NOP$ (10)

Identification code	$C_{30}H_{30}NOP$	
Empirical formula	$C_{30}H_{30}NOP$	
Formula weight	451.52	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.4229(2) Å	α= 90°
	b = 16.7050(6) Å	β= 90°
	c = 27.7408(11) Å	γ = 90°
Volume	2513.03(16) $Å^3$	
Z	4	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	0.131 mm^{-1}	
F(000)	960	

Crystal size	0.20 x 0.08 x 0.04 mm^3
Theta range for data collection	1.42 to 28.37°
Index ranges	-6<=h<=7, -22<=k<=22, -37<=l<=37
Reflections collected	65893
Independent reflections	6293 [R(int) = 0.0763]
Completeness to theta = 28.37°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9948 and 0.9742
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6293 / 0 / 313
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.0906
R indices (all data)	R1 = 0.0607, wR2 = 0.0990
Absolute structure parameter	0.01(8)
Extinction coefficient	na
Largest diff. peak and hole	0.227 and -0.202 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{30}H_{30}NOP$ (10). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	10237(1)	1920(1)	1447(1)	25(1)
O(1)	12782(2)	1714(1)	1299(1)	34(1)
N(1)	8159(3)	1429(1)	1140(1)	28(1)
C(1)	9453(3)	2960(1)	1370(1)	29(1)
C(2)	7484(4)	3226(1)	1103(1)	47(1)
C(3)	7029(5)	4042(1)	1060(1)	54(1)
C(4)	8565(5)	4584(1)	1272(1)	51(1)
C(5)	10554(6)	4327(1)	1528(1)	81(1)
C(6)	10993(5)	3517(1)	1580(1)	64(1)
C(7)	9832(3)	1752(1)	2088(1)	28(1)
C(8)	7816(4)	2046(2)	2329(1)	56(1)

C(9)	7515(5)	1903(2)	2818(1)	55(1)
C(10)	9196(5)	1470(1)	3065(1)	48(1)
C(11)	11243(6)	1201(2)	2836(1)	75(1)
C(12)	11557(5)	1340(2)	2344(1)	58(1)
C(13)	8636(4)	611(1)	964(1)	29(1)
C(14)	8128(4)	-26(1)	1339(1)	34(1)
C(15)	6030(5)	-6(1)	1619(1)	49(1)
C(16)	5611(6)	-590(2)	1964(1)	64(1)
C(17)	7274(7)	-1203(2)	2026(1)	69(1)
C(18)	9355(6)	-1231(2)	1748(1)	67(1)
C(19)	9771(5)	-646(1)	1408(1)	50(1)
C(20)	7174(4)	486(1)	490(1)	33(1)
C(21)	7710(5)	1155(1)	147(1)	49(1)
C(22)	6103(8)	1636(2)	-48(1)	79(1)
C(23)	7847(4)	-325(1)	262(1)	38(1)
C(24)	6369(5)	-520(1)	-191(1)	51(1)
C(25)	7255(4)	-1271(1)	-441(1)	37(1)
C(26)	5986(4)	-1981(1)	-406(1)	48(1)
C(27)	6824(5)	-2660(1)	-638(1)	58(1)
C(28)	8930(5)	-2649(1)	-903(1)	53(1)
C(29)	10220(4)	-1956(2)	-938(1)	54(1)
C(30)	9382(4)	-1268(1)	-711(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{30}H_{30}NOP$ (10)

P(1)-O(1)	1.4815(13)
P(1)-N(1)	1.6343(16)
P(1)-C(1)	1.8003(17)
P(1)-C(7)	1.8131(17)
N(1)-C(13)	1.473(2)
N(1)-H(1N)	0.78(2)
C(1)-C(2)	1.373(3)
C(1)-C(6)	1.380(3)
C(2)-C(3)	1.391(3)

C(2)-H(2)	0.9400
C(3)-C(4)	1.363(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.361(4)
C(4)-H(4)	0.9400
C(5)-C(6)	1.381(3)
C(5)-H(5)	0.9400
C(6)-H(6)	0.9400
C(7)-C(12)	1.361(3)
C(7)-C(8)	1.371(3)
C(8)-C(9)	1.388(3)
C(8)-H(8)	0.9400
C(9)-C(10)	1.349(3)
C(9)-H(9)	0.9400
C(10)-C(11)	1.355(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.396(3)
C(11)-H(11)	0.9400
C(12)-H(12)	0.9400
C(13)-C(14)	1.514(3)
C(13)-C(20)	1.549(3)
C(13)-H(13)	0.97(2)
C(14)-C(15)	1.378(3)
C(14)-C(19)	1.380(3)
C(15)-C(16)	1.384(3)
C(15)-H(15)	0.9400
C(16)-C(17)	1.377(4)
C(16)-H(16)	0.9400
C(17)-C(18)	1.368(4)
C(17)-H(17)	0.9400
C(18)-C(19)	1.377(3)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400
C(20)-C(21)	1.498(3)
C(20)-C(23)	1.539(3)
C(20)-H(20)	0.98(2)

C(21)-C(22)	1.301(4)
C(21)-H(21)	0.9400
C(22)-H(22A)	1.01(3)
C(22)-H(22B)	0.93(3)
C(23)-C(24)	1.527(3)
C(23)-H(23)	0.9800
C(23)-H(7B)	0.9800
C(24)-C(25)	1.512(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(25)-C(30)	1.374(3)
C(25)-C(26)	1.375(3)
C(26)-C(27)	1.381(3)
C(26)-H(26)	0.9400
C(27)-C(28)	1.359(4)
C(27)-H(27)	0.9400
C(28)-C(29)	1.357(3)
C(28)-H(28)	0.9400
C(29)-C(30)	1.387(3)
C(29)-H(29)	0.9400
C(30)-H(30)	0.9400
O(1)-P(1)-N(1)	112.31(8)
O(1)-P(1)-C(1)	114.32(8)
N(1)-P(1)-C(1)	105.06(8)
O(1)-P(1)-C(7)	110.45(8)
N(1)-P(1)-C(7)	110.49(8)
C(1)-P(1)-C(7)	103.78(7)
C(13)-N(1)-P(1)	121.21(13)
C(13)-N(1)-H(1N)	115.8(16)
P(1)-N(1)-H(1N)	117.8(16)
C(2)-C(1)-C(6)	118.66(18)
C(2)-C(1)-P(1)	124.10(14)
C(6)-C(1)-P(1)	117.20(15)
C(1)-C(2)-C(3)	120.1(2)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9

C(4)-C(3)-C(2)	120.3(2)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	120.0(2)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.0(2)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-C(5)	120.8(2)
C(1)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(12)-C(7)-C(8)	118.34(18)
C(12)-C(7)-P(1)	120.43(15)
C(8)-C(7)-P(1)	121.22(14)
C(7)-C(8)-C(9)	120.6(2)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(10)-C(9)-C(8)	120.6(2)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(9)-C(10)-C(11)	119.6(2)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	120.1(2)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(7)-C(12)-C(11)	120.7(2)
C(7)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
N(1)-C(13)-C(14)	113.10(15)
N(1)-C(13)-C(20)	108.47(15)
C(14)-C(13)-C(20)	113.26(15)
N(1)-C(13)-H(13)	105.7(12)
C(14)-C(13)-H(13)	110.4(12)
C(20)-C(13)-H(13)	105.4(11)

C(15)-C(14)-C(19)	118.22(19)
C(15)-C(14)-C(13)	121.40(17)
C(19)-C(14)-C(13)	120.37(19)
C(14)-C(15)-C(16)	120.6(2)
C(14)-C(15)-H(15)	119.7
C(16)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	120.2(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(18)-C(17)-C(16)	119.7(2)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	119.8(2)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(14)	121.5(2)
C(18)-C(19)-H(19)	119.3
C(14)-C(19)-H(19)	119.3
C(21)-C(20)-C(23)	110.45(16)
C(21)-C(20)-C(13)	109.87(16)
C(23)-C(20)-C(13)	110.28(15)
C(21)-C(20)-H(20)	107.7(12)
C(23)-C(20)-H(20)	109.2(12)
C(13)-C(20)-H(20)	109.3(12)
C(22)-C(21)-C(20)	126.4(3)
C(22)-C(21)-H(21)	116.8
C(20)-C(21)-H(21)	116.8
C(21)-C(22)-H(22A)	115.1(19)
C(21)-C(22)-H(22B)	118(2)
H(22A)-C(22)-H(22B)	126(3)
C(24)-C(23)-C(20)	113.68(17)
C(24)-C(23)-H(23)	108.8
C(20)-C(23)-H(23)	108.8
C(24)-C(23)-H(7B)	108.8
C(20)-C(23)-H(7B)	108.8
H(23)-C(23)-H(7B)	107.7

C(25)-C(24)-C(23)	112.82(18)
C(25)-C(24)-H(24A)	109.0
C(23)-C(24)-H(24A)	109.0
C(25)-C(24)-H(24B)	109.0
C(23)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
C(30)-C(25)-C(26)	117.51(19)
C(30)-C(25)-C(24)	120.9(2)
C(26)-C(25)-C(24)	121.6(2)
C(25)-C(26)-C(27)	120.7(2)
C(25)-C(26)-H(26)	119.6
C(27)-C(26)-H(26)	119.6
C(28)-C(27)-C(26)	121.2(2)
C(28)-C(27)-H(27)	119.4
C(26)-C(27)-H(27)	119.4
C(29)-C(28)-C(27)	118.9(2)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5
C(28)-C(29)-C(30)	120.4(2)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(25)-C(30)-C(29)	121.3(2)
C(25)-C(30)-H(30)	119.3
C(29)-C(30)-H(30)	119.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{30}H_{30}NOP$ (10). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	23(1)	25(1)	27(1)	-1(1)	-1(1)	2(1)

O(1)	26(1)	38(1)	40(1)	-2(1)	2(1)	3(1)
N(1)	23(1)	26(1)	36(1)	-8(1)	-4(1)	5(1)
C(1)	33(1)	28(1)	27(1)	0(1)	1(1)	2(1)
C(2)	53(1)	33(1)	56(1)	1(1)	-21(1)	2(1)
C(3)	66(2)	34(1)	63(2)	3(1)	-21(1)	11(1)
C(4)	73(2)	28(1)	53(1)	1(1)	-9(1)	6(1)
C(5)	99(2)	30(1)	114(2)	-7(1)	-49(2)	-5(1)
C(6)	64(2)	36(1)	90(2)	-1(1)	-40(1)	1(1)
C(7)	30(1)	26(1)	29(1)	-2(1)	-3(1)	-1(1)
C(8)	49(1)	80(2)	37(1)	11(1)	6(1)	27(1)
C(9)	55(1)	70(2)	39(1)	4(1)	16(1)	16(1)
C(10)	63(2)	54(1)	29(1)	8(1)	2(1)	-2(1)
C(11)	76(2)	107(2)	43(1)	29(2)	6(1)	44(2)
C(12)	54(2)	80(2)	41(1)	15(1)	9(1)	31(1)
C(13)	27(1)	27(1)	32(1)	-8(1)	-3(1)	6(1)
C(14)	38(1)	28(1)	35(1)	-7(1)	-10(1)	1(1)
C(15)	54(1)	43(1)	52(1)	8(1)	2(1)	3(1)
C(16)	73(2)	64(2)	54(1)	14(1)	6(1)	-12(2)
C(17)	102(3)	47(1)	58(2)	19(1)	-23(2)	-14(2)
C(18)	85(2)	44(1)	72(2)	15(1)	-16(2)	14(1)
C(19)	57(1)	38(1)	53(1)	-1(1)	-9(1)	17(1)
C(20)	35(1)	32(1)	32(1)	-6(1)	-7(1)	4(1)
C(21)	68(2)	42(1)	36(1)	-5(1)	-6(1)	0(1)
C(22)	118(3)	52(2)	68(2)	13(1)	-35(2)	2(2)
C(23)	42(1)	36(1)	35(1)	-9(1)	-7(1)	5(1)
C(24)	56(1)	51(1)	47(1)	-17(1)	-19(1)	10(1)
C(25)	43(1)	39(1)	28(1)	-6(1)	-10(1)	-2(1)
C(26)	47(1)	57(1)	41(1)	-9(1)	1(1)	-16(1)
C(27)	83(2)	39(1)	54(1)	-9(1)	-4(1)	-22(1)
C(28)	66(2)	51(1)	41(1)	-14(1)	-9(1)	12(1)
C(29)	44(1)	78(2)	39(1)	-10(1)	4(1)	-2(2)
C(30)	53(2)	51(1)	44(1)	-3(1)	0(1)	-18(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3)

for $C_{30}H_{30}NOP$ (10)

	x	y	z	U(eq)
H(1N)	6780(40)	1537(12)	1182(8)	34
H(2)	6441	2856	950	57
H(3)	5656	4222	884	65
H(4)	8251	5135	1241	62
H(5)	11628	4701	1670	97
H(6)	12359	3344	1761	76
H(8)	6629	2346	2161	67
H(9)	6128	2109	2979	66
H(10)	8949	1357	3393	58
H(11)	12454	919	3010	90
H(12)	12976	1148	2187	70
H(13)	10360(40)	603(11)	871(7)	35
H(15)	4874	406	1576	59
H(16)	4185	-566	2157	77
H(17)	6983	-1601	2259	83
H(18)	10498	-1649	1788	80
H(19)	11207	-669	1219	60
H(20)	5410(40)	495(12)	561(7)	39
H(21)	9371	1236	63	58
H(22A)	4370(70)	1590(20)	86(12)	95
H(22B)	6680(60)	2030(20)	-255(12)	95
H(23)	9606	-324	182	45
H(7B)	7572	-749	501	45
H(24A)	4629	-585	-104	62
H(24B)	6488	-69	-416	62
H(26)	4532	-2005	-222	58
H(27)	5922	-3139	-611	70
H(28)	9484	-3114	-1060	63
H(29)	11689	-1941	-1118	64
H(30)	10287	-791	-741	59

Table 6. Torsion angles [°] for $C_{30}H_{30}NOP$ (10)

O(1)-P(1)-N(1)-C(13)	32.32(17)
C(1)-P(1)-N(1)-C(13)	157.18(14)
C(7)-P(1)-N(1)-C(13)	-91.49(16)
O(1)-P(1)-C(1)-C(2)	123.78(17)
N(1)-P(1)-C(1)-C(2)	0.20(19)
C(7)-P(1)-C(1)-C(2)	-115.85(18)
O(1)-P(1)-C(1)-C(6)	-53.9(2)
N(1)-P(1)-C(1)-C(6)	-177.49(19)
C(7)-P(1)-C(1)-C(6)	66.5(2)
C(6)-C(1)-C(2)-C(3)	-1.8(3)
P(1)-C(1)-C(2)-C(3)	-179.48(19)
C(1)-C(2)-C(3)-C(4)	1.6(4)
C(2)-C(3)-C(4)-C(5)	-0.1(4)
C(3)-C(4)-C(5)-C(6)	-1.1(5)
C(2)-C(1)-C(6)-C(5)	0.7(4)
P(1)-C(1)-C(6)-C(5)	178.5(3)
C(4)-C(5)-C(6)-C(1)	0.8(5)
O(1)-P(1)-C(7)-C(12)	-12.0(2)
N(1)-P(1)-C(7)-C(12)	112.92(19)
C(1)-P(1)-C(7)-C(12)	-134.92(18)
O(1)-P(1)-C(7)-C(8)	166.88(17)
N(1)-P(1)-C(7)-C(8)	-68.24(19)
C(1)-P(1)-C(7)-C(8)	43.91(19)
C(12)-C(7)-C(8)-C(9)	-2.0(4)
P(1)-C(7)-C(8)-C(9)	179.1(2)
C(7)-C(8)-C(9)-C(10)	-0.2(4)
C(8)-C(9)-C(10)-C(11)	2.6(4)
C(9)-C(10)-C(11)-C(12)	-2.7(5)
C(8)-C(7)-C(12)-C(11)	1.9(4)
P(1)-C(7)-C(12)-C(11)	-179.3(2)
C(10)-C(11)-C(12)-C(7)	0.5(5)
P(1)-N(1)-C(13)-C(14)	84.0(2)
P(1)-N(1)-C(13)-C(20)	-149.53(14)

N(1)-C(13)-C(14)-C(15)	44.7(2)
C(20)-C(13)-C(14)-C(15)	-79.2(2)
N(1)-C(13)-C(14)-C(19)	-135.40(18)
C(20)-C(13)-C(14)-C(19)	100.7(2)
C(19)-C(14)-C(15)-C(16)	0.8(3)
C(13)-C(14)-C(15)-C(16)	-179.3(2)
C(14)-C(15)-C(16)-C(17)	-0.9(4)
C(15)-C(16)-C(17)-C(18)	0.5(4)
C(16)-C(17)-C(18)-C(19)	0.0(4)
C(17)-C(18)-C(19)-C(14)	-0.1(4)
C(15)-C(14)-C(19)-C(18)	-0.3(3)
C(13)-C(14)-C(19)-C(18)	179.8(2)
N(1)-C(13)-C(20)-C(21)	51.5(2)
C(14)-C(13)-C(20)-C(21)	177.98(17)
N(1)-C(13)-C(20)-C(23)	173.53(17)
C(14)-C(13)-C(20)-C(23)	-60.0(2)
C(23)-C(20)-C(21)-C(22)	115.4(3)
C(13)-C(20)-C(21)-C(22)	-122.7(3)
C(21)-C(20)-C(23)-C(24)	-61.9(3)
C(13)-C(20)-C(23)-C(24)	176.50(19)
C(20)-C(23)-C(24)-C(25)	173.42(19)
C(23)-C(24)-C(25)-C(30)	-75.9(3)
C(23)-C(24)-C(25)-C(26)	103.5(2)
C(30)-C(25)-C(26)-C(27)	-0.6(3)
C(24)-C(25)-C(26)-C(27)	179.9(2)
C(25)-C(26)-C(27)-C(28)	0.6(4)
C(26)-C(27)-C(28)-C(29)	0.1(4)
C(27)-C(28)-C(29)-C(30)	-0.7(3)
C(26)-C(25)-C(30)-C(29)	0.0(3)
C(24)-C(25)-C(30)-C(29)	179.5(2)
C(28)-C(29)-C(30)-C(25)	0.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{30}H_{30}NOP$ (10) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(1)#1	0.78(2)	2.21(2)	2.987(2)	174(2)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z

X-ray Crystal Structure of 11 (Figure 3c)

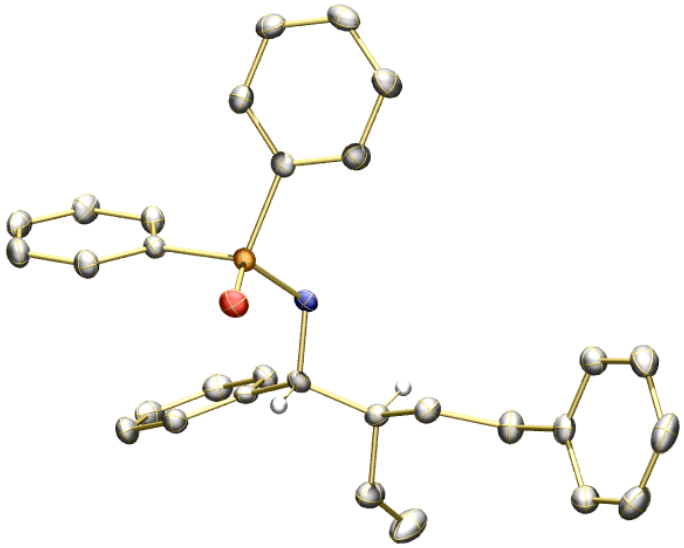

Table 1. Crystal data and structure refinement for $C_{30}H_{30}NOP$ (11)

Identification code	$C_{30}H_{30}NOP$	
Empirical formula	$C_{30}H_{30}NOP$	
Formula weight	451.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.7855(5) Å	α= 90°
	b = 10.0513(5) Å	β= 93.331(3)°
	c = 11.6042(6) Å	γ = 90°
Volume	1255.87(11) $Å^3$	
Z	2	

Density (calculated)	1.194 Mg/m^3
Absorption coefficient	0.132 mm^{-1}
F(000)	480
Crystal size	0.25 x 0.08 x 0.05 mm^3
Theta range for data collection	1.76 to 28.33°
Index ranges	-14<=h<=14, -12<=k<=13, -15<=l<=15
Reflections collected	20929
Independent reflections	6086 [R(int) = 0.0557]
Completeness to theta = 28.33°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9935 and 0.9679
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6086 / 6 / 313
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0759
R indices (all data)	R1 = 0.0599, wR2 = 0.0827
Absolute structure parameter	-0.09(7)
Extinction coefficient	na
Largest diff. peak and hole	0.289 and -0.247 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{30}H_{30}NOP$ (11). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	-133(1)	612(1)	4531(1)	16(1)
O(1)	102(1)	2053(1)	4761(1)	22(1)
N(1)	-146(1)	-242(2)	5733(1)	16(1)
C(1)	1070(2)	-166(2)	3747(2)	18(1)
C(2)	2273(2)	-174(2)	4250(2)	25(1)
C(3)	3254(2)	-654(2)	3642(2)	28(1)
C(4)	3037(2)	-1123(2)	2532(2)	26(1)
C(5)	1845(2)	-1124(2)	2025(2)	27(1)

C(6)	869(2)	-636(2)	2627(2)	24(1)
C(7)	-1556(2)	397(2)	3651(2)	18(1)
C(8)	-2129(2)	1510(2)	3138(2)	23(1)
C(9)	-3203(2)	1356(2)	2431(2)	27(1)
C(10)	-3700(2)	100(2)	2233(2)	26(1)
C(11)	-3145(2)	-1009(2)	2750(2)	26(1)
C(12)	-2074(2)	-865(2)	3464(2)	22(1)
C(13)	-906(2)	226(2)	6671(2)	17(1)
C(14)	-2240(2)	-265(2)	6510(2)	18(1)
C(15)	-3162(2)	610(2)	6114(2)	23(1)
C(16)	-4386(2)	180(2)	5924(2)	29(1)
C(17)	-4689(2)	-1129(2)	6137(2)	30(1)
C(18)	-3771(2)	-2013(2)	6529(2)	27(1)
C(19)	-2556(2)	-1583(2)	6709(2)	23(1)
C(20)	-265(2)	-147(2)	7849(2)	19(1)
C(21)	-1071(2)	234(2)	8814(2)	30(1)
C(22)	-1255(2)	-473(3)	9747(2)	46(1)
C(23)	1008(2)	542(2)	8016(2)	21(1)
C(24)	1794(2)	-29(2)	9043(2)	28(1)
C(25)	3003(2)	696(2)	9289(2)	22(1)
C(26)	4026(2)	438(2)	8655(2)	26(1)
C(27)	5127(2)	1131(2)	8865(2)	31(1)
C(28)	5209(2)	2115(2)	9700(2)	32(1)
C(29)	4202(2)	2380(2)	10329(2)	33(1)
C(30)	3110(2)	1666(2)	10136(2)	28(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{30}H_{30}NOP$ (11)

P(1)-O(1)	1.4922(13)
P(1)-N(1)	1.6385(16)
P(1)-C(1)	1.8060(19)
P(1)-C(7)	1.8061(17)
N(1)-C(13)	1.477(2)
N(1)-H(1N)	0.854(15)

C(1)-C(6)	1.388(3)
C(1)-C(2)	1.391(3)
C(2)-C(3)	1.391(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.378(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.395(3)
C(7)-C(12)	1.398(3)
C(8)-C(9)	1.389(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.385(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.386(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.389(3)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.522(2)
C(13)-C(20)	1.541(3)
C(13)-H(13)	0.976(15)
C(14)-C(15)	1.387(3)
C(14)-C(19)	1.390(3)
C(15)-C(16)	1.394(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.382(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.387(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.385(3)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

C(20)-C(21)	1.507(3)
C(20)-C(23)	1.541(2)
C(20)-H(20)	1.029(15)
C(21)-C(22)	1.318(3)
C(21)-H(21)	0.9500
C(22)-H(22A)	1.036(17)
C(22)-H(22B)	0.995(16)
C(23)-C(24)	1.534(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.506(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(30)	1.385(3)
C(25)-C(26)	1.386(3)
C(26)-C(27)	1.385(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.385(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.370(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.386(3)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
O(1)-P(1)-N(1)	111.48(8)
O(1)-P(1)-C(1)	113.01(8)
N(1)-P(1)-C(1)	104.15(8)
O(1)-P(1)-C(7)	110.32(8)
N(1)-P(1)-C(7)	111.69(8)
C(1)-P(1)-C(7)	105.95(8)
C(13)-N(1)-P(1)	119.56(12)
C(13)-N(1)-H(1N)	113.2(13)
P(1)-N(1)-H(1N)	115.6(14)
C(6)-C(1)-C(2)	118.85(17)
C(6)-C(1)-P(1)	122.79(14)
C(2)-C(1)-P(1)	118.06(14)

C(3)-C(2)-C(1)	120.43(18)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	120.01(18)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	120.02(18)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.01(19)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.67(18)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
C(8)-C(7)-C(12)	119.88(17)
C(8)-C(7)-P(1)	119.11(14)
C(12)-C(7)-P(1)	121.01(14)
C(9)-C(8)-C(7)	119.77(19)
C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	120.09(19)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	120.54(18)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(10)-C(11)-C(12)	119.84(19)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(11)-C(12)-C(7)	119.87(18)
C(11)-C(12)-H(12)	120.1
C(7)-C(12)-H(12)	120.1
N(1)-C(13)-C(14)	111.56(15)
N(1)-C(13)-C(20)	109.66(14)
C(14)-C(13)-C(20)	113.69(15)

N(1)-C(13)-H(13)	105.6(12)
C(14)-C(13)-H(13)	109.4(11)
C(20)-C(13)-H(13)	106.5(12)
C(15)-C(14)-C(19)	118.80(17)
C(15)-C(14)-C(13)	119.30(17)
C(19)-C(14)-C(13)	121.86(17)
C(14)-C(15)-C(16)	120.7(2)
C(14)-C(15)-H(15)	119.7
C(16)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	119.9(2)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	119.80(19)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(19)-C(18)-C(17)	120.0(2)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	120.79(18)
C(18)-C(19)-H(19)	119.6
C(14)-C(19)-H(19)	119.6
C(21)-C(20)-C(23)	109.95(15)
C(21)-C(20)-C(13)	110.43(15)
C(23)-C(20)-C(13)	110.68(15)
C(21)-C(20)-H(20)	106.6(11)
C(23)-C(20)-H(20)	108.1(11)
C(13)-C(20)-H(20)	111.0(12)
C(22)-C(21)-C(20)	126.5(2)
C(22)-C(21)-H(21)	116.8
C(20)-C(21)-H(21)	116.8
C(21)-C(22)-H(22A)	117.9(15)
C(21)-C(22)-H(22B)	121.8(16)
H(22A)-C(22)-H(22B)	120(2)
C(24)-C(23)-C(20)	112.22(16)
C(24)-C(23)-H(23A)	109.2
C(20)-C(23)-H(23A)	109.2

C(24)-C(23)-H(23B)	109.2
C(20)-C(23)-H(23B)	109.2
H(23A)-C(23)-H(23B)	107.9
C(25)-C(24)-C(23)	113.51(17)
C(25)-C(24)-H(24A)	108.9
C(23)-C(24)-H(24A)	108.9
C(25)-C(24)-H(24B)	108.9
C(23)-C(24)-H(24B)	108.9
H(24A)-C(24)-H(24B)	107.7
C(30)-C(25)-C(26)	118.15(18)
C(30)-C(25)-C(24)	120.71(18)
C(26)-C(25)-C(24)	121.11(19)
C(27)-C(26)-C(25)	120.9(2)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(28)-C(27)-C(26)	120.1(2)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(29)-C(28)-C(27)	119.4(2)
C(29)-C(28)-H(28)	120.3
C(27)-C(28)-H(28)	120.3
C(28)-C(29)-C(30)	120.4(2)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(25)-C(30)-C(29)	120.96(19)
C(25)-C(30)-H(30)	119.5
C(29)-C(30)-H(30)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{30}H_{30}NOP$ (11). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

P(1)	17(1)	11(1)	19(1)	0(1)	0(1)	-1(1)
O(1)	26(1)	12(1)	28(1)	-1(1)	1(1)	-2(1)
N(1)	19(1)	8(1)	21(1)	-1(1)	2(1)	1(1)
C(1)	20(1)	13(1)	21(1)	3(1)	3(1)	-1(1)
C(2)	24(1)	26(1)	26(1)	-5(1)	0(1)	-1(1)
C(3)	20(1)	29(1)	35(1)	-5(1)	2(1)	0(1)
C(4)	27(1)	20(1)	31(1)	3(1)	12(1)	2(1)
C(5)	34(1)	28(1)	19(1)	0(1)	6(1)	2(1)
C(6)	26(1)	26(1)	21(1)	3(1)	-1(1)	0(1)
C(7)	16(1)	18(1)	19(1)	1(1)	2(1)	1(1)
C(8)	23(1)	19(1)	26(1)	2(1)	0(1)	1(1)
C(9)	24(1)	28(1)	28(1)	5(1)	-2(1)	6(1)
C(10)	17(1)	39(1)	23(1)	-1(1)	-2(1)	-1(1)
C(11)	23(1)	28(1)	29(1)	-2(1)	-2(1)	-8(1)
C(12)	21(1)	19(1)	26(1)	2(1)	-1(1)	-1(1)
C(13)	18(1)	12(1)	22(1)	-2(1)	2(1)	2(1)
C(14)	20(1)	20(1)	16(1)	-4(1)	3(1)	1(1)
C(15)	22(1)	23(1)	24(1)	-3(1)	0(1)	2(1)
C(16)	20(1)	37(1)	29(1)	-2(1)	-2(1)	7(1)
C(17)	18(1)	40(1)	30(1)	-9(1)	3(1)	-4(1)
C(18)	28(1)	25(1)	29(1)	-2(1)	5(1)	-7(1)
C(19)	21(1)	20(1)	28(1)	0(1)	2(1)	2(1)
C(20)	21(1)	18(1)	18(1)	-1(1)	1(1)	-1(1)
C(21)	25(1)	40(1)	27(1)	-6(1)	2(1)	-1(1)
C(22)	37(1)	74(2)	29(1)	-4(1)	6(1)	-15(1)
C(23)	22(1)	22(1)	21(1)	0(1)	1(1)	-4(1)
C(24)	24(1)	29(1)	29(1)	6(1)	-3(1)	-2(1)
C(25)	22(1)	23(1)	21(1)	7(1)	-3(1)	0(1)
C(26)	27(1)	25(1)	26(1)	2(1)	1(1)	4(1)
C(27)	24(1)	41(1)	28(1)	7(1)	3(1)	3(1)
C(28)	29(1)	42(1)	25(1)	9(1)	-8(1)	-12(1)
C(29)	40(1)	34(1)	25(1)	-3(1)	-6(1)	-5(1)
C(30)	25(1)	35(1)	24(1)	1(1)	2(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{30}H_{30}NOP$ (11)

	x	y	z	U(eq)
H(1N)	-151(17)	-1087(16)	5655(18)	19
H(2)	2426	151	5014	30
H(3)	4072	-658	3992	34
H(4)	3708	-1446	2116	31
H(5)	1695	-1459	1264	32
H(6)	54	-624	2269	29
H(8)	-1786	2371	3273	27
H(9)	-3597	2112	2083	32
H(10)	-4427	-1	1738	32
H(11)	-3495	-1866	2616	32
H(12)	-1696	-1623	3826	26
H(13)	-895(17)	1196(15)	6627(17)	21
H(15)	-2958	1512	5970	27
H(16)	-5011	787	5649	34
H(17)	-5524	-1423	6015	35
H(18)	-3977	-2915	6673	33
H(19)	-1930	-2195	6971	28
H(20)	-127(17)	-1158(16)	7911(18)	23
H(21)	-1489	1065	8744	37
H(22A)	-790(20)	-1370(20)	9850(20)	56
H(22B)	-1780(20)	-140(30)	10363(18)	56
H(23A)	1464	435	7305	26
H(23B)	881	1506	8140	26

H(24A)	1306	8	9739	33
H(24B)	1974	-976	8888	33
H(26)	3973	-222	8069	31
H(27)	5826	930	8435	37
H(28)	5958	2602	9837	39
H(29)	4252	3058	10901	40
H(30)	2426	1844	10593	33

Table 6. Torsion angles [°] for $C_{30}H_{30}NOP$ (11)

O(1)-P(1)-N(1)-C(13)	49.52(15)
C(1)-P(1)-N(1)-C(13)	171.68(13)
C(7)-P(1)-N(1)-C(13)	-74.41(15)
O(1)-P(1)-C(1)-C(6)	-112.97(16)
N(1)-P(1)-C(1)-C(6)	125.88(16)
C(7)-P(1)-C(1)-C(6)	7.95(18)
O(1)-P(1)-C(1)-C(2)	60.64(17)
N(1)-P(1)-C(1)-C(2)	-60.51(17)
C(7)-P(1)-C(1)-C(2)	-178.45(15)
C(6)-C(1)-C(2)-C(3)	-0.5(3)
P(1)-C(1)-C(2)-C(3)	-174.31(16)
C(1)-C(2)-C(3)-C(4)	0.2(3)
C(2)-C(3)-C(4)-C(5)	-0.4(3)
C(3)-C(4)-C(5)-C(6)	0.9(3)
C(4)-C(5)-C(6)-C(1)	-1.2(3)
C(2)-C(1)-C(6)-C(5)	1.0(3)
P(1)-C(1)-C(6)-C(5)	174.51(16)
O(1)-P(1)-C(7)-C(8)	10.78(17)
N(1)-P(1)-C(7)-C(8)	135.36(14)
C(1)-P(1)-C(7)-C(8)	-111.86(15)
O(1)-P(1)-C(7)-C(12)	-170.18(14)
N(1)-P(1)-C(7)-C(12)	-45.60(17)
C(1)-P(1)-C(7)-C(12)	67.18(16)
C(12)-C(7)-C(8)-C(9)	-1.0(3)

P(1)-C(7)-C(8)-C(9)	178.07(14)
C(7)-C(8)-C(9)-C(10)	-0.2(3)
C(8)-C(9)-C(10)-C(11)	1.0(3)
C(9)-C(10)-C(11)-C(12)	-0.6(3)
C(10)-C(11)-C(12)-C(7)	-0.6(3)
C(8)-C(7)-C(12)-C(11)	1.4(3)
P(1)-C(7)-C(12)-C(11)	-177.65(15)
P(1)-N(1)-C(13)-C(14)	85.70(17)
P(1)-N(1)-C(13)-C(20)	-147.44(13)
N(1)-C(13)-C(14)-C(15)	-103.98(19)
C(20)-C(13)-C(14)-C(15)	131.38(17)
N(1)-C(13)-C(14)-C(19)	73.6(2)
C(20)-C(13)-C(14)-C(19)	-51.1(2)
C(19)-C(14)-C(15)-C(16)	0.4(3)
C(13)-C(14)-C(15)-C(16)	178.03(17)
C(14)-C(15)-C(16)-C(17)	0.3(3)
C(15)-C(16)-C(17)-C(18)	-0.6(3)
C(16)-C(17)-C(18)-C(19)	0.2(3)
C(17)-C(18)-C(19)-C(14)	0.5(3)
C(15)-C(14)-C(19)-C(18)	-0.8(3)
C(13)-C(14)-C(19)-C(18)	-178.38(18)
N(1)-C(13)-C(20)-C(21)	-175.90(16)
C(14)-C(13)-C(20)-C(21)	-50.2(2)
N(1)-C(13)-C(20)-C(23)	62.1(2)
C(14)-C(13)-C(20)-C(23)	-172.23(16)
C(23)-C(20)-C(21)-C(22)	-98.5(2)
C(13)-C(20)-C(21)-C(22)	139.1(2)
C(21)-C(20)-C(23)-C(24)	70.2(2)
C(13)-C(20)-C(23)-C(24)	-167.56(16)
C(20)-C(23)-C(24)-C(25)	-175.36(17)
C(23)-C(24)-C(25)-C(30)	97.6(2)
C(23)-C(24)-C(25)-C(26)	-80.7(2)
C(30)-C(25)-C(26)-C(27)	0.1(3)
C(24)-C(25)-C(26)-C(27)	178.41(19)
C(25)-C(26)-C(27)-C(28)	-1.4(3)
C(26)-C(27)-C(28)-C(29)	1.1(3)

C(27)-C(28)-C(29)-C(30)	0.3(3)
C(26)-C(25)-C(30)-C(29)	1.4(3)
C(24)-C(25)-C(30)-C(29)	-176.93(19)
C(28)-C(29)-C(30)-C(25)	-1.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{30}H_{30}NOP$ (11) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(1)#1	0.854(15)	1.932(16)	2.779(2)	171(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1

X-ray Crystal Structure of 13 (Figure 2c)

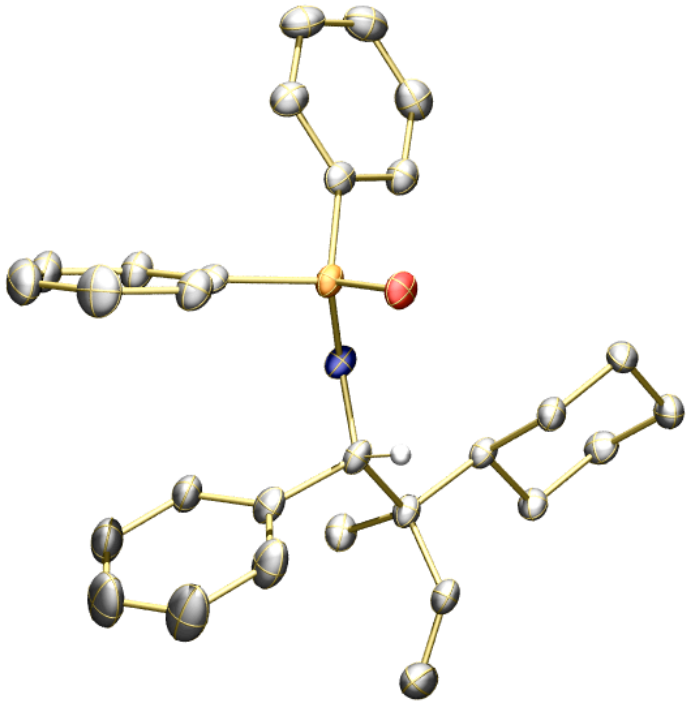

Table 1. Crystal data and structure refinement for $C_{29}H_{34}NOP$ (13)

Identification code	$C_{29}H_{34}NOP$

Empirical formula	$C_{29}H_{34}NOP$	
Formula weight	443.54	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 22.5726(15) Å	α= 90°
	b = 20.6585(13) Å	β= 119.094(4)°
	c = 23.0355(15) Å	γ = 90°
Volume	9386.5(11) $Å^3$	
Z	12	
Density (calculated)	0.942 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	2856	
Crystal size	0.15 x 0.06 x 0.05 mm^3	
Theta range for data collection	1.41 to 28.81°	
Index ranges	-30<=h<=26, -27<=k<=27, 0<=l<=31	
Reflections collected	48686	
Independent reflections	48686 [R(int) = 0.0000]	
Completeness to theta = 28.81°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9948 and 0.9845	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	48686 / 1 / 1729	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0492, wR2 = 0.1165	
R indices (all data)	R1 = 0.0702, wR2 = 0.1245	
Absolute structure parameter	-0.04(3)	
Extinction coefficient	na	
Largest diff. peak and hole	0.458 and -0.341 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{29}H_{34}NOP$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	20(1)	2748(1)	29(1)	18(1)
O(1)	-106(1)	3419(1)	180(1)	22(1)
N(1)	24(1)	2228(1)	570(1)	20(1)
C(1)	809(1)	2687(1)	20(1)	21(1)
C(2)	1116(1)	3246(1)	-40(1)	27(1)
C(3)	1714(1)	3207(1)	-69(1)	34(1)
C(4)	2002(1)	2616(1)	-46(1)	34(1)
C(5)	1701(1)	2052(1)	14(1)	32(1)
C(6)	1104(1)	2086(1)	47(1)	26(1)
C(7)	-622(1)	2507(1)	-790(1)	20(1)
C(8)	-493(1)	2454(1)	-1323(1)	26(1)
C(9)	-1020(1)	2356(1)	-1965(1)	30(1)
C(10)	-1675(1)	2312(1)	-2080(1)	31(1)
C(11)	-1813(1)	2358(1)	-1554(1)	29(1)
C(12)	-1293(1)	2457(1)	-918(1)	24(1)
C(13)	-22(1)	2444(1)	1156(1)	21(1)
C(14)	-751(1)	2391(1)	1025(1)	22(1)
C(15)	-1164(1)	1865(1)	695(1)	29(1)
C(16)	-1833(1)	1850(1)	558(1)	35(1)
C(17)	-2102(1)	2353(1)	749(1)	35(1)
C(18)	-1697(1)	2878(1)	1078(1)	33(1)
C(19)	-1027(1)	2898(1)	1213(1)	26(1)
C(20)	514(1)	2112(1)	1819(1)	23(1)
C(21)	337(1)	1400(1)	1832(1)	28(1)
C(22)	507(1)	2493(1)	2378(1)	28(1)
C(23)	402(1)	2263(1)	2857(1)	42(1)
C(24)	1232(1)	2165(1)	1867(1)	29(1)
C(25)	1800(1)	1867(1)	2513(1)	43(1)
C(26)	2485(1)	1890(1)	2533(2)	54(1)
C(27)	2683(1)	2570(1)	2452(1)	49(1)
C(28)	2129(1)	2874(1)	1813(1)	40(1)
C(29)	1442(1)	2860(1)	1801(1)	30(1)
P(2)	10484(1)	10148(1)	10524(1)	20(1)

O(2)	10410(1)	10866(1)	10490(1)	27(1)
N(2)	10115(1)	9825(1)	9779(1)	22(1)
C(30)	11363(1)	9912(1)	10986(1)	26(1)
C(31)	11572(1)	9279(1)	11010(1)	30(1)
C(32)	12242(1)	9111(1)	11377(1)	43(1)
C(33)	12717(1)	9580(2)	11735(2)	64(1)
C(34)	12524(1)	10212(2)	11709(2)	73(1)
C(35)	11848(1)	10390(1)	11340(2)	49(1)
C(36)	10058(1)	9765(1)	10924(1)	20(1)
C(37)	10326(1)	9285(1)	11403(1)	29(1)
C(38)	9943(1)	9022(1)	11667(1)	35(1)
C(39)	9293(1)	9239(1)	11455(1)	33(1)
C(40)	9022(1)	9722(1)	10986(1)	27(1)
C(41)	9402(1)	9985(1)	10720(1)	25(1)
C(42)	10108(1)	10178(1)	9223(1)	21(1)
C(43)	10784(1)	10117(1)	9224(1)	24(1)
C(44)	11049(1)	10648(1)	9058(1)	32(1)
C(45)	11674(1)	10618(1)	9087(1)	41(1)
C(46)	12052(1)	10059(1)	9295(1)	43(1)
C(47)	11796(1)	9523(1)	9461(1)	36(1)
C(48)	11163(1)	9552(1)	9421(1)	27(1)
C(49)	9471(1)	9993(1)	8551(1)	21(1)
C(50)	9561(1)	9310(1)	8351(1)	24(1)
C(51)	9402(1)	10486(1)	8040(1)	27(1)
C(52)	9368(1)	10367(1)	7458(1)	38(1)
C(53)	8820(1)	10020(1)	8632(1)	25(1)
C(54)	8171(1)	9881(1)	7977(1)	34(1)
C(55)	7543(1)	9874(1)	8067(1)	42(1)
C(56)	7465(1)	10507(1)	8360(1)	42(1)
C(57)	8108(1)	10650(1)	9014(1)	35(1)
C(58)	8733(1)	10662(1)	8922(1)	27(1)
P(3)	4815(1)	1138(1)	9976(1)	18(1)
O(3)	4684(1)	486(1)	9662(1)	23(1)
N(3)	4800(1)	1703(1)	9466(1)	19(1)
C(59)	5631(1)	1203(1)	10714(1)	20(1)
C(60)	6209(1)	1363(1)	10680(1)	27(1)

C(61)	6840(1)	1353(1)	11252(1)	33(1)
C(62)	6895(1)	1182(1)	11853(1)	31(1)
C(63)	6325(1)	1019(1)	11889(1)	36(1)
C(64)	5696(1)	1025(1)	11327(1)	29(1)
C(65)	4229(1)	1314(1)	10278(1)	21(1)
C(66)	3818(1)	827(1)	10301(1)	26(1)
C(67)	3402(1)	943(1)	10577(1)	30(1)
C(68)	3399(1)	1544(1)	10839(1)	31(1)
C(69)	3807(1)	2037(1)	10811(1)	30(1)
C(70)	4219(1)	1924(1)	10536(1)	27(1)
C(71)	4388(1)	1600(1)	8743(1)	23(1)
C(72)	3627(1)	1583(1)	8509(1)	25(1)
C(73)	3332(1)	2005(1)	8769(1)	28(1)
C(74)	2641(1)	1998(1)	8536(1)	34(1)
C(75)	2224(1)	1565(1)	8042(1)	35(1)
C(76)	2518(1)	1136(1)	7802(1)	37(1)
C(77)	3218(1)	1142(1)	8044(1)	32(1)
C(78)	4570(1)	2095(1)	8338(1)	25(1)
C(79)	4282(1)	2759(1)	8329(1)	24(1)
C(80)	4282(1)	1821(1)	7644(1)	32(1)
C(81)	3886(1)	2103(1)	7080(1)	47(1)
C(82)	5367(1)	2144(1)	8656(1)	26(1)
C(83)	5595(1)	2600(1)	8277(1)	34(1)
C(84)	6361(1)	2670(1)	8629(1)	41(1)
C(85)	6716(1)	2021(1)	8740(1)	42(1)
C(86)	6491(1)	1568(1)	9114(1)	38(1)
C(87)	5720(1)	1494(1)	8748(1)	33(1)
P(4)	4568(1)	8661(1)	9798(1)	20(1)
O(4)	4827(1)	7984(1)	9934(1)	24(1)
N(4)	5108(1)	9158(1)	9741(1)	21(1)
C(88)	4446(1)	9027(1)	10443(1)	23(1)
C(89)	4998(1)	9302(1)	10996(1)	28(1)
C(90)	4917(1)	9544(1)	11516(1)	34(1)
C(91)	4294(1)	9514(1)	11486(1)	37(1)
C(92)	3741(1)	9247(1)	10936(1)	35(1)
C(93)	3819(1)	9007(1)	10422(1)	28(1)

C(94)	3755(1)	8693(1)	9056(1)	21(1)
C(95)	3413(1)	9279(1)	8830(1)	28(1)
C(96)	2798(1)	9301(1)	8256(1)	34(1)
C(97)	2519(1)	8744(1)	7893(1)	39(1)
C(98)	2858(1)	8158(1)	8112(1)	41(1)
C(99)	3472(1)	8131(1)	8687(1)	29(1)
C(100)	5451(1)	8937(1)	9372(1)	21(1)
C(101)	4997(1)	8986(1)	8622(1)	27(1)
C(102)	4581(1)	9519(1)	8330(1)	30(1)
C(103)	4187(1)	9564(1)	7644(1)	44(1)
C(104)	4191(1)	9069(2)	7244(1)	55(1)
C(105)	4593(1)	8535(2)	7526(1)	55(1)
C(106)	4989(1)	8486(1)	8214(1)	40(1)
C(107)	6147(1)	9296(1)	9618(1)	21(1)
C(108)	6027(1)	9982(1)	9352(1)	27(1)
C(109)	6539(1)	8902(1)	9364(1)	24(1)
C(110)	6687(1)	9044(1)	8897(1)	41(1)
C(111)	6541(1)	9322(1)	10396(1)	20(1)
C(112)	7243(1)	9636(1)	10657(1)	24(1)
C(113)	7614(1)	9695(1)	11416(1)	28(1)
C(114)	7689(1)	9037(1)	11741(1)	29(1)
C(115)	6995(1)	8733(1)	11495(1)	28(1)
C(116)	6618(1)	8668(1)	10735(1)	24(1)
P(5)	9858(1)	1825(1)	4923(1)	19(1)
O(5)	9798(1)	1153(1)	5125(1)	23(1)
N(5)	9598(1)	2369(1)	5267(1)	20(1)
C(117)	9393(1)	1912(1)	4033(1)	22(1)
C(118)	9191(1)	1356(1)	3637(1)	30(1)
C(119)	8839(1)	1414(1)	2952(1)	34(1)
C(120)	8685(1)	2014(1)	2656(1)	35(1)
C(121)	8884(1)	2565(1)	3046(1)	33(1)
C(122)	9234(1)	2517(1)	3732(1)	25(1)
C(123)	10723(1)	2028(1)	5154(1)	24(1)
C(124)	10965(1)	1995(1)	4703(1)	38(1)
C(125)	11641(1)	2093(2)	4909(2)	52(1)
C(126)	12088(1)	2225(1)	5570(2)	49(1)

C(127)	11858(1)	2251(1)	6025(1)	45(1)
C(128)	11182(1)	2160(1)	5823(1)	35(1)
C(129)	9313(1)	2191(1)	5696(1)	22(1)
C(130)	9818(1)	2313(1)	6423(1)	22(1)
C(131)	10225(1)	2861(1)	6633(1)	27(1)
C(132)	10673(1)	2958(1)	7305(1)	32(1)
C(133)	10720(1)	2515(1)	7771(1)	33(1)
C(134)	10330(1)	1962(1)	7567(1)	38(1)
C(135)	9883(1)	1862(1)	6896(1)	31(1)
C(136)	8602(1)	2510(1)	5474(1)	24(1)
C(137)	8687(1)	3235(1)	5649(1)	32(1)
C(138)	8288(1)	2147(1)	5828(1)	34(1)
C(139)	8046(1)	2394(2)	6199(1)	55(1)
C(140)	8138(1)	2433(1)	4701(1)	27(1)
C(141)	7435(1)	2738(1)	4444(1)	42(1)
C(142)	7014(1)	2696(1)	3693(1)	53(1)
C(143)	6932(1)	1999(1)	3445(1)	46(1)
C(144)	7630(1)	1692(1)	3701(1)	36(1)
C(145)	8044(1)	1731(1)	4458(1)	27(1)
P(6)	10247(1)	9399(1)	4945(1)	22(1)
O(6)	10179(1)	8682(1)	4925(1)	29(1)
N(6)	9641(1)	9746(1)	5041(1)	22(1)
C(146)	10146(1)	9732(1)	4177(1)	23(1)
C(147)	9535(1)	9616(1)	3602(1)	28(1)
C(148)	9441(1)	9818(1)	2992(1)	31(1)
C(149)	9949(1)	10144(1)	2943(1)	36(1)
C(150)	10554(1)	10274(1)	3507(1)	42(1)
C(151)	10656(1)	10060(1)	4123(1)	36(1)
C(152)	11079(1)	9646(1)	5571(1)	25(1)
C(153)	11582(1)	9185(1)	5907(1)	36(1)
C(154)	12230(1)	9383(1)	6365(1)	52(1)
C(155)	12377(1)	10026(2)	6487(2)	57(1)
C(156)	11882(1)	10489(1)	6163(1)	44(1)
C(157)	11230(1)	10301(1)	5709(1)	31(1)
C(158)	9414(1)	9418(1)	5466(1)	24(1)
C(159)	9920(1)	9494(1)	6208(1)	26(1)

C(160)	10271(1)	10067(1)	6469(1)	28(1)
C(161)	10730(1)	10111(1)	7145(1)	37(1)
C(162)	10846(1)	9586(2)	7556(1)	45(1)
C(163)	10504(1)	9018(1)	7298(1)	42(1)
C(164)	10048(1)	8969(1)	6629(1)	35(1)
C(165)	8677(1)	9610(1)	5285(1)	26(1)
C(166)	8676(1)	10292(1)	5541(1)	27(1)
C(167)	8441(1)	9118(1)	5615(1)	37(1)
C(168)	8250(2)	9221(2)	6059(1)	54(1)
C(169)	8204(1)	9591(1)	4514(1)	32(1)
C(170)	7464(1)	9752(2)	4306(1)	48(1)
C(171)	7007(1)	9763(2)	3548(1)	58(1)
C(172)	7051(2)	9122(2)	3243(1)	62(1)
C(173)	7784(2)	8976(2)	3440(1)	51(1)
C(174)	8227(1)	8956(1)	4188(1)	41(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{29}H_{34}NOP$ (13)

P(1)-O(1)	1.4897(13)
P(1)-N(1)	1.6401(16)
P(1)-C(1)	1.7961(19)
P(1)-C(7)	1.8040(19)
N(1)-C(13)	1.472(2)
N(1)-H(1N)	0.8800
C(1)-C(2)	1.386(3)
C(1)-C(6)	1.397(3)
C(2)-C(3)	1.386(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.372(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.391(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.387(3)
C(5)-H(5A)	0.9500

C(6)-H(6A)	0.9500
C(7)-C(8)	1.394(3)
C(7)-C(12)	1.400(3)
C(8)-C(9)	1.390(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.374(3)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.392(3)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.377(3)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-C(14)	1.526(3)
C(13)-C(20)	1.571(3)
C(13)-H(13A)	1.0000
C(14)-C(15)	1.392(3)
C(14)-C(19)	1.392(3)
C(15)-C(16)	1.384(3)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.379(3)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.382(3)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.390(3)
C(18)-H(18A)	0.9500
C(19)-H(19A)	0.9500
C(20)-C(22)	1.516(3)
C(20)-C(21)	1.529(3)
C(20)-C(24)	1.572(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.325(3)
C(22)-H(22A)	0.9500
C(23)-H(23A)	0.9500
C(23)-H(23B)	0.9500

C(24)-C(29)	1.541(3)
C(24)-C(25)	1.542(3)
C(24)-H(24A)	1.0000
C(25)-C(26)	1.524(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.515(4)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.527(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.537(3)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
P(2)-O(2)	1.4899(14)
P(2)-N(2)	1.6415(17)
P(2)-C(30)	1.804(2)
P(2)-C(36)	1.8048(19)
N(2)-C(42)	1.467(2)
N(2)-H(2N)	0.8800
C(30)-C(31)	1.382(3)
C(30)-C(35)	1.404(3)
C(31)-C(32)	1.372(3)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.381(4)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.368(5)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.387(4)
C(34)-H(34A)	0.9500
C(35)-H(35A)	0.9500
C(36)-C(37)	1.386(3)
C(36)-C(41)	1.393(3)

C(37)-C(38)	1.387(3)
C(37)-H(37A)	0.9500
C(38)-C(39)	1.376(3)
C(38)-H(38A)	0.9500
C(39)-C(40)	1.377(3)
C(39)-H(39A)	0.9500
C(40)-C(41)	1.385(3)
C(40)-H(40A)	0.9500
C(41)-H(41A)	0.9500
C(42)-C(43)	1.529(3)
C(42)-C(49)	1.564(3)
C(42)-H(42A)	1.0000
C(43)-C(48)	1.387(3)
C(43)-C(44)	1.389(3)
C(44)-C(45)	1.383(3)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.377(4)
C(45)-H(45A)	0.9500
C(46)-C(47)	1.386(4)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.388(3)
C(47)-H(47A)	0.9500
C(48)-H(48A)	0.9500
C(49)-C(51)	1.505(3)
C(49)-C(50)	1.529(3)
C(49)-C(53)	1.570(3)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.328(3)
C(51)-H(51A)	0.9500
C(52)-H(52A)	0.9500
C(52)-H(52B)	0.9500
C(53)-C(54)	1.535(3)
C(53)-C(58)	1.540(3)
C(53)-H(53A)	1.0000

C(54)-C(55)	1.528(3)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.522(3)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-C(57)	1.530(3)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.525(3)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
P(3)-O(3)	1.4903(14)
P(3)-N(3)	1.6441(16)
P(3)-C(59)	1.8039(19)
P(3)-C(65)	1.807(2)
N(3)-C(71)	1.476(2)
N(3)-H(3N)	0.8800
C(59)-C(60)	1.385(3)
C(59)-C(64)	1.397(3)
C(60)-C(61)	1.393(3)
C(60)-H(60A)	0.9500
C(61)-C(62)	1.376(3)
C(61)-H(61A)	0.9500
C(62)-C(63)	1.370(3)
C(62)-H(62A)	0.9500
C(63)-C(64)	1.380(3)
C(63)-H(63A)	0.9500
C(64)-H(64A)	0.9500
C(65)-C(66)	1.385(3)
C(65)-C(70)	1.400(3)
C(66)-C(67)	1.388(3)
C(66)-H(66A)	0.9500
C(67)-C(68)	1.381(3)

C(67)-H(67A)	0.9500
C(68)-C(69)	1.394(3)
C(68)-H(68A)	0.9500
C(69)-C(70)	1.376(3)
C(69)-H(69A)	0.9500
C(70)-H(70A)	0.9500
C(71)-C(72)	1.531(3)
C(71)-C(78)	1.569(3)
C(71)-H(71A)	1.0000
C(72)-C(77)	1.368(3)
C(72)-C(73)	1.395(3)
C(73)-C(74)	1.381(3)
C(73)-H(73A)	0.9500
C(74)-C(75)	1.394(3)
C(74)-H(74A)	0.9500
C(75)-C(76)	1.373(3)
C(75)-H(75A)	0.9500
C(76)-C(77)	1.398(3)
C(76)-H(76A)	0.9500
C(77)-H(77A)	0.9500
C(78)-C(80)	1.513(3)
C(78)-C(79)	1.514(3)
C(78)-C(82)	1.580(3)
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(80)-C(81)	1.303(3)
C(80)-H(80A)	0.9500
C(81)-H(81A)	0.9500
C(81)-H(81B)	0.9500
C(82)-C(87)	1.525(3)
C(82)-C(83)	1.536(3)
C(82)-H(82A)	1.0000
C(83)-C(84)	1.517(3)
C(83)-H(83A)	0.9900
C(83)-H(83B)	0.9900

C(84)-C(85)	1.518(3)
C(84)-H(84A)	0.9900
C(84)-H(84B)	0.9900
C(85)-C(86)	1.517(3)
C(85)-H(85A)	0.9900
C(85)-H(85B)	0.9900
C(86)-C(87)	1.527(3)
C(86)-H(86A)	0.9900
C(86)-H(86B)	0.9900
C(87)-H(87A)	0.9900
C(87)-H(87B)	0.9900
P(4)-O(4)	1.4894(14)
P(4)-N(4)	1.6464(16)
P(4)-C(94)	1.8016(19)
P(4)-C(88)	1.804(2)
N(4)-C(100)	1.474(2)
N(4)-H(4N)	0.8800
C(88)-C(93)	1.391(3)
C(88)-C(89)	1.398(3)
C(89)-C(90)	1.389(3)
C(89)-H(89A)	0.9500
C(90)-C(91)	1.376(3)
C(90)-H(90A)	0.9500
C(91)-C(92)	1.389(3)
C(91)-H(91A)	0.9500
C(92)-C(93)	1.374(3)
C(92)-H(92A)	0.9500
C(93)-H(93A)	0.9500
C(94)-C(95)	1.391(3)
C(94)-C(99)	1.398(3)
C(95)-C(96)	1.376(3)
C(95)-H(95A)	0.9500
C(96)-C(97)	1.381(4)
C(96)-H(96A)	0.9500
C(97)-C(98)	1.389(4)
C(97)-H(97A)	0.9500

C(98)-C(99)	1.376(3)
C(98)-H(98A)	0.9500
C(99)-H(99A)	0.9500
C(100)-C(101)	1.523(3)
C(100)-C(107)	1.573(3)
C(100)-H(10B)	1.0000
C(101)-C(102)	1.389(3)
C(101)-C(106)	1.391(3)
C(102)-C(103)	1.388(3)
C(102)-H(10C)	0.9500
C(103)-C(104)	1.378(4)
C(103)-H(10D)	0.9500
C(104)-C(105)	1.375(4)
C(104)-H(10E)	0.9500
C(105)-C(106)	1.394(3)
C(105)-H(10F)	0.9500
C(106)-H(10G)	0.9500
C(107)-C(109)	1.513(3)
C(107)-C(108)	1.514(3)
C(107)-C(111)	1.568(3)
C(108)-H(10H)	0.9800
C(108)-H(10I)	0.9800
C(108)-H(10J)	0.9800
C(109)-C(110)	1.305(3)
C(109)-H(10K)	0.9500
C(110)-H(11B)	0.9500
C(110)-H(11C)	0.9500
C(111)-C(116)	1.528(3)
C(111)-C(112)	1.539(3)
C(111)-H(11E)	1.0000
C(112)-C(113)	1.532(3)
C(112)-H(11F)	0.9900
C(112)-H(11G)	0.9900
C(113)-C(114)	1.522(3)
C(113)-H(11H)	0.9900
C(113)-H(11I)	0.9900

C(114)-C(115)	1.519(3)
C(114)-H(11J)	0.9900
C(114)-H(11K)	0.9900
C(115)-C(116)	1.536(3)
C(115)-H(11L)	0.9900
C(115)-H(11M)	0.9900
C(116)-H(11N)	0.9900
C(116)-H(11O)	0.9900
P(5)-O(5)	1.4915(14)
P(5)-N(5)	1.6398(16)
P(5)-C(117)	1.8002(19)
P(5)-C(123)	1.805(2)
N(5)-C(129)	1.463(2)
N(5)-H(5N)	0.8800
C(117)-C(122)	1.389(3)
C(117)-C(118)	1.398(3)
C(118)-C(119)	1.384(3)
C(118)-H(11P)	0.9500
C(119)-C(120)	1.376(3)
C(119)-H(11Q)	0.9500
C(120)-C(121)	1.382(3)
C(120)-H(12B)	0.9500
C(121)-C(122)	1.383(3)
C(121)-H(12C)	0.9500
C(122)-H(12D)	0.9500
C(123)-C(124)	1.391(3)
C(123)-C(128)	1.403(3)
C(124)-C(125)	1.375(3)
C(124)-H(12E)	0.9500
C(125)-C(126)	1.385(4)
C(125)-H(12F)	0.9500
C(126)-C(127)	1.379(4)
C(126)-H(12G)	0.9500
C(127)-C(128)	1.374(3)
C(127)-H(12H)	0.9500
C(128)-H(12I)	0.9500

C(129)-C(130)	1.521(3)
C(129)-C(136)	1.574(3)
C(129)-H(12J)	1.0000
C(130)-C(135)	1.386(3)
C(130)-C(131)	1.390(3)
C(131)-C(132)	1.391(3)
C(131)-H(13B)	0.9500
C(132)-C(133)	1.375(3)
C(132)-H(13C)	0.9500
C(133)-C(134)	1.378(4)
C(133)-H(13D)	0.9500
C(134)-C(135)	1.391(3)
C(134)-H(13E)	0.9500
C(135)-H(13F)	0.9500
C(136)-C(138)	1.515(3)
C(136)-C(137)	1.538(3)
C(136)-C(140)	1.575(3)
C(137)-H(13G)	0.9800
C(137)-H(13H)	0.9800
C(137)-H(13I)	0.9800
C(138)-C(139)	1.321(4)
C(138)-H(13J)	0.9500
C(139)-H(13K)	0.9500
C(139)-H(13L)	0.9500
C(140)-C(145)	1.532(3)
C(140)-C(141)	1.534(3)
C(140)-H(14A)	1.0000
C(141)-C(142)	1.519(3)
C(141)-H(14B)	0.9900
C(141)-H(14C)	0.9900
C(142)-C(143)	1.528(4)
C(142)-H(14D)	0.9900
C(142)-H(14E)	0.9900
C(143)-C(144)	1.526(3)
C(143)-H(14F)	0.9900
C(143)-H(14G)	0.9900

C(144)-C(145)	1.529(3)
C(144)-H(14H)	0.9900
C(144)-H(14I)	0.9900
C(145)-H(14J)	0.9900
C(145)-H(14K)	0.9900
P(6)-O(6)	1.4880(15)
P(6)-N(6)	1.6515(17)
P(6)-C(152)	1.798(2)
P(6)-C(146)	1.806(2)
N(6)-C(158)	1.472(2)
N(6)-H(6N)	0.8800
C(146)-C(151)	1.392(3)
C(146)-C(147)	1.393(3)
C(147)-C(148)	1.380(3)
C(147)-H(14L)	0.9500
C(148)-C(149)	1.381(3)
C(148)-H(14M)	0.9500
C(149)-C(150)	1.378(3)
C(149)-H(14N)	0.9500
C(150)-C(151)	1.396(3)
C(150)-H(15B)	0.9500
C(151)-H(15C)	0.9500
C(152)-C(153)	1.392(3)
C(152)-C(157)	1.395(3)
C(153)-C(154)	1.386(4)
C(153)-H(15D)	0.9500
C(154)-C(155)	1.366(4)
C(154)-H(15E)	0.9500
C(155)-C(156)	1.382(4)
C(155)-H(15F)	0.9500
C(156)-C(157)	1.383(3)
C(156)-H(15G)	0.9500
C(157)-H(15H)	0.9500
C(158)-C(159)	1.534(3)
C(158)-C(165)	1.558(3)
C(158)-H(15I)	1.0000

C(159)-C(164)	1.388(3)
C(159)-C(160)	1.389(3)
C(160)-C(161)	1.392(3)
C(160)-H(16B)	0.9500
C(161)-C(162)	1.380(4)
C(161)-H(16C)	0.9500
C(162)-C(163)	1.371(4)
C(162)-H(16D)	0.9500
C(163)-C(164)	1.379(3)
C(163)-H(16E)	0.9500
C(164)-H(16F)	0.9500
C(165)-C(167)	1.512(3)
C(165)-C(166)	1.526(3)
C(165)-C(169)	1.567(3)
C(166)-H(16G)	0.9800
C(166)-H(16H)	0.9800
C(166)-H(16I)	0.9800
C(167)-C(168)	1.306(4)
C(167)-H(16J)	0.9500
C(168)-H(16K)	0.9500
C(168)-H(16L)	0.9500
C(169)-C(174)	1.526(3)
C(169)-C(170)	1.534(3)
C(169)-H(16N)	1.0000
C(170)-C(171)	1.536(4)
C(170)-H(17B)	0.9900
C(170)-H(17C)	0.9900
C(171)-C(172)	1.526(5)
C(171)-H(17D)	0.9900
C(171)-H(17E)	0.9900
C(172)-C(173)	1.517(4)
C(172)-H(17F)	0.9900
C(172)-H(17G)	0.9900
C(173)-C(174)	1.514(3)
C(173)-H(17H)	0.9900
C(173)-H(17I)	0.9900

C(174)-H(17J)	0.9900
C(174)-H(17K)	0.9900
O(1)-P(1)-N(1)	111.29(8)
O(1)-P(1)-C(1)	111.77(9)
N(1)-P(1)-C(1)	108.90(9)
O(1)-P(1)-C(7)	110.71(8)
N(1)-P(1)-C(7)	108.61(8)
C(1)-P(1)-C(7)	105.33(9)
C(13)-N(1)-P(1)	121.44(13)
C(13)-N(1)-H(1N)	119.3
P(1)-N(1)-H(1N)	119.3
C(2)-C(1)-C(6)	119.69(18)
C(2)-C(1)-P(1)	119.25(16)
C(6)-C(1)-P(1)	121.02(15)
C(3)-C(2)-C(1)	120.0(2)
C(3)-C(2)-H(2A)	120.0
C(1)-C(2)-H(2A)	120.0
C(4)-C(3)-C(2)	120.4(2)
C(4)-C(3)-H(3A)	119.8
C(2)-C(3)-H(3A)	119.8
C(3)-C(4)-C(5)	120.2(2)
C(3)-C(4)-H(4A)	119.9
C(5)-C(4)-H(4A)	119.9
C(6)-C(5)-C(4)	119.9(2)
C(6)-C(5)-H(5A)	120.1
C(4)-C(5)-H(5A)	120.1
C(5)-C(6)-C(1)	119.80(19)
C(5)-C(6)-H(6A)	120.1
C(1)-C(6)-H(6A)	120.1
C(8)-C(7)-C(12)	118.51(18)
C(8)-C(7)-P(1)	122.49(15)
C(12)-C(7)-P(1)	118.41(15)
C(9)-C(8)-C(7)	120.74(19)
C(9)-C(8)-H(8A)	119.6
C(7)-C(8)-H(8A)	119.6
C(10)-C(9)-C(8)	119.85(19)

C(10)-C(9)-H(9A)	120.1
C(8)-C(9)-H(9A)	120.1
C(9)-C(10)-C(11)	120.2(2)
C(9)-C(10)-H(10A)	119.9
C(11)-C(10)-H(10A)	119.9
C(12)-C(11)-C(10)	120.10(19)
C(12)-C(11)-H(11A)	119.9
C(10)-C(11)-H(11A)	119.9
C(11)-C(12)-C(7)	120.58(18)
C(11)-C(12)-H(12A)	119.7
C(7)-C(12)-H(12A)	119.7
N(1)-C(13)-C(14)	110.40(15)
N(1)-C(13)-C(20)	113.24(15)
C(14)-C(13)-C(20)	114.06(15)
N(1)-C(13)-H(13A)	106.2
C(14)-C(13)-H(13A)	106.2
C(20)-C(13)-H(13A)	106.2
C(15)-C(14)-C(19)	118.30(19)
C(15)-C(14)-C(13)	122.41(18)
C(19)-C(14)-C(13)	119.21(17)
C(16)-C(15)-C(14)	120.7(2)
C(16)-C(15)-H(15A)	119.7
C(14)-C(15)-H(15A)	119.7
C(17)-C(16)-C(15)	120.6(2)
C(17)-C(16)-H(16A)	119.7
C(15)-C(16)-H(16A)	119.7
C(16)-C(17)-C(18)	119.4(2)
C(16)-C(17)-H(17A)	120.3
C(18)-C(17)-H(17A)	120.3
C(17)-C(18)-C(19)	120.1(2)
C(17)-C(18)-H(18A)	119.9
C(19)-C(18)-H(18A)	119.9
C(18)-C(19)-C(14)	120.8(2)
C(18)-C(19)-H(19A)	119.6
C(14)-C(19)-H(19A)	119.6
C(22)-C(20)-C(21)	111.77(17)

C(22)-C(20)-C(13)	106.16(16)
C(21)-C(20)-C(13)	110.65(16)
C(22)-C(20)-C(24)	109.85(16)
C(21)-C(20)-C(24)	109.70(16)
C(13)-C(20)-C(24)	108.63(16)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(20)	127.0(2)
C(23)-C(22)-H(22A)	116.5
C(20)-C(22)-H(22A)	116.5
C(22)-C(23)-H(23A)	120.0
C(22)-C(23)-H(23B)	120.0
H(23A)-C(23)-H(23B)	120.0
C(29)-C(24)-C(25)	108.45(18)
C(29)-C(24)-C(20)	114.43(17)
C(25)-C(24)-C(20)	112.66(18)
C(29)-C(24)-H(24A)	107.0
C(25)-C(24)-H(24A)	107.0
C(20)-C(24)-H(24A)	107.0
C(26)-C(25)-C(24)	111.9(2)
C(26)-C(25)-H(25A)	109.2
C(24)-C(25)-H(25A)	109.2
C(26)-C(25)-H(25B)	109.2
C(24)-C(25)-H(25B)	109.2
H(25A)-C(25)-H(25B)	107.9
C(27)-C(26)-C(25)	112.4(2)
C(27)-C(26)-H(26A)	109.1
C(25)-C(26)-H(26A)	109.1
C(27)-C(26)-H(26B)	109.1
C(25)-C(26)-H(26B)	109.1
H(26A)-C(26)-H(26B)	107.9
C(26)-C(27)-C(28)	110.3(2)

C(26)-C(27)-H(27A)	109.6
C(28)-C(27)-H(27A)	109.6
C(26)-C(27)-H(27B)	109.6
C(28)-C(27)-H(27B)	109.6
H(27A)-C(27)-H(27B)	108.1
C(27)-C(28)-C(29)	110.9(2)
C(27)-C(28)-H(28A)	109.5
C(29)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
C(29)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	108.0
C(28)-C(29)-C(24)	111.82(18)
C(28)-C(29)-H(29A)	109.3
C(24)-C(29)-H(29A)	109.3
C(28)-C(29)-H(29B)	109.3
C(24)-C(29)-H(29B)	109.3
H(29A)-C(29)-H(29B)	107.9
O(2)-P(2)-N(2)	111.27(8)
O(2)-P(2)-C(30)	111.24(9)
N(2)-P(2)-C(30)	111.14(9)
O(2)-P(2)-C(36)	112.89(8)
N(2)-P(2)-C(36)	103.32(9)
C(30)-P(2)-C(36)	106.65(9)
C(42)-N(2)-P(2)	119.67(13)
C(42)-N(2)-H(2N)	120.2
P(2)-N(2)-H(2N)	120.2
C(31)-C(30)-C(35)	119.2(2)
C(31)-C(30)-P(2)	122.37(16)
C(35)-C(30)-P(2)	118.43(18)
C(32)-C(31)-C(30)	121.1(2)
C(32)-C(31)-H(31A)	119.4
C(30)-C(31)-H(31A)	119.4
C(31)-C(32)-C(33)	119.6(3)
C(31)-C(32)-H(32A)	120.2
C(33)-C(32)-H(32A)	120.2
C(34)-C(33)-C(32)	120.3(3)

C(34)-C(33)-H(33A)	119.9
C(32)-C(33)-H(33A)	119.9
C(33)-C(34)-C(35)	120.9(3)
C(33)-C(34)-H(34A)	119.6
C(35)-C(34)-H(34A)	119.6
C(34)-C(35)-C(30)	118.9(3)
C(34)-C(35)-H(35A)	120.6
C(30)-C(35)-H(35A)	120.6
C(37)-C(36)-C(41)	118.90(18)
C(37)-C(36)-P(2)	125.82(15)
C(41)-C(36)-P(2)	115.28(15)
C(36)-C(37)-C(38)	120.3(2)
C(36)-C(37)-H(37A)	119.8
C(38)-C(37)-H(37A)	119.8
C(39)-C(38)-C(37)	120.2(2)
C(39)-C(38)-H(38A)	119.9
C(37)-C(38)-H(38A)	119.9
C(38)-C(39)-C(40)	120.21(19)
C(38)-C(39)-H(39A)	119.9
C(40)-C(39)-H(39A)	119.9
C(39)-C(40)-C(41)	119.8(2)
C(39)-C(40)-H(40A)	120.1
C(41)-C(40)-H(40A)	120.1
C(40)-C(41)-C(36)	120.5(2)
C(40)-C(41)-H(41A)	119.7
C(36)-C(41)-H(41A)	119.7
N(2)-C(42)-C(43)	111.80(16)
N(2)-C(42)-C(49)	110.85(15)
C(43)-C(42)-C(49)	114.71(15)
N(2)-C(42)-H(42A)	106.3
C(43)-C(42)-H(42A)	106.3
C(49)-C(42)-H(42A)	106.3
C(48)-C(43)-C(44)	118.4(2)
C(48)-C(43)-C(42)	121.72(18)
C(44)-C(43)-C(42)	119.75(19)
C(45)-C(44)-C(43)	121.2(2)

C(45)-C(44)-H(44A)	119.4
C(43)-C(44)-H(44A)	119.4
C(46)-C(45)-C(44)	120.0(2)
C(46)-C(45)-H(45A)	120.0
C(44)-C(45)-H(45A)	120.0
C(45)-C(46)-C(47)	119.7(2)
C(45)-C(46)-H(46A)	120.2
C(47)-C(46)-H(46A)	120.2
C(46)-C(47)-C(48)	120.2(2)
C(46)-C(47)-H(47A)	119.9
C(48)-C(47)-H(47A)	119.9
C(43)-C(48)-C(47)	120.6(2)
C(43)-C(48)-H(48A)	119.7
C(47)-C(48)-H(48A)	119.7
C(51)-C(49)-C(50)	111.47(16)
C(51)-C(49)-C(42)	107.72(16)
C(50)-C(49)-C(42)	109.28(15)
C(51)-C(49)-C(53)	108.81(16)
C(50)-C(49)-C(53)	109.77(15)
C(42)-C(49)-C(53)	109.75(15)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-C(49)	126.7(2)
C(52)-C(51)-H(51A)	116.7
C(49)-C(51)-H(51A)	116.7
C(51)-C(52)-H(52A)	120.0
C(51)-C(52)-H(52B)	120.0
H(52A)-C(52)-H(52B)	120.0
C(54)-C(53)-C(58)	109.03(17)
C(54)-C(53)-C(49)	112.18(16)
C(58)-C(53)-C(49)	113.92(16)
C(54)-C(53)-H(53A)	107.1

C(58)-C(53)-H(53A)	107.1
C(49)-C(53)-H(53A)	107.1
C(55)-C(54)-C(53)	111.85(19)
C(55)-C(54)-H(54A)	109.2
C(53)-C(54)-H(54A)	109.2
C(55)-C(54)-H(54B)	109.2
C(53)-C(54)-H(54B)	109.2
H(54A)-C(54)-H(54B)	107.9
C(56)-C(55)-C(54)	111.6(2)
C(56)-C(55)-H(55A)	109.3
C(54)-C(55)-H(55A)	109.3
C(56)-C(55)-H(55B)	109.3
C(54)-C(55)-H(55B)	109.3
H(55A)-C(55)-H(55B)	108.0
C(55)-C(56)-C(57)	110.1(2)
C(55)-C(56)-H(56A)	109.6
C(57)-C(56)-H(56A)	109.6
C(55)-C(56)-H(56B)	109.6
C(57)-C(56)-H(56B)	109.6
H(56A)-C(56)-H(56B)	108.2
C(58)-C(57)-C(56)	111.45(19)
C(58)-C(57)-H(57A)	109.3
C(56)-C(57)-H(57A)	109.3
C(58)-C(57)-H(57B)	109.3
C(56)-C(57)-H(57B)	109.3
H(57A)-C(57)-H(57B)	108.0
C(57)-C(58)-C(53)	111.63(17)
C(57)-C(58)-H(58A)	109.3
C(53)-C(58)-H(58A)	109.3
C(57)-C(58)-H(58B)	109.3
C(53)-C(58)-H(58B)	109.3
H(58A)-C(58)-H(58B)	108.0
O(3)-P(3)-N(3)	111.43(8)
O(3)-P(3)-C(59)	113.29(8)
N(3)-P(3)-C(59)	106.09(8)
O(3)-P(3)-C(65)	111.00(8)

N(3)-P(3)-C(65)	111.62(8)
C(59)-P(3)-C(65)	103.05(9)
C(71)-N(3)-P(3)	119.08(12)
C(71)-N(3)-H(3N)	120.5
P(3)-N(3)-H(3N)	120.5
C(60)-C(59)-C(64)	118.76(18)
C(60)-C(59)-P(3)	121.52(15)
C(64)-C(59)-P(3)	119.40(15)
C(59)-C(60)-C(61)	120.0(2)
C(59)-C(60)-H(60A)	120.0
C(61)-C(60)-H(60A)	120.0
C(62)-C(61)-C(60)	120.4(2)
C(62)-C(61)-H(61A)	119.8
C(60)-C(61)-H(61A)	119.8
C(63)-C(62)-C(61)	119.9(2)
C(63)-C(62)-H(62A)	120.1
C(61)-C(62)-H(62A)	120.1
C(62)-C(63)-C(64)	120.5(2)
C(62)-C(63)-H(63A)	119.7
C(64)-C(63)-H(63A)	119.7
C(63)-C(64)-C(59)	120.4(2)
C(63)-C(64)-H(64A)	119.8
C(59)-C(64)-H(64A)	119.8
C(66)-C(65)-C(70)	119.26(18)
C(66)-C(65)-P(3)	119.92(15)
C(70)-C(65)-P(3)	120.64(15)
C(65)-C(66)-C(67)	120.52(19)
C(65)-C(66)-H(66A)	119.7
C(67)-C(66)-H(66A)	119.7
C(68)-C(67)-C(66)	120.12(19)
C(68)-C(67)-H(67A)	119.9
C(66)-C(67)-H(67A)	119.9
C(67)-C(68)-C(69)	119.6(2)
C(67)-C(68)-H(68A)	120.2
C(69)-C(68)-H(68A)	120.2
C(70)-C(69)-C(68)	120.5(2)

C(70)-C(69)-H(69A)	119.8
C(68)-C(69)-H(69A)	119.8
C(69)-C(70)-C(65)	120.06(19)
C(69)-C(70)-H(70A)	120.0
C(65)-C(70)-H(70A)	120.0
N(3)-C(71)-C(72)	112.62(16)
N(3)-C(71)-C(78)	111.92(15)
C(72)-C(71)-C(78)	112.36(16)
N(3)-C(71)-H(71A)	106.5
C(72)-C(71)-H(71A)	106.5
C(78)-C(71)-H(71A)	106.5
C(77)-C(72)-C(73)	118.25(19)
C(77)-C(72)-C(71)	120.26(18)
C(73)-C(72)-C(71)	121.47(18)
C(74)-C(73)-C(72)	120.7(2)
C(74)-C(73)-H(73A)	119.6
C(72)-C(73)-H(73A)	119.6
C(73)-C(74)-C(75)	120.7(2)
C(73)-C(74)-H(74A)	119.6
C(75)-C(74)-H(74A)	119.6
C(76)-C(75)-C(74)	118.4(2)
C(76)-C(75)-H(75A)	120.8
C(74)-C(75)-H(75A)	120.8
C(75)-C(76)-C(77)	120.6(2)
C(75)-C(76)-H(76A)	119.7
C(77)-C(76)-H(76A)	119.7
C(72)-C(77)-C(76)	121.2(2)
C(72)-C(77)-H(77A)	119.4
C(76)-C(77)-H(77A)	119.4
C(80)-C(78)-C(79)	111.29(17)
C(80)-C(78)-C(71)	106.44(16)
C(79)-C(78)-C(71)	111.24(16)
C(80)-C(78)-C(82)	108.84(17)
C(79)-C(78)-C(82)	109.41(16)
C(71)-C(78)-C(82)	109.55(16)
C(78)-C(79)-H(79A)	109.5

C(78)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(78)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(81)-C(80)-C(78)	128.4(2)
C(81)-C(80)-H(80A)	115.8
C(78)-C(80)-H(80A)	115.8
C(80)-C(81)-H(81A)	120.0
C(80)-C(81)-H(81B)	120.0
H(81A)-C(81)-H(81B)	120.0
C(87)-C(82)-C(83)	108.74(17)
C(87)-C(82)-C(78)	114.06(17)
C(83)-C(82)-C(78)	113.34(17)
C(87)-C(82)-H(82A)	106.7
C(83)-C(82)-H(82A)	106.7
C(78)-C(82)-H(82A)	106.7
C(84)-C(83)-C(82)	111.31(19)
C(84)-C(83)-H(83A)	109.4
C(82)-C(83)-H(83A)	109.4
C(84)-C(83)-H(83B)	109.4
C(82)-C(83)-H(83B)	109.4
H(83A)-C(83)-H(83B)	108.0
C(83)-C(84)-C(85)	112.2(2)
C(83)-C(84)-H(84A)	109.2
C(85)-C(84)-H(84A)	109.2
C(83)-C(84)-H(84B)	109.2
C(85)-C(84)-H(84B)	109.2
H(84A)-C(84)-H(84B)	107.9
C(86)-C(85)-C(84)	110.18(19)
C(86)-C(85)-H(85A)	109.6
C(84)-C(85)-H(85A)	109.6
C(86)-C(85)-H(85B)	109.6
C(84)-C(85)-H(85B)	109.6
H(85A)-C(85)-H(85B)	108.1
C(85)-C(86)-C(87)	110.8(2)

C(85)-C(86)-H(86A)	109.5
C(87)-C(86)-H(86A)	109.5
C(85)-C(86)-H(86B)	109.5
C(87)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	108.1
C(82)-C(87)-C(86)	111.50(18)
C(82)-C(87)-H(87A)	109.3
C(86)-C(87)-H(87A)	109.3
C(82)-C(87)-H(87B)	109.3
C(86)-C(87)-H(87B)	109.3
H(87A)-C(87)-H(87B)	108.0
O(4)-P(4)-N(4)	111.86(8)
O(4)-P(4)-C(94)	110.46(9)
N(4)-P(4)-C(94)	110.72(8)
O(4)-P(4)-C(88)	114.94(9)
N(4)-P(4)-C(88)	102.72(9)
C(94)-P(4)-C(88)	105.77(9)
C(100)-N(4)-P(4)	118.03(13)
C(100)-N(4)-H(4N)	121.0
P(4)-N(4)-H(4N)	121.0
C(93)-C(88)-C(89)	118.96(19)
C(93)-C(88)-P(4)	121.25(16)
C(89)-C(88)-P(4)	119.68(15)
C(90)-C(89)-C(88)	119.9(2)
C(90)-C(89)-H(89A)	120.0
C(88)-C(89)-H(89A)	120.0
C(91)-C(90)-C(89)	120.1(2)
C(91)-C(90)-H(90A)	120.0
C(89)-C(90)-H(90A)	120.0
C(90)-C(91)-C(92)	120.5(2)
C(90)-C(91)-H(91A)	119.8
C(92)-C(91)-H(91A)	119.8
C(93)-C(92)-C(91)	119.6(2)
C(93)-C(92)-H(92A)	120.2
C(91)-C(92)-H(92A)	120.2
C(92)-C(93)-C(88)	121.0(2)

C(92)-C(93)-H(93A)	119.5
C(88)-C(93)-H(93A)	119.5
C(95)-C(94)-C(99)	119.27(18)
C(95)-C(94)-P(4)	120.71(15)
C(99)-C(94)-P(4)	119.98(15)
C(96)-C(95)-C(94)	120.3(2)
C(96)-C(95)-H(95A)	119.8
C(94)-C(95)-H(95A)	119.8
C(95)-C(96)-C(97)	120.3(2)
C(95)-C(96)-H(96A)	119.8
C(97)-C(96)-H(96A)	119.8
C(96)-C(97)-C(98)	119.8(2)
C(96)-C(97)-H(97A)	120.1
C(98)-C(97)-H(97A)	120.1
C(99)-C(98)-C(97)	120.3(2)
C(99)-C(98)-H(98A)	119.8
C(97)-C(98)-H(98A)	119.8
C(98)-C(99)-C(94)	120.0(2)
C(98)-C(99)-H(99A)	120.0
C(94)-C(99)-H(99A)	120.0
N(4)-C(100)-C(101)	112.40(15)
N(4)-C(100)-C(107)	111.05(15)
C(101)-C(100)-C(107)	112.38(16)
N(4)-C(100)-H(10B)	106.9
C(101)-C(100)-H(10B)	106.9
C(107)-C(100)-H(10B)	106.9
C(102)-C(101)-C(106)	118.4(2)
C(102)-C(101)-C(100)	121.74(19)
C(106)-C(101)-C(100)	119.83(19)
C(103)-C(102)-C(101)	120.9(2)
C(103)-C(102)-H(10C)	119.6
C(101)-C(102)-H(10C)	119.6
C(104)-C(103)-C(102)	120.1(2)
C(104)-C(103)-H(10D)	120.0
C(102)-C(103)-H(10D)	120.0
C(105)-C(104)-C(103)	119.9(2)

C(105)-C(104)-H(10E)	120.1
C(103)-C(104)-H(10E)	120.1
C(104)-C(105)-C(106)	120.3(2)
C(104)-C(105)-H(10F)	119.9
C(106)-C(105)-H(10F)	119.9
C(101)-C(106)-C(105)	120.4(2)
C(101)-C(106)-H(10G)	119.8
C(105)-C(106)-H(10G)	119.8
C(109)-C(107)-C(108)	111.77(17)
C(109)-C(107)-C(111)	110.35(15)
C(108)-C(107)-C(111)	108.70(16)
C(109)-C(107)-C(100)	106.05(15)
C(108)-C(107)-C(100)	110.12(15)
C(111)-C(107)-C(100)	109.83(15)
C(107)-C(108)-H(10H)	109.5
C(107)-C(108)-H(10I)	109.5
H(10H)-C(108)-H(10I)	109.5
C(107)-C(108)-H(10J)	109.5
H(10H)-C(108)-H(10J)	109.5
H(10I)-C(108)-H(10J)	109.5
C(110)-C(109)-C(107)	129.0(2)
C(110)-C(109)-H(10K)	115.5
C(107)-C(109)-H(10K)	115.5
C(109)-C(110)-H(11B)	120.0
C(109)-C(110)-H(11C)	120.0
H(11B)-C(110)-H(11C)	120.0
C(116)-C(111)-C(112)	109.50(15)
C(116)-C(111)-C(107)	114.51(15)
C(112)-C(111)-C(107)	111.32(15)
C(116)-C(111)-H(11E)	107.0
C(112)-C(111)-H(11E)	107.0
C(107)-C(111)-H(11E)	107.0
C(113)-C(112)-C(111)	111.52(16)
C(113)-C(112)-H(11F)	109.3
C(111)-C(112)-H(11F)	109.3
C(113)-C(112)-H(11G)	109.3

C(111)-C(112)-H(11G)	109.3
H(11F)-C(112)-H(11G)	108.0
C(114)-C(113)-C(112)	111.05(17)
C(114)-C(113)-H(11H)	109.4
C(112)-C(113)-H(11H)	109.4
C(114)-C(113)-H(11I)	109.4
C(112)-C(113)-H(11I)	109.4
H(11H)-C(113)-H(11I)	108.0
C(115)-C(114)-C(113)	109.77(17)
C(115)-C(114)-H(11J)	109.7
C(113)-C(114)-H(11J)	109.7
C(115)-C(114)-H(11K)	109.7
C(113)-C(114)-H(11K)	109.7
H(11J)-C(114)-H(11K)	108.2
C(114)-C(115)-C(116)	111.12(17)
C(114)-C(115)-H(11L)	109.4
C(116)-C(115)-H(11L)	109.4
C(114)-C(115)-H(11M)	109.4
C(116)-C(115)-H(11M)	109.4
H(11L)-C(115)-H(11M)	108.0
C(111)-C(116)-C(115)	111.53(17)
C(111)-C(116)-H(11N)	109.3
C(115)-C(116)-H(11N)	109.3
C(111)-C(116)-H(11O)	109.3
C(115)-C(116)-H(11O)	109.3
H(11N)-C(116)-H(11O)	108.0
O(5)-P(5)-N(5)	112.21(8)
O(5)-P(5)-C(117)	110.88(9)
N(5)-P(5)-C(117)	109.54(8)
O(5)-P(5)-C(123)	111.93(8)
N(5)-P(5)-C(123)	106.79(9)
C(117)-P(5)-C(123)	105.16(9)
C(129)-N(5)-P(5)	122.21(12)
C(129)-N(5)-H(5N)	118.9
P(5)-N(5)-H(5N)	118.9
C(122)-C(117)-C(118)	119.31(18)

C(122)-C(117)-P(5)	121.60(15)
C(118)-C(117)-P(5)	119.09(15)
C(119)-C(118)-C(117)	119.8(2)
C(119)-C(118)-H(11P)	120.1
C(117)-C(118)-H(11P)	120.1
C(120)-C(119)-C(118)	120.6(2)
C(120)-C(119)-H(11Q)	119.7
C(118)-C(119)-H(11Q)	119.7
C(119)-C(120)-C(121)	119.7(2)
C(119)-C(120)-H(12B)	120.2
C(121)-C(120)-H(12B)	120.2
C(120)-C(121)-C(122)	120.6(2)
C(120)-C(121)-H(12C)	119.7
C(122)-C(121)-H(12C)	119.7
C(121)-C(122)-C(117)	120.0(2)
C(121)-C(122)-H(12D)	120.0
C(117)-C(122)-H(12D)	120.0
C(124)-C(123)-C(128)	118.8(2)
C(124)-C(123)-P(5)	121.90(17)
C(128)-C(123)-P(5)	119.00(16)
C(125)-C(124)-C(123)	120.5(2)
C(125)-C(124)-H(12E)	119.8
C(123)-C(124)-H(12E)	119.8
C(124)-C(125)-C(126)	120.1(2)
C(124)-C(125)-H(12F)	119.9
C(126)-C(125)-H(12F)	119.9
C(127)-C(126)-C(125)	120.1(2)
C(127)-C(126)-H(12G)	120.0
C(125)-C(126)-H(12G)	120.0
C(128)-C(127)-C(126)	120.2(3)
C(128)-C(127)-H(12H)	119.9
C(126)-C(127)-H(12H)	119.9
C(127)-C(128)-C(123)	120.3(2)
C(127)-C(128)-H(12I)	119.8
C(123)-C(128)-H(12I)	119.8
N(5)-C(129)-C(130)	111.22(16)

N(5)-C(129)-C(136)	112.91(15)
C(130)-C(129)-C(136)	112.81(16)
N(5)-C(129)-H(12J)	106.5
C(130)-C(129)-H(12J)	106.5
C(136)-C(129)-H(12J)	106.5
C(135)-C(130)-C(131)	118.28(18)
C(135)-C(130)-C(129)	119.45(18)
C(131)-C(130)-C(129)	122.26(17)
C(130)-C(131)-C(132)	120.33(19)
C(130)-C(131)-H(13B)	119.8
C(132)-C(131)-H(13B)	119.8
C(133)-C(132)-C(131)	120.7(2)
C(133)-C(132)-H(13C)	119.6
C(131)-C(132)-H(13C)	119.6
C(132)-C(133)-C(134)	119.5(2)
C(132)-C(133)-H(13D)	120.2
C(134)-C(133)-H(13D)	120.2
C(133)-C(134)-C(135)	119.9(2)
C(133)-C(134)-H(13E)	120.1
C(135)-C(134)-H(13E)	120.1
C(130)-C(135)-C(134)	121.2(2)
C(130)-C(135)-H(13F)	119.4
C(134)-C(135)-H(13F)	119.4
C(138)-C(136)-C(137)	111.96(18)
C(138)-C(136)-C(129)	106.73(17)
C(137)-C(136)-C(129)	110.21(16)
C(138)-C(136)-C(140)	109.35(16)
C(137)-C(136)-C(140)	108.97(17)
C(129)-C(136)-C(140)	109.59(16)
C(136)-C(137)-H(13G)	109.5
C(136)-C(137)-H(13H)	109.5
H(13G)-C(137)-H(13H)	109.5
C(136)-C(137)-H(13I)	109.5
H(13G)-C(137)-H(13I)	109.5
H(13H)-C(137)-H(13I)	109.5
C(139)-C(138)-C(136)	127.3(3)

C(139)-C(138)-H(13J)	116.4
C(136)-C(138)-H(13J)	116.4
C(138)-C(139)-H(13K)	120.0
C(138)-C(139)-H(13L)	120.0
H(13K)-C(139)-H(13L)	120.0
C(145)-C(140)-C(141)	108.34(18)
C(145)-C(140)-C(136)	114.06(17)
C(141)-C(140)-C(136)	112.79(18)
C(145)-C(140)-H(14A)	107.1
C(141)-C(140)-H(14A)	107.1
C(136)-C(140)-H(14A)	107.1
C(142)-C(141)-C(140)	111.9(2)
C(142)-C(141)-H(14B)	109.2
C(140)-C(141)-H(14B)	109.2
C(142)-C(141)-H(14C)	109.2
C(140)-C(141)-H(14C)	109.2
H(14B)-C(141)-H(14C)	107.9
C(141)-C(142)-C(143)	112.0(2)
C(141)-C(142)-H(14D)	109.2
C(143)-C(142)-H(14D)	109.2
C(141)-C(142)-H(14E)	109.2
C(143)-C(142)-H(14E)	109.2
H(14D)-C(142)-H(14E)	107.9
C(144)-C(143)-C(142)	109.4(2)
C(144)-C(143)-H(14F)	109.8
C(142)-C(143)-H(14F)	109.8
C(144)-C(143)-H(14G)	109.8
C(142)-C(143)-H(14G)	109.8
H(14F)-C(143)-H(14G)	108.2
C(143)-C(144)-C(145)	111.3(2)
C(143)-C(144)-H(14H)	109.4
C(145)-C(144)-H(14H)	109.4
C(143)-C(144)-H(14I)	109.4
C(145)-C(144)-H(14I)	109.4
H(14H)-C(144)-H(14I)	108.0
C(144)-C(145)-C(140)	111.41(17)

C(144)-C(145)-H(14J)	109.3
C(140)-C(145)-H(14J)	109.3
C(144)-C(145)-H(14K)	109.3
C(140)-C(145)-H(14K)	109.3
H(14J)-C(145)-H(14K)	108.0
O(6)-P(6)-N(6)	110.90(9)
O(6)-P(6)-C(152)	111.01(9)
N(6)-P(6)-C(152)	112.32(9)
O(6)-P(6)-C(146)	112.79(9)
N(6)-P(6)-C(146)	104.33(8)
C(152)-P(6)-C(146)	105.23(10)
C(158)-N(6)-P(6)	117.85(13)
C(158)-N(6)-H(6N)	121.1
P(6)-N(6)-H(6N)	121.1
C(151)-C(146)-C(147)	118.64(18)
C(151)-C(146)-P(6)	123.86(16)
C(147)-C(146)-P(6)	117.38(16)
C(148)-C(147)-C(146)	120.4(2)
C(148)-C(147)-H(14L)	119.8
C(146)-C(147)-H(14L)	119.8
C(147)-C(148)-C(149)	120.7(2)
C(147)-C(148)-H(14M)	119.7
C(149)-C(148)-H(14M)	119.7
C(150)-C(149)-C(148)	119.9(2)
C(150)-C(149)-H(14N)	120.0
C(148)-C(149)-H(14N)	120.0
C(149)-C(150)-C(151)	119.7(2)
C(149)-C(150)-H(15B)	120.2
C(151)-C(150)-H(15B)	120.2
C(146)-C(151)-C(150)	120.7(2)
C(146)-C(151)-H(15C)	119.7
C(150)-C(151)-H(15C)	119.7
C(153)-C(152)-C(157)	119.6(2)
C(153)-C(152)-P(6)	120.22(17)
C(157)-C(152)-P(6)	120.14(15)
C(154)-C(153)-C(152)	119.7(2)

C(154)-C(153)-H(15D)	120.2
C(152)-C(153)-H(15D)	120.2
C(155)-C(154)-C(153)	120.3(2)
C(155)-C(154)-H(15E)	119.9
C(153)-C(154)-H(15E)	119.9
C(154)-C(155)-C(156)	120.8(2)
C(154)-C(155)-H(15F)	119.6
C(156)-C(155)-H(15F)	119.6
C(155)-C(156)-C(157)	119.8(2)
C(155)-C(156)-H(15G)	120.1
C(157)-C(156)-H(15G)	120.1
C(156)-C(157)-C(152)	119.8(2)
C(156)-C(157)-H(15H)	120.1
C(152)-C(157)-H(15H)	120.1
N(6)-C(158)-C(159)	112.44(16)
N(6)-C(158)-C(165)	112.12(15)
C(159)-C(158)-C(165)	113.06(16)
N(6)-C(158)-H(15I)	106.2
C(159)-C(158)-H(15I)	106.2
C(165)-C(158)-H(15I)	106.2
C(164)-C(159)-C(160)	118.8(2)
C(164)-C(159)-C(158)	119.19(19)
C(160)-C(159)-C(158)	121.96(18)
C(159)-C(160)-C(161)	119.9(2)
C(159)-C(160)-H(16B)	120.0
C(161)-C(160)-H(16B)	120.0
C(162)-C(161)-C(160)	120.4(2)
C(162)-C(161)-H(16C)	119.8
C(160)-C(161)-H(16C)	119.8
C(163)-C(162)-C(161)	119.8(2)
C(163)-C(162)-H(16D)	120.1
C(161)-C(162)-H(16D)	120.1
C(162)-C(163)-C(164)	120.3(2)
C(162)-C(163)-H(16E)	119.8
C(164)-C(163)-H(16E)	119.8
C(163)-C(164)-C(159)	120.8(2)

C(163)-C(164)-H(16F)	119.6
C(159)-C(164)-H(16F)	119.6
C(167)-C(165)-C(166)	111.10(18)
C(167)-C(165)-C(158)	106.57(17)
C(166)-C(165)-C(158)	109.55(16)
C(167)-C(165)-C(169)	109.89(17)
C(166)-C(165)-C(169)	109.43(17)
C(158)-C(165)-C(169)	110.27(17)
C(165)-C(166)-H(16G)	109.5
C(165)-C(166)-H(16H)	109.5
H(16G)-C(166)-H(16H)	109.5
C(165)-C(166)-H(16I)	109.5
H(16G)-C(166)-H(16I)	109.5
H(16H)-C(166)-H(16I)	109.5
C(168)-C(167)-C(165)	128.0(2)
C(168)-C(167)-H(16J)	116.0
C(165)-C(167)-H(16J)	116.0
C(167)-C(168)-H(16K)	120.0
C(167)-C(168)-H(16L)	120.0
H(16K)-C(168)-H(16L)	120.0
C(174)-C(169)-C(170)	109.05(19)
C(174)-C(169)-C(165)	114.35(19)
C(170)-C(169)-C(165)	112.72(19)
C(174)-C(169)-H(16N)	106.7
C(170)-C(169)-H(16N)	106.7
C(165)-C(169)-H(16N)	106.7
C(169)-C(170)-C(171)	112.6(2)
C(169)-C(170)-H(17B)	109.1
C(171)-C(170)-H(17B)	109.1
C(169)-C(170)-H(17C)	109.1
C(171)-C(170)-H(17C)	109.1
H(17B)-C(170)-H(17C)	107.8
C(172)-C(171)-C(170)	110.7(3)
C(172)-C(171)-H(17D)	109.5
C(170)-C(171)-H(17D)	109.5
C(172)-C(171)-H(17E)	109.5

C(170)-C(171)-H(17E)	109.5
H(17D)-C(171)-H(17E)	108.1
C(173)-C(172)-C(171)	109.8(2)
C(173)-C(172)-H(17F)	109.7
C(171)-C(172)-H(17F)	109.7
C(173)-C(172)-H(17G)	109.7
C(171)-C(172)-H(17G)	109.7
H(17F)-C(172)-H(17G)	108.2
C(174)-C(173)-C(172)	111.6(2)
C(174)-C(173)-H(17H)	109.3
C(172)-C(173)-H(17H)	109.3
C(174)-C(173)-H(17I)	109.3
C(172)-C(173)-H(17I)	109.3
H(17H)-C(173)-H(17I)	108.0
C(173)-C(174)-C(169)	111.9(2)
C(173)-C(174)-H(17J)	109.2
C(169)-C(174)-H(17J)	109.2
C(173)-C(174)-H(17K)	109.2
C(169)-C(174)-H(17K)	109.2
H(17J)-C(174)-H(17K)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{29}H_{34}NOP$ (13). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	23(1)	14(1)	19(1)	-1(1)	12(1)	-1(1)
O(1)	30(1)	14(1)	24(1)	0(1)	15(1)	1(1)
N(1)	31(1)	13(1)	22(1)	0(1)	17(1)	1(1)
C(1)	22(1)	22(1)	22(1)	-2(1)	12(1)	-5(1)
C(2)	26(1)	21(1)	30(1)	6(1)	10(1)	-1(1)

C(3)	24(1)	32(1)	43(1)	13(1)	13(1)	-4(1)
C(4)	22(1)	40(1)	41(1)	3(1)	18(1)	-1(1)
C(5)	28(1)	27(1)	42(1)	-6(1)	19(1)	-2(1)
C(6)	28(1)	19(1)	35(1)	-4(1)	17(1)	-5(1)
C(7)	26(1)	13(1)	21(1)	1(1)	12(1)	-2(1)
C(8)	26(1)	29(1)	26(1)	-2(1)	16(1)	-5(1)
C(9)	37(1)	33(1)	26(1)	-4(1)	19(1)	-5(1)
C(10)	33(1)	32(1)	21(1)	0(1)	8(1)	-3(1)
C(11)	24(1)	32(1)	31(1)	3(1)	13(1)	0(1)
C(12)	28(1)	26(1)	25(1)	0(1)	17(1)	-2(1)
C(13)	29(1)	16(1)	21(1)	-3(1)	14(1)	-2(1)
C(14)	27(1)	23(1)	18(1)	3(1)	13(1)	-2(1)
C(15)	36(1)	23(1)	33(1)	-2(1)	20(1)	-4(1)
C(16)	32(1)	31(1)	40(1)	2(1)	17(1)	-9(1)
C(17)	29(1)	42(1)	41(1)	8(1)	22(1)	-3(1)
C(18)	38(1)	37(1)	33(1)	6(1)	24(1)	7(1)
C(19)	34(1)	27(1)	24(1)	-2(1)	20(1)	-2(1)
C(20)	31(1)	18(1)	19(1)	0(1)	11(1)	2(1)
C(21)	40(1)	20(1)	25(1)	1(1)	16(1)	1(1)
C(22)	40(1)	21(1)	22(1)	-1(1)	13(1)	3(1)
C(23)	68(2)	34(1)	29(1)	1(1)	27(1)	9(1)
C(24)	29(1)	25(1)	29(1)	-2(1)	10(1)	1(1)
C(25)	37(1)	36(1)	39(1)	5(1)	4(1)	3(1)
C(26)	32(1)	47(2)	58(2)	-1(1)	2(1)	4(1)
C(27)	30(1)	46(2)	53(2)	-8(1)	7(1)	-3(1)
C(28)	29(1)	37(1)	52(2)	-10(1)	18(1)	-6(1)
C(29)	28(1)	23(1)	36(1)	-5(1)	13(1)	-3(1)
P(2)	27(1)	16(1)	23(1)	-3(1)	17(1)	-4(1)
O(2)	42(1)	16(1)	31(1)	-3(1)	24(1)	-4(1)
N(2)	31(1)	17(1)	23(1)	-1(1)	18(1)	-6(1)
C(30)	26(1)	31(1)	25(1)	-6(1)	16(1)	-5(1)
C(31)	31(1)	35(1)	30(1)	-5(1)	19(1)	-1(1)
C(32)	32(1)	54(2)	44(1)	-13(1)	20(1)	7(1)
C(33)	25(1)	85(2)	76(2)	-35(2)	19(1)	-1(1)
C(34)	29(1)	74(2)	111(3)	-52(2)	29(2)	-19(1)
C(35)	38(1)	42(2)	68(2)	-28(1)	28(1)	-13(1)

C(36)	25(1)	19(1)	22(1)	-5(1)	16(1)	-6(1)
C(37)	34(1)	30(1)	29(1)	5(1)	20(1)	4(1)
C(38)	52(1)	29(1)	33(1)	4(1)	29(1)	0(1)
C(39)	47(1)	32(1)	35(1)	-10(1)	32(1)	-15(1)
C(40)	26(1)	30(1)	31(1)	-7(1)	17(1)	-5(1)
C(41)	29(1)	22(1)	30(1)	-4(1)	18(1)	-3(1)
C(42)	30(1)	15(1)	23(1)	0(1)	18(1)	-1(1)
C(43)	29(1)	25(1)	20(1)	-4(1)	15(1)	-5(1)
C(44)	40(1)	31(1)	29(1)	-4(1)	21(1)	-11(1)
C(45)	47(1)	53(2)	36(1)	-14(1)	30(1)	-25(1)
C(46)	30(1)	68(2)	37(1)	-22(1)	22(1)	-13(1)
C(47)	31(1)	51(2)	25(1)	-10(1)	12(1)	4(1)
C(48)	30(1)	29(1)	22(1)	-2(1)	13(1)	-1(1)
C(49)	28(1)	14(1)	25(1)	2(1)	16(1)	0(1)
C(50)	30(1)	21(1)	22(1)	-2(1)	14(1)	-2(1)
C(51)	34(1)	20(1)	28(1)	2(1)	16(1)	-2(1)
C(52)	53(1)	31(1)	29(1)	7(1)	19(1)	-6(1)
C(53)	28(1)	19(1)	31(1)	1(1)	17(1)	1(1)
C(54)	34(1)	33(1)	37(1)	-8(1)	18(1)	-3(1)
C(55)	29(1)	45(1)	55(2)	-12(1)	22(1)	-5(1)
C(56)	32(1)	43(1)	52(2)	-6(1)	22(1)	3(1)
C(57)	36(1)	32(1)	43(1)	-3(1)	25(1)	6(1)
C(58)	32(1)	21(1)	32(1)	-1(1)	19(1)	2(1)
P(3)	19(1)	14(1)	21(1)	0(1)	9(1)	-1(1)
O(3)	25(1)	18(1)	25(1)	0(1)	11(1)	0(1)
N(3)	21(1)	12(1)	21(1)	-2(1)	8(1)	-4(1)
C(59)	22(1)	15(1)	21(1)	-1(1)	8(1)	0(1)
C(60)	26(1)	27(1)	29(1)	4(1)	14(1)	2(1)
C(61)	24(1)	34(1)	36(1)	5(1)	11(1)	-1(1)
C(62)	25(1)	27(1)	29(1)	-2(1)	4(1)	-1(1)
C(63)	35(1)	46(1)	22(1)	4(1)	10(1)	-3(1)
C(64)	26(1)	36(1)	25(1)	2(1)	12(1)	-4(1)
C(65)	20(1)	18(1)	26(1)	0(1)	11(1)	1(1)
C(66)	25(1)	21(1)	29(1)	-3(1)	11(1)	-2(1)
C(67)	28(1)	26(1)	40(1)	2(1)	20(1)	-5(1)
C(68)	25(1)	31(1)	44(1)	1(1)	23(1)	4(1)

C(69)	33(1)	20(1)	44(1)	-4(1)	24(1)	1(1)
C(70)	27(1)	18(1)	38(1)	-2(1)	18(1)	-3(1)
C(71)	29(1)	17(1)	24(1)	-2(1)	13(1)	0(1)
C(72)	27(1)	22(1)	26(1)	-1(1)	13(1)	-2(1)
C(73)	27(1)	25(1)	30(1)	-4(1)	13(1)	-1(1)
C(74)	32(1)	29(1)	46(1)	0(1)	23(1)	1(1)
C(75)	24(1)	31(1)	49(1)	6(1)	17(1)	0(1)
C(76)	30(1)	32(1)	41(1)	-8(1)	11(1)	-9(1)
C(77)	29(1)	24(1)	42(1)	-3(1)	16(1)	0(1)
C(78)	30(1)	20(1)	27(1)	-1(1)	16(1)	0(1)
C(79)	26(1)	18(1)	29(1)	6(1)	13(1)	2(1)
C(80)	39(1)	32(1)	28(1)	-3(1)	18(1)	0(1)
C(81)	62(2)	45(2)	25(1)	1(1)	14(1)	3(1)
C(82)	28(1)	22(1)	33(1)	0(1)	19(1)	0(1)
C(83)	40(1)	28(1)	44(1)	5(1)	28(1)	-1(1)
C(84)	42(1)	28(1)	66(2)	3(1)	37(1)	-3(1)
C(85)	43(1)	32(1)	69(2)	4(1)	43(1)	4(1)
C(86)	34(1)	27(1)	63(2)	4(1)	32(1)	3(1)
C(87)	37(1)	21(1)	52(1)	1(1)	30(1)	0(1)
P(4)	17(1)	15(1)	25(1)	1(1)	9(1)	1(1)
O(4)	25(1)	16(1)	32(1)	3(1)	14(1)	3(1)
N(4)	18(1)	15(1)	30(1)	-1(1)	12(1)	-1(1)
C(88)	25(1)	17(1)	29(1)	3(1)	14(1)	2(1)
C(89)	25(1)	25(1)	32(1)	1(1)	13(1)	1(1)
C(90)	41(1)	26(1)	31(1)	-2(1)	15(1)	1(1)
C(91)	50(1)	32(1)	38(1)	0(1)	29(1)	1(1)
C(92)	38(1)	32(1)	46(1)	-1(1)	29(1)	-3(1)
C(93)	28(1)	23(1)	36(1)	-1(1)	18(1)	-2(1)
C(94)	18(1)	19(1)	27(1)	2(1)	13(1)	-4(1)
C(95)	23(1)	24(1)	33(1)	3(1)	10(1)	1(1)
C(96)	23(1)	36(1)	40(1)	13(1)	12(1)	4(1)
C(97)	24(1)	49(2)	33(1)	5(1)	6(1)	-4(1)
C(98)	35(1)	37(1)	39(1)	-11(1)	10(1)	-12(1)
C(99)	24(1)	25(1)	36(1)	-1(1)	12(1)	-3(1)
C(100)	16(1)	17(1)	29(1)	-2(1)	9(1)	2(1)
C(101)	16(1)	30(1)	30(1)	-2(1)	8(1)	-1(1)

C(102)	21(1)	36(1)	30(1)	1(1)	9(1)	7(1)
C(103)	30(1)	59(2)	32(1)	0(1)	7(1)	17(1)
C(104)	38(1)	76(2)	28(1)	-13(1)	-1(1)	12(1)
C(105)	42(1)	64(2)	39(1)	-26(1)	4(1)	9(1)
C(106)	26(1)	42(1)	36(1)	-12(1)	4(1)	3(1)
C(107)	16(1)	19(1)	26(1)	1(1)	8(1)	-1(1)
C(108)	23(1)	22(1)	33(1)	4(1)	10(1)	-2(1)
C(109)	17(1)	26(1)	28(1)	1(1)	8(1)	2(1)
C(110)	39(1)	49(2)	42(1)	10(1)	25(1)	13(1)
C(111)	16(1)	17(1)	27(1)	0(1)	10(1)	0(1)
C(112)	19(1)	23(1)	27(1)	3(1)	10(1)	-2(1)
C(113)	21(1)	32(1)	30(1)	-4(1)	11(1)	-5(1)
C(114)	23(1)	36(1)	24(1)	3(1)	8(1)	1(1)
C(115)	24(1)	32(1)	28(1)	8(1)	13(1)	2(1)
C(116)	19(1)	23(1)	28(1)	3(1)	9(1)	1(1)
P(5)	24(1)	13(1)	19(1)	2(1)	10(1)	1(1)
O(5)	28(1)	14(1)	24(1)	2(1)	11(1)	1(1)
N(5)	32(1)	10(1)	21(1)	1(1)	16(1)	0(1)
C(117)	25(1)	24(1)	17(1)	2(1)	10(1)	6(1)
C(118)	35(1)	23(1)	26(1)	-1(1)	10(1)	6(1)
C(119)	33(1)	41(1)	24(1)	-8(1)	10(1)	4(1)
C(120)	29(1)	50(2)	20(1)	4(1)	8(1)	2(1)
C(121)	29(1)	35(1)	31(1)	15(1)	11(1)	3(1)
C(122)	26(1)	21(1)	29(1)	4(1)	13(1)	2(1)
C(123)	26(1)	17(1)	31(1)	4(1)	14(1)	2(1)
C(124)	33(1)	50(2)	33(1)	13(1)	19(1)	9(1)
C(125)	41(1)	67(2)	63(2)	19(2)	37(1)	13(1)
C(126)	30(1)	44(2)	71(2)	12(1)	24(1)	4(1)
C(127)	32(1)	36(1)	54(2)	-8(1)	10(1)	-5(1)
C(128)	33(1)	31(1)	36(1)	-8(1)	15(1)	-3(1)
C(129)	27(1)	18(1)	21(1)	0(1)	12(1)	-2(1)
C(130)	26(1)	20(1)	21(1)	0(1)	12(1)	1(1)
C(131)	33(1)	21(1)	24(1)	-1(1)	13(1)	-2(1)
C(132)	32(1)	29(1)	26(1)	-9(1)	8(1)	-2(1)
C(133)	27(1)	48(1)	20(1)	-3(1)	8(1)	6(1)
C(134)	38(1)	53(2)	24(1)	13(1)	15(1)	4(1)

C(135)	31(1)	32(1)	28(1)	7(1)	14(1)	-4(1)
C(136)	24(1)	26(1)	24(1)	-1(1)	12(1)	-2(1)
C(137)	33(1)	27(1)	34(1)	-8(1)	15(1)	4(1)
C(138)	28(1)	48(1)	29(1)	-1(1)	14(1)	-8(1)
C(139)	46(2)	86(2)	45(2)	-4(2)	31(1)	-6(1)
C(140)	25(1)	26(1)	24(1)	0(1)	9(1)	-1(1)
C(141)	27(1)	43(1)	40(1)	-8(1)	5(1)	7(1)
C(142)	40(1)	48(2)	44(2)	-3(1)	0(1)	14(1)
C(143)	35(1)	46(2)	34(1)	-3(1)	0(1)	-1(1)
C(144)	36(1)	31(1)	30(1)	-4(1)	8(1)	-7(1)
C(145)	28(1)	24(1)	26(1)	-1(1)	11(1)	-4(1)
P(6)	30(1)	15(1)	18(1)	1(1)	11(1)	3(1)
O(6)	41(1)	16(1)	29(1)	1(1)	17(1)	4(1)
N(6)	31(1)	15(1)	20(1)	4(1)	13(1)	5(1)
C(146)	33(1)	16(1)	20(1)	1(1)	14(1)	7(1)
C(147)	35(1)	22(1)	26(1)	-3(1)	14(1)	-5(1)
C(148)	40(1)	26(1)	21(1)	-3(1)	10(1)	0(1)
C(149)	50(1)	34(1)	26(1)	2(1)	21(1)	0(1)
C(150)	45(1)	51(2)	36(1)	4(1)	23(1)	-10(1)
C(151)	32(1)	46(2)	29(1)	2(1)	14(1)	-2(1)
C(152)	29(1)	25(1)	20(1)	0(1)	9(1)	5(1)
C(153)	42(1)	26(1)	28(1)	1(1)	9(1)	12(1)
C(154)	43(1)	43(2)	41(1)	-2(1)	0(1)	22(1)
C(155)	31(1)	55(2)	54(2)	-15(1)	-3(1)	6(1)
C(156)	37(1)	31(1)	46(1)	-6(1)	6(1)	-1(1)
C(157)	31(1)	22(1)	31(1)	3(1)	8(1)	5(1)
C(158)	38(1)	13(1)	24(1)	2(1)	18(1)	-2(1)
C(159)	35(1)	24(1)	22(1)	6(1)	16(1)	8(1)
C(160)	32(1)	31(1)	23(1)	2(1)	15(1)	3(1)
C(161)	32(1)	51(2)	26(1)	-10(1)	13(1)	-1(1)
C(162)	42(1)	75(2)	17(1)	8(1)	12(1)	26(1)
C(163)	60(2)	45(2)	33(1)	18(1)	30(1)	26(1)
C(164)	56(1)	28(1)	32(1)	10(1)	30(1)	13(1)
C(165)	34(1)	22(1)	25(1)	-2(1)	16(1)	-7(1)
C(166)	27(1)	28(1)	25(1)	-2(1)	12(1)	0(1)
C(167)	43(1)	32(1)	38(1)	-2(1)	22(1)	-11(1)

C(168)	69(2)	52(2)	57(2)	-5(1)	43(2)	-22(1)
C(169)	36(1)	30(1)	25(1)	-2(1)	12(1)	-9(1)
C(170)	36(1)	56(2)	41(1)	-12(1)	11(1)	-12(1)
C(171)	37(1)	83(2)	38(2)	-11(2)	5(1)	-12(1)
C(172)	56(2)	82(2)	35(1)	-17(2)	12(1)	-29(2)
C(173)	64(2)	52(2)	33(1)	-12(1)	22(1)	-22(1)
C(174)	55(2)	36(1)	33(1)	-12(1)	22(1)	-18(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{29}H_{34}NOP$ (13)

	x	y	z	U(eq)
H(1N)	55	1812	508	25
H(2A)	915	3656	-62	32
H(3A)	1925	3591	-105	41
H(4A)	2410	2593	-70	40
H(5A)	1903	1644	32	38
H(6A)	897	1701	89	32
H(8A)	-41	2485	-1245	31
H(9A)	-927	2321	-2324	36
H(10A)	-2036	2248	-2519	37
H(11A)	-2266	2323	-1635	35
H(12A)	-1390	2491	-561	29
H(13A)	90	2916	1208	25
H(15A)	-985	1514	563	35
H(16A)	-2109	1489	330	42
H(17A)	-2560	2339	656	42
H(18A)	-1878	3226	1213	40
H(19A)	-754	3263	1436	31
H(21A)	-113	1369	1796	42
H(21B)	674	1203	2250	42
H(21C)	335	1172	1458	42
H(22A)	587	2945	2385	34

H(23A)	320	1814	2873	51
H(23B)	409	2547	3185	51
H(24A)	1212	1909	1490	35
H(25A)	1831	2106	2899	52
H(25B)	1684	1411	2547	52
H(26A)	2836	1711	2963	65
H(26B)	2467	1613	2174	65
H(27A)	3114	2558	2437	59
H(27B)	2755	2837	2838	59
H(28A)	2093	2634	1426	48
H(28B)	2252	3327	1781	48
H(29A)	1091	3050	1378	36
H(29B)	1470	3128	2170	36
H(2N)	9921	9442	9713	26
H(31A)	11246	8955	10768	36
H(32A)	12379	8675	11386	51
H(33A)	13180	9464	12000	77
H(34A)	12856	10532	11947	88
H(35A)	11716	10829	11327	58
H(37A)	10775	9134	11551	35
H(38A)	10129	8693	11995	42
H(39A)	9030	9054	11633	39
H(40A)	8576	9875	10846	33
H(41A)	9214	10317	10395	30
H(42A)	10057	10646	9300	25
H(44A)	10795	11039	8922	38
H(45A)	11844	10984	8964	50
H(46A)	12487	10040	9325	52
H(47A)	12054	9135	9602	43
H(48A)	10988	9181	9530	32
H(50A)	9966	9297	8297	36
H(50B)	9162	9193	7930	36
H(50C)	9614	9003	8697	36
H(51A)	9381	10927	8145	32
H(52A)	9387	9934	7330	45
H(52B)	9325	10715	7170	45

H(53A)	8865	9669	8950	30
H(54A)	8114	10217	7647	41
H(54B)	8214	9457	7801	41
H(55A)	7135	9800	7631	51
H(55B)	7580	9512	8364	51
H(56A)	7072	10477	8440	51
H(56B)	7378	10864	8042	51
H(57A)	8061	11075	9188	42
H(57B)	8167	10316	9346	42
H(58A)	9141	10741	9357	32
H(58B)	8692	11021	8621	32
H(3N)	5035	2062	9622	23
H(60A)	6176	1480	10266	32
H(61A)	7236	1464	11227	39
H(62A)	7326	1178	12243	37
H(63A)	6363	900	12305	43
H(64A)	5305	908	11358	35
H(66A)	3822	411	10127	31
H(67A)	3117	608	10586	36
H(68A)	3122	1621	11037	37
H(69A)	3800	2453	10984	36
H(70A)	4497	2262	10522	32
H(71A)	4510	1161	8650	28
H(73A)	3610	2300	9110	34
H(74A)	2448	2292	8715	41
H(75A)	1747	1566	7874	42
H(76A)	2242	833	7469	44
H(77A)	3414	833	7882	38
H(79A)	3788	2728	8133	36
H(79B)	4393	3054	8063	36
H(79C)	4477	2924	8784	36
H(80A)	4406	1387	7615	39
H(81A)	3743	2536	7073	57
H(81B)	3739	1874	6675	57
H(82A)	5539	2333	9110	31
H(83A)	5437	2429	7823	41

H(83B)	5386	3032	8235	41
H(84A)	6513	2884	9063	49
H(84B)	6491	2950	8361	49
H(85A)	6608	1827	8307	50
H(85B)	7213	2085	8999	50
H(86A)	6641	1741	9565	46
H(86B)	6704	1139	9160	46
H(87A)	5574	1296	8307	40
H(87B)	5585	1200	9002	40
H(4N)	5189	9544	9926	25
H(89A)	5427	9325	11016	33
H(90A)	5292	9730	11892	41
H(91A)	4242	9676	11845	44
H(92A)	3310	9231	10916	42
H(93A)	3441	8824	10047	34
H(95A)	3606	9665	9074	33
H(96A)	2566	9701	8107	41
H(97A)	2095	8761	7495	47
H(98A)	2666	7775	7863	49
H(99A)	3703	7729	8834	35
H(10B)	5557	8468	9477	25
H(10C)	4567	9857	8602	36
H(10D)	3914	9936	7450	53
H(10E)	3916	9098	6776	66
H(10F)	4601	8197	7250	66
H(10G)	5255	8110	8405	47
H(10H)	6463	10200	9506	41
H(10I)	5759	10217	9514	41
H(10J)	5781	9972	8866	41
H(10K)	6700	8495	9573	29
H(11B)	6542	9444	8667	49
H(11C)	6939	8748	8788	49
H(11E)	6274	9607	10536	24
H(11F)	7518	9372	10518	29
H(11G)	7188	10072	10458	29
H(11H)	8069	9885	11567	34

H(11I)	7358	9989	11553	34
H(11J)	7973	8751	11632	35
H(11K)	7916	9088	12230	35
H(11L)	6724	9004	11634	33
H(11M)	7047	8300	11698	33
H(11N)	6871	8368	10599	29
H(11O)	6164	8479	10589	29
H(5N)	9630	2781	5191	24
H(11P)	9295	940	3837	37
H(11Q)	8703	1036	2684	41
H(12B)	8444	2050	2185	42
H(12C)	8778	2979	2842	40
H(12D)	9367	2897	3996	30
H(12E)	10660	1904	4249	45
H(12F)	11801	2070	4597	63
H(12G)	12554	2298	5710	59
H(12H)	12168	2332	6480	54
H(12I)	11025	2187	6137	42
H(12J)	9235	1713	5647	26
H(13B)	10198	3172	6317	32
H(13C)	10949	3335	7443	38
H(13D)	11018	2590	8230	40
H(13E)	10368	1648	7885	46
H(13F)	9617	1479	6760	37
H(13G)	8976	3288	6129	48
H(13H)	8242	3428	5512	48
H(13I)	8897	3451	5416	48
H(13J)	8262	1689	5778	41
H(13K)	8058	2849	6267	66
H(13L)	7859	2118	6399	66
H(14A)	8366	2669	4485	32
H(14B)	7194	2514	4647	50
H(14C)	7488	3198	4581	50
H(14D)	7235	2954	3489	63
H(14E)	6561	2885	3550	63
H(14F)	6666	1748	3606	55

H(14G)	6684	1992	2953	55
H(14H)	7876	1918	3503	43
H(14I)	7576	1233	3561	43
H(14J)	8494	1530	4608	32
H(14K)	7811	1483	4656	32
H(6N)	9460	10116	4844	26
H(14L)	9180	9395	3630	34
H(14M)	9023	9733	2603	37
H(14N)	9881	10278	2520	43
H(15B)	10900	10507	3476	51
H(15C)	11077	10140	4510	43
H(15D)	11481	8737	5822	43
H(15E)	12574	9069	6595	62
H(15F)	12825	10157	6797	68
H(15G)	11989	10936	6253	53
H(15H)	10887	10618	5492	37
H(15I)	9400	8945	5366	29
H(16B)	10197	10428	6187	34
H(16C)	10965	10506	7324	44
H(16D)	11161	9617	8017	55
H(16E)	10582	8656	7581	51
H(16F)	9819	8571	6454	42
H(16G)	8969	10304	6023	40
H(16H)	8213	10411	5431	40
H(16I)	8845	10599	5331	40
H(16J)	8431	8681	5483	44
H(16K)	8249	9648	6211	65
H(16L)	8112	8868	6230	65
H(16N)	8367	9936	4322	39
H(17B)	7445	10181	4489	57
H(17C)	7288	9427	4500	57
H(17D)	6532	9843	3441	70
H(17E)	7149	10120	3357	70
H(17F)	6865	8769	3399	74
H(17G)	6777	9146	2753	74
H(17H)	7809	8554	3250	61

H(17I)	7955	9313	3255	61
H(17J)	8701	8865	4297	49
H(17K)	8074	8599	4370	49

Table 6. Torsion angles [°] for $C_{29}H_{34}NOP$ (13)

O(1)-P(1)-N(1)-C(13)	-5.86(17)
C(1)-P(1)-N(1)-C(13)	117.80(15)
C(7)-P(1)-N(1)-C(13)	-127.98(15)
O(1)-P(1)-C(1)-C(2)	-17.79(19)
N(1)-P(1)-C(1)-C(2)	-141.16(16)
C(7)-P(1)-C(1)-C(2)	102.50(17)
O(1)-P(1)-C(1)-C(6)	164.56(15)
N(1)-P(1)-C(1)-C(6)	41.19(18)
C(7)-P(1)-C(1)-C(6)	-75.15(18)
C(6)-C(1)-C(2)-C(3)	-0.4(3)
P(1)-C(1)-C(2)-C(3)	-178.03(16)
C(1)-C(2)-C(3)-C(4)	0.7(3)
C(2)-C(3)-C(4)-C(5)	-0.7(3)
C(3)-C(4)-C(5)-C(6)	0.3(3)
C(4)-C(5)-C(6)-C(1)	0.1(3)
C(2)-C(1)-C(6)-C(5)	0.0(3)
P(1)-C(1)-C(6)-C(5)	177.62(16)
O(1)-P(1)-C(7)-C(8)	107.14(17)
N(1)-P(1)-C(7)-C(8)	-130.38(17)
C(1)-P(1)-C(7)-C(8)	-13.84(19)
O(1)-P(1)-C(7)-C(12)	-63.94(17)
N(1)-P(1)-C(7)-C(12)	58.54(17)
C(1)-P(1)-C(7)-C(12)	175.08(15)
C(12)-C(7)-C(8)-C(9)	0.2(3)
P(1)-C(7)-C(8)-C(9)	-170.88(16)
C(7)-C(8)-C(9)-C(10)	0.1(3)
C(8)-C(9)-C(10)-C(11)	-0.5(3)
C(9)-C(10)-C(11)-C(12)	0.7(3)

C(10)-C(11)-C(12)-C(7)	-0.4(3)
C(8)-C(7)-C(12)-C(11)	0.0(3)
P(1)-C(7)-C(12)-C(11)	171.42(16)
P(1)-N(1)-C(13)-C(14)	97.76(17)
P(1)-N(1)-C(13)-C(20)	-132.96(15)
N(1)-C(13)-C(14)-C(15)	41.2(2)
C(20)-C(13)-C(14)-C(15)	-87.6(2)
N(1)-C(13)-C(14)-C(19)	-135.59(18)
C(20)-C(13)-C(14)-C(19)	95.6(2)
C(19)-C(14)-C(15)-C(16)	0.0(3)
C(13)-C(14)-C(15)-C(16)	-176.83(19)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
C(15)-C(16)-C(17)-C(18)	0.3(3)
C(16)-C(17)-C(18)-C(19)	0.2(3)
C(17)-C(18)-C(19)-C(14)	-0.6(3)
C(15)-C(14)-C(19)-C(18)	0.5(3)
C(13)-C(14)-C(19)-C(18)	177.42(18)
N(1)-C(13)-C(20)-C(22)	167.21(16)
C(14)-C(13)-C(20)-C(22)	-65.4(2)
N(1)-C(13)-C(20)-C(21)	-71.3(2)
C(14)-C(13)-C(20)-C(21)	56.0(2)
N(1)-C(13)-C(20)-C(24)	49.1(2)
C(14)-C(13)-C(20)-C(24)	176.52(15)
C(21)-C(20)-C(22)-C(23)	3.6(3)
C(13)-C(20)-C(22)-C(23)	124.4(3)
C(24)-C(20)-C(22)-C(23)	-118.4(3)
C(22)-C(20)-C(24)-C(29)	-61.6(2)
C(21)-C(20)-C(24)-C(29)	175.20(17)
C(13)-C(20)-C(24)-C(29)	54.1(2)
C(22)-C(20)-C(24)-C(25)	62.9(2)
C(21)-C(20)-C(24)-C(25)	-60.3(2)
C(13)-C(20)-C(24)-C(25)	178.63(18)
C(29)-C(24)-C(25)-C(26)	-55.4(3)
C(20)-C(24)-C(25)-C(26)	176.9(2)
C(24)-C(25)-C(26)-C(27)	56.4(3)
C(25)-C(26)-C(27)-C(28)	-55.3(3)

C(26)-C(27)-C(28)-C(29)	55.5(3)
C(27)-C(28)-C(29)-C(24)	-57.7(3)
C(25)-C(24)-C(29)-C(28)	56.5(2)
C(20)-C(24)-C(29)-C(28)	-176.81(18)
O(2)-P(2)-N(2)-C(42)	33.75(17)
C(30)-P(2)-N(2)-C(42)	-90.82(16)
C(36)-P(2)-N(2)-C(42)	155.16(14)
O(2)-P(2)-C(30)-C(31)	-170.72(16)
N(2)-P(2)-C(30)-C(31)	-46.1(2)
C(36)-P(2)-C(30)-C(31)	65.80(19)
O(2)-P(2)-C(30)-C(35)	10.1(2)
N(2)-P(2)-C(30)-C(35)	134.69(19)
C(36)-P(2)-C(30)-C(35)	-113.4(2)
C(35)-C(30)-C(31)-C(32)	0.6(3)
P(2)-C(30)-C(31)-C(32)	-178.56(18)
C(30)-C(31)-C(32)-C(33)	0.6(4)
C(31)-C(32)-C(33)-C(34)	-1.8(5)
C(32)-C(33)-C(34)-C(35)	1.8(6)
C(33)-C(34)-C(35)-C(30)	-0.6(5)
C(31)-C(30)-C(35)-C(34)	-0.6(4)
P(2)-C(30)-C(35)-C(34)	178.6(2)
O(2)-P(2)-C(36)-C(37)	-134.23(18)
N(2)-P(2)-C(36)-C(37)	105.46(19)
C(30)-P(2)-C(36)-C(37)	-11.8(2)
O(2)-P(2)-C(36)-C(41)	45.76(17)
N(2)-P(2)-C(36)-C(41)	-74.55(16)
C(30)-P(2)-C(36)-C(41)	168.22(15)
C(41)-C(36)-C(37)-C(38)	0.9(3)
P(2)-C(36)-C(37)-C(38)	-179.15(17)
C(36)-C(37)-C(38)-C(39)	-0.1(3)
C(37)-C(38)-C(39)-C(40)	-0.8(3)
C(38)-C(39)-C(40)-C(41)	0.9(3)
C(39)-C(40)-C(41)-C(36)	-0.2(3)
C(37)-C(36)-C(41)-C(40)	-0.7(3)
P(2)-C(36)-C(41)-C(40)	179.30(15)
P(2)-N(2)-C(42)-C(43)	79.29(18)

P(2)-N(2)-C(42)-C(49)	-151.37(13)
N(2)-C(42)-C(43)-C(48)	35.6(2)
C(49)-C(42)-C(43)-C(48)	-91.7(2)
N(2)-C(42)-C(43)-C(44)	-140.93(18)
C(49)-C(42)-C(43)-C(44)	91.8(2)
C(48)-C(43)-C(44)-C(45)	0.0(3)
C(42)-C(43)-C(44)-C(45)	176.59(19)
C(43)-C(44)-C(45)-C(46)	-1.1(3)
C(44)-C(45)-C(46)-C(47)	1.3(3)
C(45)-C(46)-C(47)-C(48)	-0.4(3)
C(44)-C(43)-C(48)-C(47)	1.0(3)
C(42)-C(43)-C(48)-C(47)	-175.56(18)
C(46)-C(47)-C(48)-C(43)	-0.8(3)
N(2)-C(42)-C(49)-C(51)	165.82(16)
C(43)-C(42)-C(49)-C(51)	-66.4(2)
N(2)-C(42)-C(49)-C(50)	-72.92(19)
C(43)-C(42)-C(49)-C(50)	54.9(2)
N(2)-C(42)-C(49)-C(53)	47.5(2)
C(43)-C(42)-C(49)-C(53)	175.28(16)
C(50)-C(49)-C(51)-C(52)	5.0(3)
C(42)-C(49)-C(51)-C(52)	124.9(2)
C(53)-C(49)-C(51)-C(52)	-116.2(2)
C(51)-C(49)-C(53)-C(54)	59.0(2)
C(50)-C(49)-C(53)-C(54)	-63.2(2)
C(42)-C(49)-C(53)-C(54)	176.68(17)
C(51)-C(49)-C(53)-C(58)	-65.4(2)
C(50)-C(49)-C(53)-C(58)	172.33(17)
C(42)-C(49)-C(53)-C(58)	52.2(2)
C(58)-C(53)-C(54)-C(55)	-55.8(2)
C(49)-C(53)-C(54)-C(55)	177.10(19)
C(53)-C(54)-C(55)-C(56)	56.8(3)
C(54)-C(55)-C(56)-C(57)	-55.6(3)
C(55)-C(56)-C(57)-C(58)	55.9(3)
C(56)-C(57)-C(58)-C(53)	-57.2(2)
C(54)-C(53)-C(58)-C(57)	56.0(2)
C(49)-C(53)-C(58)-C(57)	-177.83(17)

O(3)-P(3)-N(3)-C(71)	27.24(16)
C(59)-P(3)-N(3)-C(71)	150.96(14)
C(65)-P(3)-N(3)-C(71)	-97.50(15)
O(3)-P(3)-C(59)-C(60)	86.49(18)
N(3)-P(3)-C(59)-C(60)	-36.06(18)
C(65)-P(3)-C(59)-C(60)	-153.49(16)
O(3)-P(3)-C(59)-C(64)	-86.94(17)
N(3)-P(3)-C(59)-C(64)	150.50(16)
C(65)-P(3)-C(59)-C(64)	33.08(18)
C(64)-C(59)-C(60)-C(61)	-0.8(3)
P(3)-C(59)-C(60)-C(61)	-174.27(17)
C(59)-C(60)-C(61)-C(62)	0.2(3)
C(60)-C(61)-C(62)-C(63)	0.3(3)
C(61)-C(62)-C(63)-C(64)	-0.2(4)
C(62)-C(63)-C(64)-C(59)	-0.4(4)
C(60)-C(59)-C(64)-C(63)	0.9(3)
P(3)-C(59)-C(64)-C(63)	174.52(18)
O(3)-P(3)-C(65)-C(66)	10.76(19)
N(3)-P(3)-C(65)-C(66)	135.73(16)
C(59)-P(3)-C(65)-C(66)	-110.82(17)
O(3)-P(3)-C(65)-C(70)	-174.08(15)
N(3)-P(3)-C(65)-C(70)	-49.11(18)
C(59)-P(3)-C(65)-C(70)	64.35(18)
C(70)-C(65)-C(66)-C(67)	0.0(3)
P(3)-C(65)-C(66)-C(67)	175.28(16)
C(65)-C(66)-C(67)-C(68)	-0.8(3)
C(66)-C(67)-C(68)-C(69)	1.4(3)
C(67)-C(68)-C(69)-C(70)	-1.2(3)
C(68)-C(69)-C(70)-C(65)	0.4(3)
C(66)-C(65)-C(70)-C(69)	0.2(3)
P(3)-C(65)-C(70)-C(69)	-175.01(17)
P(3)-N(3)-C(71)-C(72)	66.48(19)
P(3)-N(3)-C(71)-C(78)	-165.79(13)
N(3)-C(71)-C(72)-C(77)	-139.0(2)
C(78)-C(71)-C(72)-C(77)	93.5(2)
N(3)-C(71)-C(72)-C(73)	39.8(3)

C(78)-C(71)-C(72)-C(73)	-87.7(2)
C(77)-C(72)-C(73)-C(74)	-3.4(3)
C(71)-C(72)-C(73)-C(74)	177.75(19)
C(72)-C(73)-C(74)-C(75)	0.8(3)
C(73)-C(74)-C(75)-C(76)	1.4(4)
C(74)-C(75)-C(76)-C(77)	-0.8(4)
C(73)-C(72)-C(77)-C(76)	3.9(3)
C(71)-C(72)-C(77)-C(76)	-177.2(2)
C(75)-C(76)-C(77)-C(72)	-1.9(4)
N(3)-C(71)-C(78)-C(80)	163.30(16)
C(72)-C(71)-C(78)-C(80)	-68.8(2)
N(3)-C(71)-C(78)-C(79)	-75.3(2)
C(72)-C(71)-C(78)-C(79)	52.6(2)
N(3)-C(71)-C(78)-C(82)	45.8(2)
C(72)-C(71)-C(78)-C(82)	173.65(16)
C(79)-C(78)-C(80)-C(81)	6.1(3)
C(71)-C(78)-C(80)-C(81)	127.4(3)
C(82)-C(78)-C(80)-C(81)	-114.6(3)
C(80)-C(78)-C(82)-C(87)	-63.3(2)
C(79)-C(78)-C(82)-C(87)	174.91(18)
C(71)-C(78)-C(82)-C(87)	52.7(2)
C(80)-C(78)-C(82)-C(83)	61.9(2)
C(79)-C(78)-C(82)-C(83)	-59.9(2)
C(71)-C(78)-C(82)-C(83)	177.87(17)
C(87)-C(82)-C(83)-C(84)	-56.2(2)
C(78)-C(82)-C(83)-C(84)	175.86(18)
C(82)-C(83)-C(84)-C(85)	56.3(3)
C(83)-C(84)-C(85)-C(86)	-55.3(3)
C(84)-C(85)-C(86)-C(87)	55.8(3)
C(83)-C(82)-C(87)-C(86)	57.6(2)
C(78)-C(82)-C(87)-C(86)	-174.83(19)
C(85)-C(86)-C(87)-C(82)	-58.5(3)
O(4)-P(4)-N(4)-C(100)	42.26(16)
C(94)-P(4)-N(4)-C(100)	-81.41(15)
C(88)-P(4)-N(4)-C(100)	166.05(14)
O(4)-P(4)-C(88)-C(93)	-93.59(18)

N(4)-P(4)-C(88)-C(93)	144.69(17)
C(94)-P(4)-C(88)-C(93)	28.54(19)
O(4)-P(4)-C(88)-C(89)	82.49(18)
N(4)-P(4)-C(88)-C(89)	-39.23(18)
C(94)-P(4)-C(88)-C(89)	-155.38(16)
C(93)-C(88)-C(89)-C(90)	0.7(3)
P(4)-C(88)-C(89)-C(90)	-175.44(16)
C(88)-C(89)-C(90)-C(91)	-0.2(3)
C(89)-C(90)-C(91)-C(92)	-0.5(4)
C(90)-C(91)-C(92)-C(93)	0.6(4)
C(91)-C(92)-C(93)-C(88)	-0.1(3)
C(89)-C(88)-C(93)-C(92)	-0.6(3)
P(4)-C(88)-C(93)-C(92)	175.54(17)
O(4)-P(4)-C(94)-C(95)	-179.96(16)
N(4)-P(4)-C(94)-C(95)	-55.50(18)
C(88)-P(4)-C(94)-C(95)	55.08(18)
O(4)-P(4)-C(94)-C(99)	-2.38(19)
N(4)-P(4)-C(94)-C(99)	122.08(16)
C(88)-P(4)-C(94)-C(99)	-127.34(16)
C(99)-C(94)-C(95)-C(96)	1.0(3)
P(4)-C(94)-C(95)-C(96)	178.64(17)
C(94)-C(95)-C(96)-C(97)	-0.8(3)
C(95)-C(96)-C(97)-C(98)	0.3(4)
C(96)-C(97)-C(98)-C(99)	-0.1(4)
C(97)-C(98)-C(99)-C(94)	0.3(4)
C(95)-C(94)-C(99)-C(98)	-0.8(3)
P(4)-C(94)-C(99)-C(98)	-178.40(18)
P(4)-N(4)-C(100)-C(101)	78.44(18)
P(4)-N(4)-C(100)-C(107)	-154.70(13)
N(4)-C(100)-C(101)-C(102)	41.9(3)
C(107)-C(100)-C(101)-C(102)	-84.3(2)
N(4)-C(100)-C(101)-C(106)	-137.7(2)
C(107)-C(100)-C(101)-C(106)	96.2(2)
C(106)-C(101)-C(102)-C(103)	-2.5(3)
C(100)-C(101)-C(102)-C(103)	178.0(2)
C(101)-C(102)-C(103)-C(104)	1.6(4)

C(102)-C(103)-C(104)-C(105)	-0.8(5)
C(103)-C(104)-C(105)-C(106)	1.0(5)
C(102)-C(101)-C(106)-C(105)	2.6(4)
C(100)-C(101)-C(106)-C(105)	-177.9(2)
C(104)-C(105)-C(106)-C(101)	-1.9(4)
N(4)-C(100)-C(107)-C(109)	163.53(15)
C(101)-C(100)-C(107)-C(109)	-69.60(19)
N(4)-C(100)-C(107)-C(108)	-75.4(2)
C(101)-C(100)-C(107)-C(108)	51.5(2)
N(4)-C(100)-C(107)-C(111)	44.3(2)
C(101)-C(100)-C(107)-C(111)	171.17(15)
C(108)-C(107)-C(109)-C(110)	-10.8(3)
C(111)-C(107)-C(109)-C(110)	-131.9(2)
C(100)-C(107)-C(109)-C(110)	109.3(3)
C(109)-C(107)-C(111)-C(116)	-64.6(2)
C(108)-C(107)-C(111)-C(116)	172.48(16)
C(100)-C(107)-C(111)-C(116)	51.9(2)
C(109)-C(107)-C(111)-C(112)	60.3(2)
C(108)-C(107)-C(111)-C(112)	-62.6(2)
C(100)-C(107)-C(111)-C(112)	176.82(15)
C(116)-C(111)-C(112)-C(113)	-55.4(2)
C(107)-C(111)-C(112)-C(113)	177.01(16)
C(111)-C(112)-C(113)-C(114)	57.2(2)
C(112)-C(113)-C(114)-C(115)	-57.4(2)
C(113)-C(114)-C(115)-C(116)	57.5(2)
C(112)-C(111)-C(116)-C(115)	55.4(2)
C(107)-C(111)-C(116)-C(115)	-178.81(15)
C(114)-C(115)-C(116)-C(111)	-57.5(2)
O(5)-P(5)-N(5)-C(129)	-2.62(17)
C(117)-P(5)-N(5)-C(129)	120.99(15)
C(123)-P(5)-N(5)-C(129)	-125.62(15)
O(5)-P(5)-C(117)-C(122)	164.31(15)
N(5)-P(5)-C(117)-C(122)	39.93(19)
C(123)-P(5)-C(117)-C(122)	-74.52(18)
O(5)-P(5)-C(117)-C(118)	-16.08(19)
N(5)-P(5)-C(117)-C(118)	-140.47(16)

C(123)-P(5)-C(117)-C(118)	105.09(17)
C(122)-C(117)-C(118)-C(119)	0.3(3)
P(5)-C(117)-C(118)-C(119)	-179.32(17)
C(117)-C(118)-C(119)-C(120)	-0.1(3)
C(118)-C(119)-C(120)-C(121)	0.0(3)
C(119)-C(120)-C(121)-C(122)	-0.1(3)
C(120)-C(121)-C(122)-C(117)	0.3(3)
C(118)-C(117)-C(122)-C(121)	-0.4(3)
P(5)-C(117)-C(122)-C(121)	179.19(16)
O(5)-P(5)-C(123)-C(124)	98.62(19)
N(5)-P(5)-C(123)-C(124)	-138.21(18)
C(117)-P(5)-C(123)-C(124)	-21.9(2)
O(5)-P(5)-C(123)-C(128)	-74.83(18)
N(5)-P(5)-C(123)-C(128)	48.35(18)
C(117)-P(5)-C(123)-C(128)	164.69(16)
C(128)-C(123)-C(124)-C(125)	-0.3(4)
P(5)-C(123)-C(124)-C(125)	-173.8(2)
C(123)-C(124)-C(125)-C(126)	0.1(4)
C(124)-C(125)-C(126)-C(127)	0.8(4)
C(125)-C(126)-C(127)-C(128)	-1.5(4)
C(126)-C(127)-C(128)-C(123)	1.2(4)
C(124)-C(123)-C(128)-C(127)	-0.3(3)
P(5)-C(123)-C(128)-C(127)	173.34(19)
P(5)-N(5)-C(129)-C(130)	104.68(17)
P(5)-N(5)-C(129)-C(136)	-127.32(15)
N(5)-C(129)-C(130)-C(135)	-138.55(19)
C(136)-C(129)-C(130)-C(135)	93.4(2)
N(5)-C(129)-C(130)-C(131)	40.9(2)
C(136)-C(129)-C(130)-C(131)	-87.2(2)
C(135)-C(130)-C(131)-C(132)	-1.6(3)
C(129)-C(130)-C(131)-C(132)	178.96(19)
C(130)-C(131)-C(132)-C(133)	0.0(3)
C(131)-C(132)-C(133)-C(134)	1.6(3)
C(132)-C(133)-C(134)-C(135)	-1.5(3)
C(131)-C(130)-C(135)-C(134)	1.7(3)
C(129)-C(130)-C(135)-C(134)	-178.9(2)

C(133)-C(134)-C(135)-C(130)	-0.2(4)
N(5)-C(129)-C(136)-C(138)	164.53(16)
C(130)-C(129)-C(136)-C(138)	-68.3(2)
N(5)-C(129)-C(136)-C(137)	-73.7(2)
C(130)-C(129)-C(136)-C(137)	53.5(2)
N(5)-C(129)-C(136)-C(140)	46.2(2)
C(130)-C(129)-C(136)-C(140)	173.39(16)
C(137)-C(136)-C(138)-C(139)	6.1(3)
C(129)-C(136)-C(138)-C(139)	126.8(3)
C(140)-C(136)-C(138)-C(139)	-114.8(3)
C(138)-C(136)-C(140)-C(145)	-60.4(2)
C(137)-C(136)-C(140)-C(145)	176.98(18)
C(129)-C(136)-C(140)-C(145)	56.3(2)
C(138)-C(136)-C(140)-C(141)	63.8(2)
C(137)-C(136)-C(140)-C(141)	-58.9(2)
C(129)-C(136)-C(140)-C(141)	-179.54(18)
C(145)-C(140)-C(141)-C(142)	-56.5(3)
C(136)-C(140)-C(141)-C(142)	176.3(2)
C(140)-C(141)-C(142)-C(143)	57.0(3)
C(141)-C(142)-C(143)-C(144)	-55.4(3)
C(142)-C(143)-C(144)-C(145)	56.0(3)
C(143)-C(144)-C(145)-C(140)	-58.7(2)
C(141)-C(140)-C(145)-C(144)	57.3(2)
C(136)-C(140)-C(145)-C(144)	-176.22(17)
O(6)-P(6)-N(6)-C(158)	35.89(16)
C(152)-P(6)-N(6)-C(158)	-88.97(16)
C(146)-P(6)-N(6)-C(158)	157.59(14)
O(6)-P(6)-C(146)-C(151)	-116.69(19)
N(6)-P(6)-C(146)-C(151)	122.87(18)
C(152)-P(6)-C(146)-C(151)	4.5(2)
O(6)-P(6)-C(146)-C(147)	59.19(18)
N(6)-P(6)-C(146)-C(147)	-61.25(17)
C(152)-P(6)-C(146)-C(147)	-179.66(15)
C(151)-C(146)-C(147)-C(148)	0.5(3)
P(6)-C(146)-C(147)-C(148)	-175.61(16)
C(146)-C(147)-C(148)-C(149)	-0.5(3)

C(147)-C(148)-C(149)-C(150)	-0.5(4)
C(148)-C(149)-C(150)-C(151)	1.6(4)
C(147)-C(146)-C(151)-C(150)	0.6(3)
P(6)-C(146)-C(151)-C(150)	176.43(19)
C(149)-C(150)-C(151)-C(146)	-1.7(4)
O(6)-P(6)-C(152)-C(153)	7.3(2)
N(6)-P(6)-C(152)-C(153)	132.13(18)
C(146)-P(6)-C(152)-C(153)	-114.98(18)
O(6)-P(6)-C(152)-C(157)	-174.65(17)
N(6)-P(6)-C(152)-C(157)	-49.9(2)
C(146)-P(6)-C(152)-C(157)	63.03(19)
C(157)-C(152)-C(153)-C(154)	-1.2(4)
P(6)-C(152)-C(153)-C(154)	176.8(2)
C(152)-C(153)-C(154)-C(155)	-0.1(4)
C(153)-C(154)-C(155)-C(156)	0.8(5)
C(154)-C(155)-C(156)-C(157)	-0.2(5)
C(155)-C(156)-C(157)-C(152)	-1.1(4)
C(153)-C(152)-C(157)-C(156)	1.8(3)
P(6)-C(152)-C(157)-C(156)	-176.21(19)
P(6)-N(6)-C(158)-C(159)	75.68(18)
P(6)-N(6)-C(158)-C(165)	-155.60(13)
N(6)-C(158)-C(159)-C(164)	-139.86(19)
C(165)-C(158)-C(159)-C(164)	91.9(2)
N(6)-C(158)-C(159)-C(160)	38.2(3)
C(165)-C(158)-C(159)-C(160)	-90.0(2)
C(164)-C(159)-C(160)-C(161)	-1.3(3)
C(158)-C(159)-C(160)-C(161)	-179.45(19)
C(159)-C(160)-C(161)-C(162)	0.8(3)
C(160)-C(161)-C(162)-C(163)	-0.3(3)
C(161)-C(162)-C(163)-C(164)	0.3(4)
C(162)-C(163)-C(164)-C(159)	-0.8(4)
C(160)-C(159)-C(164)-C(163)	1.3(3)
C(158)-C(159)-C(164)-C(163)	179.5(2)
N(6)-C(158)-C(165)-C(167)	164.93(16)
C(159)-C(158)-C(165)-C(167)	-66.7(2)
N(6)-C(158)-C(165)-C(166)	-74.8(2)

C(159)-C(158)-C(165)-C(166)	53.6(2)
N(6)-C(158)-C(165)-C(169)	45.7(2)
C(159)-C(158)-C(165)-C(169)	174.09(16)
C(166)-C(165)-C(167)-C(168)	0.4(4)
C(158)-C(165)-C(167)-C(168)	119.6(3)
C(169)-C(165)-C(167)-C(168)	-120.9(3)
C(167)-C(165)-C(169)-C(174)	-64.6(2)
C(166)-C(165)-C(169)-C(174)	173.13(19)
C(158)-C(165)-C(169)-C(174)	52.6(2)
C(167)-C(165)-C(169)-C(170)	60.7(3)
C(166)-C(165)-C(169)-C(170)	-61.6(2)
C(158)-C(165)-C(169)-C(170)	177.87(19)
C(174)-C(169)-C(170)-C(171)	-54.5(3)
C(165)-C(169)-C(170)-C(171)	177.4(2)
C(169)-C(170)-C(171)-C(172)	55.8(3)
C(170)-C(171)-C(172)-C(173)	-55.8(3)
C(171)-C(172)-C(173)-C(174)	57.5(3)
C(172)-C(173)-C(174)-C(169)	-58.3(3)
C(170)-C(169)-C(174)-C(173)	55.3(3)
C(165)-C(169)-C(174)-C(173)	-177.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{29}H_{34}NOP$ (13) [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(2)#1	0.88	2.12	2.979(2)	164.7
N(2)-H(2N)...O(1)#2	0.88	2.15	2.907(2)	144.4
N(3)-H(3N)...O(4)#3	0.88	2.11	2.913(2)	151.1
N(4)-H(4N)...O(3)#4	0.88	2.19	2.882(2)	135.5
N(5)-H(5N)...O(6)#5	0.88	1.96	2.833(2)	173.0
N(6)-H(6N)...O(5)#4	0.88	2.26	2.923(2)	131.8

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y-1,z-1 #2 -x+1,y+1/2,-z+1 #3 -x+1,y-1/2,-z+2
#4 x,y+1,z #5 -x+2,y-1/2,-z+1

Absolute Stereochemical Identity of 15a (Figure 3a)

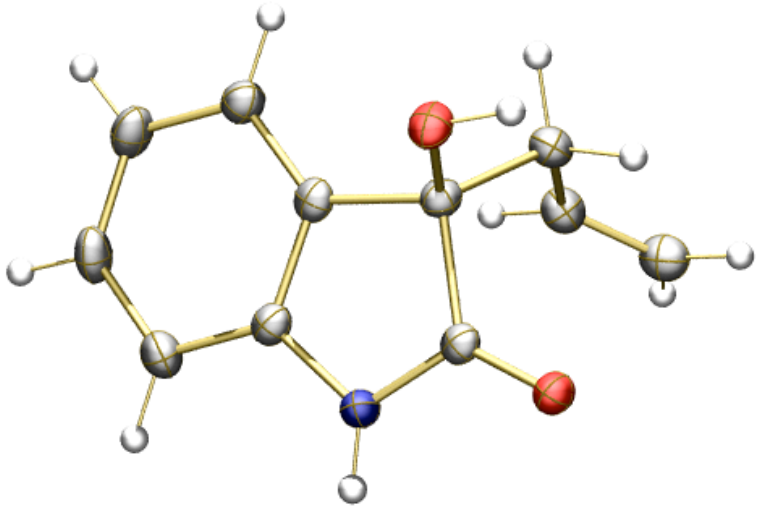

Table 1. Crystal data and structure refinement for $C_{11}H_{11}NO_2$ (15a)

Identification code	$C_{11}H_{11}NO_2$	
Empirical formula	$C_{11}H_{11}NO_2$	
Formula weight	189.21	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.4763(3) Å	α= 90º
	b = 7.5057(3) Å	β= 90º
	c = 16.9951(7) Å	γ = 90º
Volume	953.68(7) $Å^3$	
Z	4	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.745 mm^{-1}	
F(000)	400	
Crystal size	0.20 x 0.10 x 0.07 mm^3	

Theta range for data collection	5.20 to 67.32º
Index ranges	-6<=h<=8, -8<=k<=8, -20<=l<=19
Reflections collected	5081
Independent reflections	1626 [R(int) = 0.0390]
Completeness to theta = 67.32º	97.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9497 and 0.8652
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1626 / 0 / 134
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0746
R indices (all data)	R1 = 0.0308, wR2 = 0.0751
Absolute structure parameter	0.0(2)
Extinction coefficient	0.0093(12)
Largest diff. peak and hole	0.213 and -0.186 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{11}H_{11}NO_2$ (15a). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

O(1)	2482(1)	7117(1)	10115(1)	21(1)
O(2)	4795(1)	7911(1)	8720(1)	22(1)
N(1)	616(2)	6638(2)	9063(1)	20(1)
C(1)	2220(2)	6744(2)	9414(1)	18(1)
C(2)	3694(2)	6381(2)	8795(1)	19(1)
C(3)	2590(2)	6138(2)	8062(1)	19(1)
C(4)	3115(2)	5825(2)	7292(1)	23(1)
C(5)	1792(2)	5651(2)	6720(1)	28(1)
C(6)	-3(2)	5773(2)	6921(1)	27(1)
C(7)	-546(2)	6101(2)	7695(1)	24(1)
C(8)	792(2)	6280(2)	8248(1)	20(1)
C(9)	4814(2)	4750(2)	9025(1)	21(1)
C(10)	3789(2)	3043(2)	9088(1)	24(1)
C(11)	3807(2)	1972(2)	9698(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{11}H_{11}NO_2$ (15a)

O(1)-C(1)	1.2390(17)
O(2)-C(2)	1.4187(17)
O(2)-H(2O)	0.86(2)
N(1)-C(1)	1.341(2)
N(1)-C(8)	1.4179(17)
N(1)-H(1N)	0.846(19)
C(1)-C(2)	1.5477(19)
C(2)-C(3)	1.5064(19)
C(2)-C(9)	1.533(2)
C(3)-C(4)	1.3852(19)
C(3)-C(8)	1.386(2)
C(4)-C(5)	1.394(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.398(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.379(2)
C(7)-H(7)	0.9500
C(9)-C(10)	1.497(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.312(2)
C(10)-H(10)	0.9500
C(11)-H(11A)	0.9500
C(11)-H(11B)	0.9500
C(2)-O(2)-H(2O)	108.3(14)
C(1)-N(1)-C(8)	111.26(12)
C(1)-N(1)-H(1N)	120.1(12)
C(8)-N(1)-H(1N)	128.1(12)
O(1)-C(1)-N(1)	125.55(13)
O(1)-C(1)-C(2)	125.49(13)
N(1)-C(1)-C(2)	108.93(11)

O(2)-C(2)-C(3)	109.98(11)
O(2)-C(2)-C(9)	110.65(11)
C(3)-C(2)-C(9)	114.43(11)
O(2)-C(2)-C(1)	109.34(11)
C(3)-C(2)-C(1)	101.16(11)
C(9)-C(2)-C(1)	110.86(11)
C(4)-C(3)-C(8)	120.25(13)
C(4)-C(3)-C(2)	130.28(14)
C(8)-C(3)-C(2)	109.47(11)
C(3)-C(4)-C(5)	118.27(14)
C(3)-C(4)-H(4)	120.9
C(5)-C(4)-H(4)	120.9
C(6)-C(5)-C(4)	120.55(13)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(7)	121.58(14)
C(5)-C(6)-H(6)	119.2
C(7)-C(6)-H(6)	119.2
C(8)-C(7)-C(6)	116.63(14)
C(8)-C(7)-H(7)	121.7
C(6)-C(7)-H(7)	121.7
C(7)-C(8)-C(3)	122.71(13)
C(7)-C(8)-N(1)	128.16(14)
C(3)-C(8)-N(1)	109.14(13)
C(10)-C(9)-C(2)	114.96(12)
C(10)-C(9)-H(9A)	108.5
C(2)-C(9)-H(9A)	108.5
C(10)-C(9)-H(9B)	108.5
C(2)-C(9)-H(9B)	108.5
H(9A)-C(9)-H(9B)	107.5
C(11)-C(10)-C(9)	125.14(14)
C(11)-C(10)-H(10)	117.4
C(9)-C(10)-H(10)	117.4
C(10)-C(11)-H(11A)	120.0
C(10)-C(11)-H(11B)	120.0
H(11A)-C(11)-H(11B)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{11}H_{11}NO_2$ (15a). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	23(1)	18(1)	-1(1)	0(1)	0(1)
O(2)	24(1)	21(1)	22(1)	2(1)	-1(1)	-6(1)
N(1)	18(1)	25(1)	18(1)	-1(1)	1(1)	2(1)
C(1)	21(1)	14(1)	18(1)	2(1)	1(1)	0(1)
C(2)	19(1)	19(1)	18(1)	0(1)	1(1)	-2(1)
C(3)	24(1)	14(1)	20(1)	1(1)	0(1)	1(1)
C(4)	26(1)	22(1)	21(1)	0(1)	2(1)	3(1)
C(5)	39(1)	26(1)	18(1)	-3(1)	-1(1)	7(1)
C(6)	35(1)	26(1)	22(1)	-4(1)	-10(1)	7(1)
C(7)	24(1)	24(1)	26(1)	0(1)	-4(1)	3(1)
C(8)	23(1)	17(1)	18(1)	0(1)	1(1)	1(1)
C(9)	19(1)	22(1)	23(1)	-1(1)	0(1)	1(1)
C(10)	24(1)	22(1)	26(1)	-3(1)	-2(1)	0(1)
C(11)	29(1)	22(1)	33(1)	0(1)	3(1)	1(1)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{11}H_{11}NO_2$ (15a)

	x	y	z	U(eq)
H(2O)	5560(30)	7910(30)	9102(11)	33
H(1N)	-320(30)	6910(20)	9315(10)	24
H(4)	4345	5731	7158	28
H(5)	2121	5447	6187	33
H(6)	-885	5630	6523	33
H(7)	-1773	6195	7833	29

H(9A)	5774	4593	8630	26
H(9B)	5394	4991	9538	26
H(10)	3068	2708	8652	29
H(11A)	4510	2259	10146	34
H(11B)	3116	909	9692	34

Table 6. Torsion angles [º] for $C_{11}H_{11}NO_2$ (15a)

C(8)-N(1)-C(1)-O(1)	176.77(13)
C(8)-N(1)-C(1)-C(2)	-1.54(15)
O(1)-C(1)-C(2)-O(2)	-60.30(18)
N(1)-C(1)-C(2)-O(2)	118.01(12)
O(1)-C(1)-C(2)-C(3)	-176.30(13)
N(1)-C(1)-C(2)-C(3)	2.01(14)
O(1)-C(1)-C(2)-C(9)	61.95(17)
N(1)-C(1)-C(2)-C(9)	-119.74(12)
O(2)-C(2)-C(3)-C(4)	62.35(19)
C(9)-C(2)-C(3)-C(4)	-62.90(19)
C(1)-C(2)-C(3)-C(4)	177.88(15)
O(2)-C(2)-C(3)-C(8)	-117.33(12)
C(9)-C(2)-C(3)-C(8)	117.42(13)
C(1)-C(2)-C(3)-C(8)	-1.80(14)
C(8)-C(3)-C(4)-C(5)	-0.3(2)
C(2)-C(3)-C(4)-C(5)	180.00(14)
C(3)-C(4)-C(5)-C(6)	-0.6(2)
C(4)-C(5)-C(6)-C(7)	1.1(2)
C(5)-C(6)-C(7)-C(8)	-0.6(2)
C(6)-C(7)-C(8)-C(3)	-0.4(2)
C(6)-C(7)-C(8)-N(1)	179.05(14)
C(4)-C(3)-C(8)-C(7)	0.8(2)
C(2)-C(3)-C(8)-C(7)	-179.43(12)
C(4)-C(3)-C(8)-N(1)	-178.67(13)
C(2)-C(3)-C(8)-N(1)	1.05(15)
C(1)-N(1)-C(8)-C(7)	-179.15(14)
C(1)-N(1)-C(8)-C(3)	0.34(16)

O(2)-C(2)-C(9)-C(10)	-177.65(11)
C(3)-C(2)-C(9)-C(10)	-52.74(17)
C(1)-C(2)-C(9)-C(10)	60.87(16)
C(2)-C(9)-C(10)-C(11)	-127.70(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{11}H_{11}NO_2$ (15a) [Å and º]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(1)#1	0.86(2)	1.96(2)	2.8209(14)	174.0(18)
N(1)-H(1N)...O(1)#2	0.846(19)	2.04(2)	2.8836(16)	173.0(17)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+3/2,-z+2 #2 x-1/2,-y+3/2,-z+2

X-ray Crystal Structure of 21 (Figure 3c)

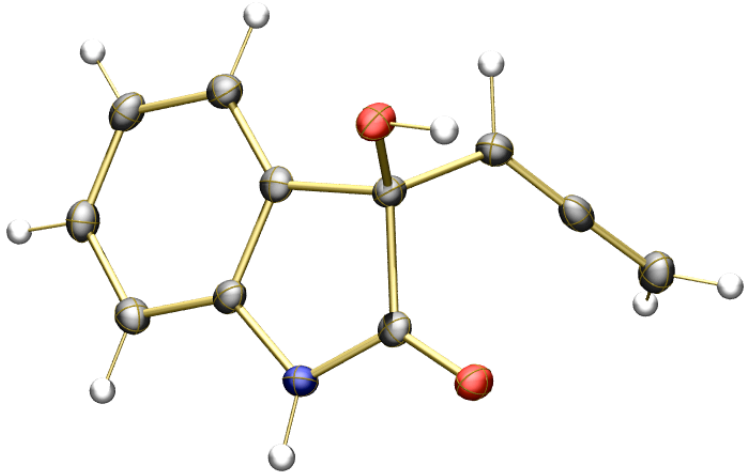

Table 1. Crystal data and structure refinement for $C_{11}H_9NO_2$ (21)

Identification code	$C_{11}H_9NO_2$
Empirical formula	$C_{11}H_9NO_2$
Formula weight	187.19
Temperature	100(2) K
Wavelength	1.54178 Å

Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.0851(7) Å	α= 90º
	b = 7.1233(7) Å	β= 90º
	c = 17.6028(16) Å	γ = 90º
Volume	888.40(15) $Å^3$	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	0.800 mm^{-1}	
F(000)	392	
Crystal size	0.15 x 0.12 x 0.06 mm^3	
Theta range for data collection	5.02 to 68.81º.	
Index ranges	-8<=h<=8, -8<=k<=8, -21<=l<=18	
Reflections collected	10395	
Independent reflections	1579 [R(int) = 0.0346]	
Completeness to theta = 68.00º	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9536 and 0.8895	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1579 / 0 / 142	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0250, wR2 = 0.0641	
R indices (all data)	R1 = 0.0260, wR2 = 0.0652	
Absolute structure parameter	0.21(19)	
Extinction coefficient	na	
Largest diff. peak and hole	0.146 and -0.176 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_{11}H_9NO_2$ (21). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2374(1)	1954(1)	10038(1)	18(1)
O(2)	4912(1)	2864(1)	8733(1)	18(1)
N(1)	412(2)	1808(2)	9004(1)	16(1)

C(1)	2085(2)	1710(2)	9352(1)	15(1)
C(2)	3632(2)	1335(2)	8749(1)	15(1)
C(3)	2481(2)	1311(2)	8024(1)	15(1)
C(4)	3020(2)	1036(2)	7280(1)	18(1)
C(5)	1632(2)	1064(2)	6717(1)	20(1)
C(6)	-256(2)	1347(2)	6908(1)	20(1)
C(7)	-816(2)	1598(2)	7662(1)	19(1)
C(8)	584(2)	1576(2)	8207(1)	16(1)
C(9)	4648(2)	-509(2)	8866(1)	18(1)
C(10)	4259(2)	-1798(2)	9364(1)	18(1)
C(11)	3899(2)	-3140(2)	9842(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for $C_{11}H_9NO_2$ (21)

O(1)-C(1)	1.2370(15)
O(2)-C(2)	1.4177(16)
O(2)-H(2O)	0.858(19)
N(1)-C(1)	1.3361(17)
N(1)-C(8)	1.4176(16)
N(1)-H(1N)	0.882(18)
C(1)-C(2)	1.5500(17)
C(2)-C(9)	1.5124(19)
C(2)-C(3)	1.5132(17)
C(3)-C(4)	1.3798(18)
C(3)-C(8)	1.3944(18)
C(4)-C(5)	1.3960(19)
C(4)-H(4)	0.9500
C(5)-C(6)	1.394(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.3961(18)
C(6)-H(6)	0.9500
C(7)-C(8)	1.3807(19)
C(7)-H(7)	0.9500
C(9)-C(10)	1.299(2)

C(9)-H(9)	0.989(17)
C(10)-C(11)	1.299(2)
C(11)-H(11A)	0.946(18)
C(11)-H(11B)	0.975(19)

C(2)-O(2)-H(2O)	107.7(13)
C(1)-N(1)-C(8)	111.82(11)
C(1)-N(1)-H(1N)	122.2(11)
C(8)-N(1)-H(1N)	125.2(11)
O(1)-C(1)-N(1)	125.98(11)
O(1)-C(1)-C(2)	125.21(11)
N(1)-C(1)-C(2)	108.75(10)
O(2)-C(2)-C(9)	111.41(10)
O(2)-C(2)-C(3)	109.71(10)
C(9)-C(2)-C(3)	111.19(11)
O(2)-C(2)-C(1)	109.46(10)
C(9)-C(2)-C(1)	113.18(11)
C(3)-C(2)-C(1)	101.45(10)
C(4)-C(3)-C(8)	120.33(12)
C(4)-C(3)-C(2)	130.78(12)
C(8)-C(3)-C(2)	108.87(11)
C(3)-C(4)-C(5)	118.54(12)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	120.42(13)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	121.36(12)
C(5)-C(6)-H(6)	119.3
C(7)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	117.11(12)
C(8)-C(7)-H(7)	121.4
C(6)-C(7)-H(7)	121.4
C(7)-C(8)-C(3)	122.23(12)
C(7)-C(8)-N(1)	128.68(12)
C(3)-C(8)-N(1)	109.09(11)

C(10)-C(9)-C(2)	127.19(12)
C(10)-C(9)-H(9)	121.7(10)
C(2)-C(9)-H(9)	111.1(10)
C(11)-C(10)-C(9)	177.59(14)
C(10)-C(11)-H(11A)	120.1(11)
C(10)-C(11)-H(11B)	123.5(10)
H(11A)-C(11)-H(11B)	116.3(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{11}H_9NO_2$ (21). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	22(1)	14(1)	-1(1)	0(1)	-1(1)
O(2)	18(1)	20(1)	15(1)	1(1)	-1(1)	-5(1)
N(1)	14(1)	20(1)	15(1)	0(1)	2(1)	2(1)
C(1)	17(1)	11(1)	16(1)	1(1)	0(1)	-1(1)
C(2)	15(1)	17(1)	13(1)	1(1)	1(1)	-1(1)
C(3)	17(1)	12(1)	17(1)	0(1)	0(1)	-2(1)
C(4)	19(1)	17(1)	18(1)	0(1)	2(1)	0(1)
C(5)	28(1)	19(1)	14(1)	-1(1)	1(1)	-1(1)
C(6)	23(1)	20(1)	17(1)	0(1)	-5(1)	0(1)
C(7)	17(1)	18(1)	21(1)	1(1)	-1(1)	-1(1)
C(8)	19(1)	14(1)	14(1)	0(1)	2(1)	1(1)
C(9)	17(1)	20(1)	18(1)	0(1)	2(1)	2(1)
C(10)	16(1)	20(1)	19(1)	-5(1)	-2(1)	5(1)
C(11)	28(1)	20(1)	21(1)	2(1)	0(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{11}H_9NO_2$ (21)

	x	y	z	U(eq)
H(2O)	5500(30)	2880(30)	9159(11)	27
H(1N)	-620(30)	2170(20)	9242(9)	20
H(4)	4306	831	7152	22
H(5)	1976	888	6200	24
H(6)	-1181	1371	6517	24
H(7)	-2104	1775	7793	22
H(9)	5680(20)	-670(20)	8493(9)	22
H(11A)	4500(20)	-3160(30)	10323(10)	28
H(11B)	3010(20)	-4160(30)	9740(10)	28

Table 6. Torsion angles [º] for $C_{11}H_9NO_2$ (21)

C(8)-N(1)-C(1)-O(1)	176.22(12)
C(8)-N(1)-C(1)-C(2)	-1.07(14)
O(1)-C(1)-C(2)-O(2)	-59.86(16)
N(1)-C(1)-C(2)-O(2)	117.46(11)
O(1)-C(1)-C(2)-C(9)	65.06(16)
N(1)-C(1)-C(2)-C(9)	-117.62(12)
O(1)-C(1)-C(2)-C(3)	-175.74(12)
N(1)-C(1)-C(2)-C(3)	1.58(13)
O(2)-C(2)-C(3)-C(4)	64.53(17)
C(9)-C(2)-C(3)-C(4)	-59.16(18)
C(1)-C(2)-C(3)-C(4)	-179.77(13)
O(2)-C(2)-C(3)-C(8)	-117.25(11)
C(9)-C(2)-C(3)-C(8)	119.06(12)
C(1)-C(2)-C(3)-C(8)	-1.55(13)
C(8)-C(3)-C(4)-C(5)	1.14(19)
C(2)-C(3)-C(4)-C(5)	179.19(13)
C(3)-C(4)-C(5)-C(6)	-0.6(2)
C(4)-C(5)-C(6)-C(7)	-0.4(2)

C(5)-C(6)-C(7)-C(8)	0.8(2)
C(6)-C(7)-C(8)-C(3)	-0.25(19)
C(6)-C(7)-C(8)-N(1)	179.48(13)
C(4)-C(3)-C(8)-C(7)	-0.74(19)
C(2)-C(3)-C(8)-C(7)	-179.18(12)
C(4)-C(3)-C(8)-N(1)	179.48(11)
C(2)-C(3)-C(8)-N(1)	1.04(14)
C(1)-N(1)-C(8)-C(7)	-179.73(13)
C(1)-N(1)-C(8)-C(3)	0.03(15)
O(2)-C(2)-C(9)-C(10)	129.44(14)
C(3)-C(2)-C(9)-C(10)	-107.84(16)
C(1)-C(2)-C(9)-C(10)	5.6(2)
C(2)-C(9)-C(10)-C(11)	152(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for $C_{11}H_9NO_2$ (21) [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(1)#1	0.858(19)	1.942(19)	2.7812(13)	165.6(17)
N(1)-H(1N)...O(1)#2	0.882(18)	2.003(18)	2.8729(15)	168.6(15)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,-z+2 #2 x-1/2,-y+1/2,-z+2