Supporting Information

"Enantioselective Reductive Coupling of 1,3-Enynes to Heterocyclic Aromatic Aldehydes and Ketones *via* Rhodium Catalyzed Asymmetric Hydrogenation: Mechanistic Insight into the Role of Brønsted Acid Additives"

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I. Experimental Section

General: All reactions were run under an atmosphere of argon, unless otherwise indicated. Anhydrous solvents were transferred by an oven-dried syringe. Flasks were flame-dried and cooled under a stream of nitrogen. Dichloroethane (DCE) was distilled from calcium hydride. $Rh(COD)_2OTf$, (*R*)-*tol*-BINAP and (*R*)-*xylyl*-WALPHOS were used as received from Strem Chemicals. All the 1,3-enynes were prepared following the literature procedure.[1] The aldehyde substrates are either commercially available or prepared using literature procedure, for example *N*-4-methoxybenzyl-2-imidazole carboxaldehyde, [2] *N*-phenyl-5-pyrazine-2-carboxaldehyde,[3] 5-methyl-2-thiazocarboxaldehyde.[4] All the ketone substrates used for reductive coupling reactions are commercially available. All the hydrogen mediated reductive coupling reactions were carried out in 13 x 100 mm test tubes. Analytical thin-layer chromatography (TLC) was carried out using 0.2-mm commercial silica gel plates (DC-Fertigplatten Kieselgel 60 F_{254}). Preparative column chromatography employing silica gel was performed according to the method of Still.[5] Solvents for chromatography are listed as volume/volume ratios. Infrared spectra were recorded on a Perkin-Elmer 1600 spectrometer. High-resolution mass spectra (HRMS) were obtained on a Karatos MS9 and are reported as m/z (relative intensity). Accurate masses are reported for the molecular ion [M] or a suitable fragment ion. Proton nucolorless magnetic resonance (^{1}H-NMR) spectra were recorded with a Varian Gemini (400 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane. Coupling constants are reported in Hertz (Hz). Carbon-13 nucolorless magnetic resonance (^{13}C-NMR) spectra were recorded with a Varian Gemini 400 (100 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, ppm relative to the center of the triplet at 77.0 ppm for deuteriochloroform. ^{13}C NMR spectra were routinely run with broadband decoupling.

General procedure for the reductive coupling of 1, 3-enynes and heterocyclic aromatic aldehydes and ketones

To a degassed solution of $Rh(COD)_2OTf$ (4.4 mg, 9.3 μmol, 2 mol%), (*R*)-*tol*-BINAP (6.3 mg, 9.3 μmol, 2 mol%) and triphenylacetic acid (2.7 mg, 9.3 μmol, 2 mol%)in DCE (1.0 mL) in a 13 x 100 mm test tube, a solution of aldehyde (0.466 mmol, 100 mol%) and the enyne (0.932 mmol, 200 mol%) in DCE (1.4 mL, total volume, 2.4 mL, 0.2 M) was added. The system was then purged with argon gas followed by hydrogen gas. The reaction was allowed to stir at 40 ^{o}C under 1 atm of hydrogen until complete consumption of the aldehyde. The solvent was evaporated *in vacuo* and the crude reaction mixture was purified by flash chromatography.

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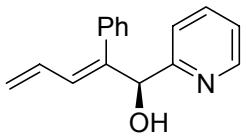
(1) Sonagashira, K.; Tohada, Y.; Hagihara, N. *Tetrahedron Lett*. **1975**, *16*, 4467.
(2) Werner, A., Sánchez-Migallan, A., Fruchier A., Elguero, J., Fernández-Castiño, C., Foces-Foces, C. *Tetrahedron* **1995**, *51*, 4779.
(3) Murphy, W. V., Hadden, S. K.; Watcher, M. P. *J. Heterocycl. Chem*. **1993**, *27*, 1933.
(4) Palle, E, V.; Hennings, L. *Acta Chem. Scand.* **1966**, *20*, 2649.
(5) Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923.

II. Full characterization data

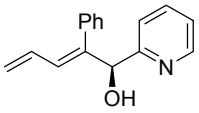
2-Phenyl-1-pyridin-2-yl-penta-2,4-dien-1-ol



2

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1b** (120.0 mg, 0.932 mmol, 200 mol%) was coupled to pyridine-2-carboxaldehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (100.7 mg, 0.424 mmol) as a colorless oil in 94% yield after purification by flash column chromatography (R_f = 0.20, 35% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 8.35 (dd, *J* = 3.2, 1.0 Hz, 1H), 7.46 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.15 (m, 3H), 7.03 (m, 3H), 6.96 (m, 3H), 6.50 (d, *J* = 11.2 Hz, 1H), 6.22 (ddd, *J* = 16.8, 10.8, 10.4 Hz, 1H), 5.26 (dd, *J* = 16.8, 1.6, 2H), 5.0 (dd, *J* = 10.0, 2.0 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 159.1, 147.6, 144.0, 137.1, 136.3, 133.6, 129.4, 127.7, 127.0, 122.2, 118.8, 76.7.
HRMS Calcd. for $C_{16}H_{15}NO$ (M): 237.1154, Found: 237.1158.
FTIR (NaCl Film): 3374, 3080, 3053, 3017, 2973, 2874, 1594, 1570, 1470, 1437, 1396, 1208, 1076, 999, 914, 801, 768, 743, 673 cm^{-1}.



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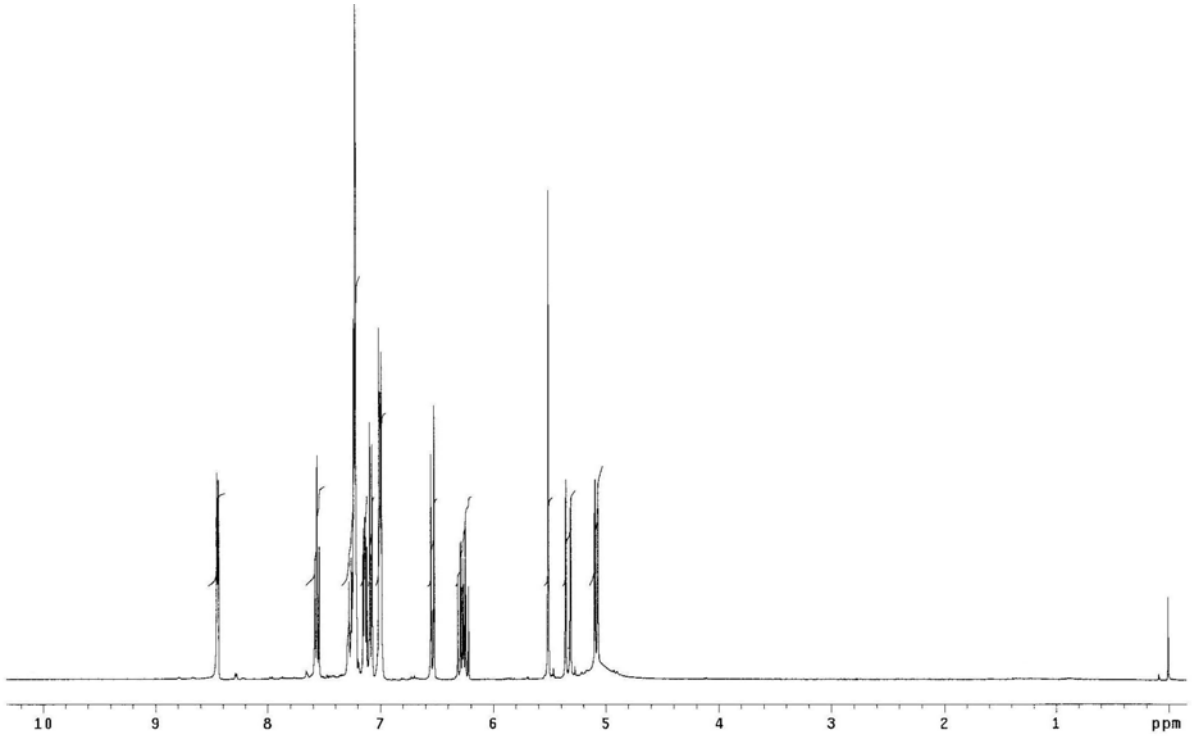
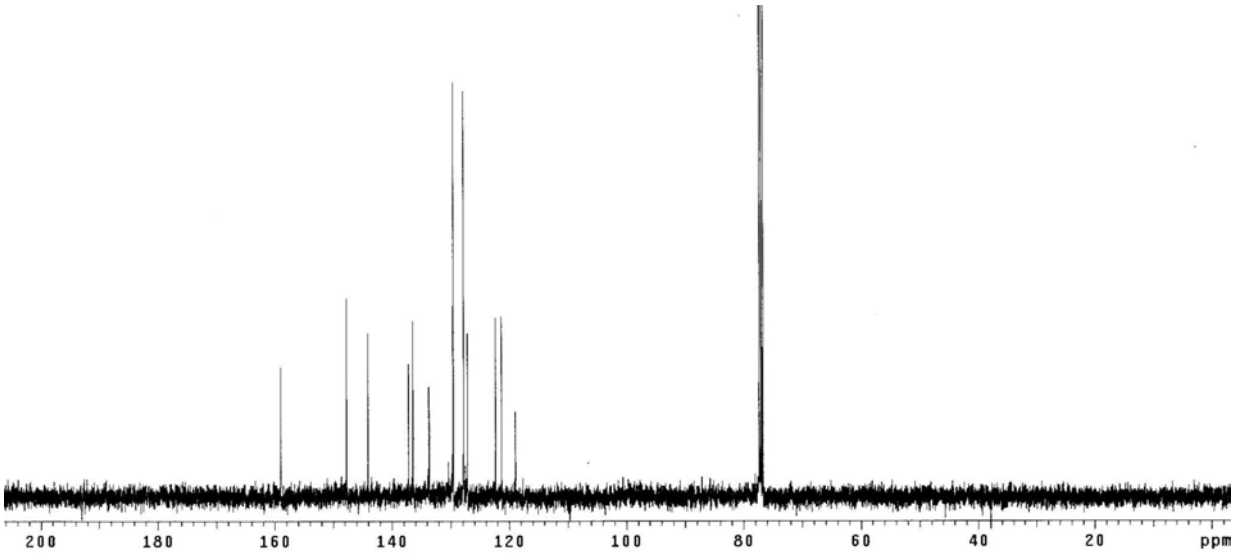
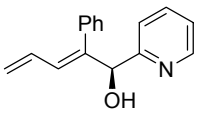
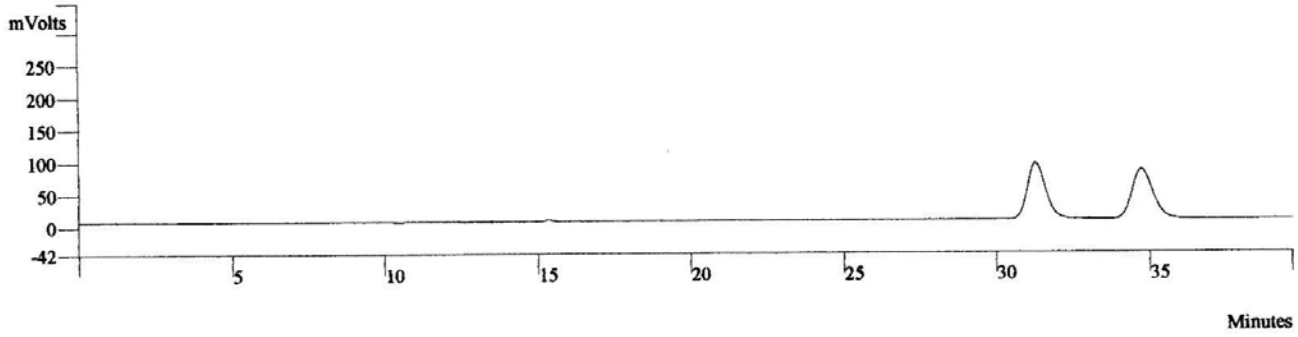






2

HPLC (Chiralcel OD-H column, 5% *i*-PrOH/hexanes, 0.3 mL/min, 254 nm): t_{minor} = 31.2 min, t_{major} = 34.5 min; ee = 92%.



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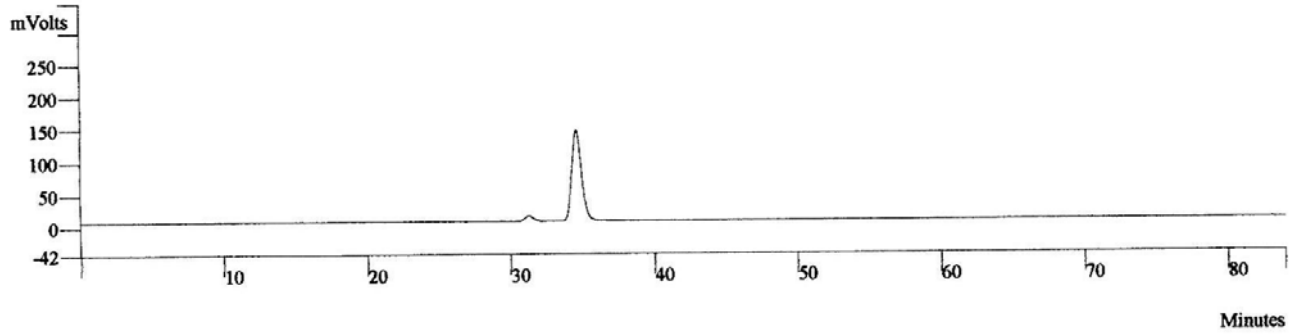

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1		3.7756	31.261	0.000	255853	0.00	BB	33.6		0
2		96.2244	34.574	0.000	6520560	0.00	BB	43.5		0
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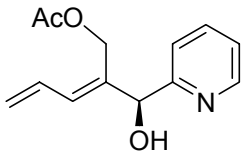
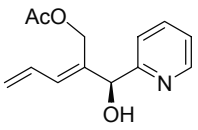
Acetic acid 2-(hydroxy-pyridin-2-yl-methyl)-penta-2,4-dienyl ester



3

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1b** (116.0 mg, 0.932 mmol, 200 mol%) was coupled to pyridine-2-carboxaldehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (100.0 mg, 0.429 mmol) as a colorless oil in 94% yield after purification by flash column chromatography (R_f = 0.22, 45% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 8.54 (d, *J* = 4.8 Hz, 1H), 7.67 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.22 (dd, *J* = 7.2, 4.8 Hz, 1H), 6.70 (ddd, *J* = 16.8, 11.2, 10.4 Hz, 1H), 6.44 (d, *J* = 11.6 Hz, 1H), 5.41 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.32 (dd, *J* =10.0, 1.2, 1H), 5.27 (s, 1H) 5.20 (s, 1H), 4.68 (q, *J* = 12.8 Hz, 2H) 1.80 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.6, 159.2, 147.8, 136.6, 136.3, 133.9, 131.5, 122.4, 121.3, 122.1, 76.0, 58.4, 20.5.
HRMS Calcd. for $C_{13}H_{15}NO_3$ (M): 233.1052, Found: 233.1052.
FTIR (NaCl Film): 3384, 3083, 3051, 3011, 2961, 1737, 1592, 1467, 1436, 1239, 1039, 995, 914, 671.



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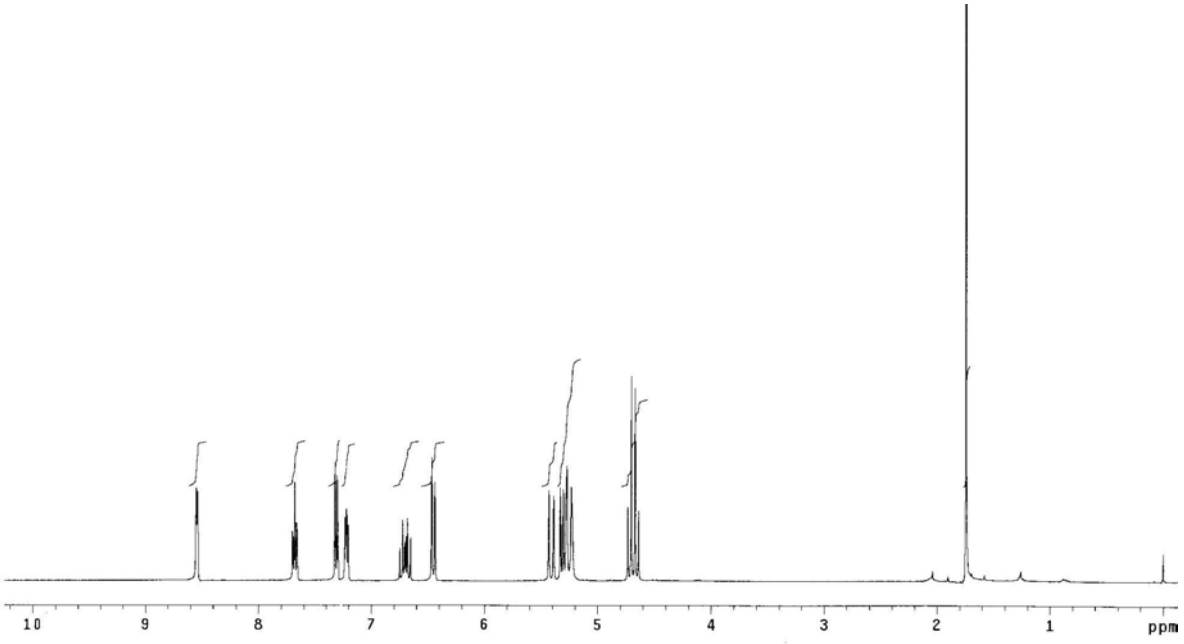
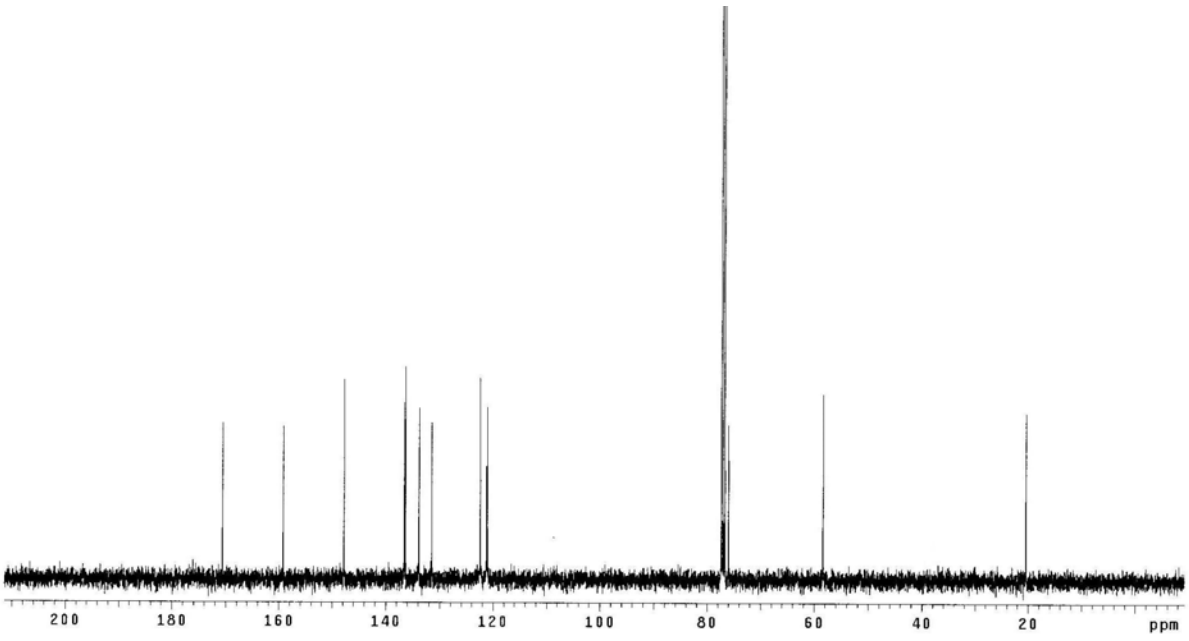
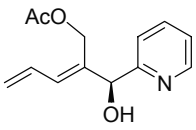
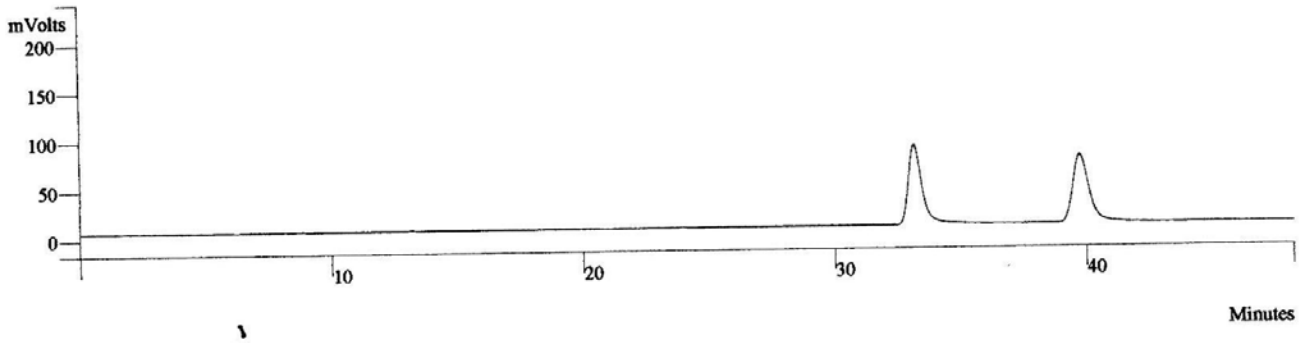






3

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor}=32.0 min, t_{major} = 38.4 min; ee = 95%.



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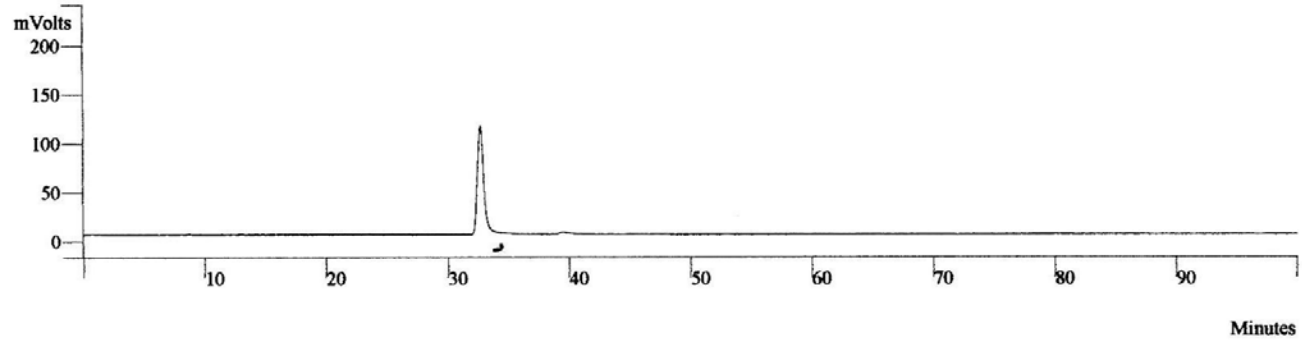
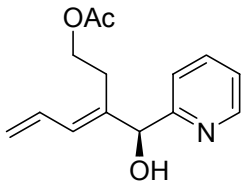


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		97.4675	32.690	0.000	4031690	0.00	BB	32.7		0
2		2.3874	39.533	0.000	98754	0.00	BB	42.3		0
3		0.1451	98.180	0.000	6000	0.00	BB	0.1		0
	Totals	**100.0000**		**0.000**	**4136444**					

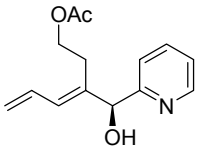
Acetic acid 3-(hydroxy-pyridin-2-yl-methyl)-hexa-3,5-dienyl ester



4

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1e** (120.0 mg, 0.932 mmol, 200 mol%) was coupled to pyridine-2-carboxaldehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (105.0 mg, 0.425 mmol) as a colorless oil in 93% yield after purification by flash column chromatography (R_f = 0.25, 40% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 8.54 (d, *J* = 4.8 Hz, 1H), 7.67 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.22 (dd, *J* = 6.4, 5.2 Hz, 1H), 6.64 (dt, *J* = 16.8, 10.8 Hz, 1H), 6.35 (d, *J* = 11.2 Hz, 1H), 5.33 (d, *J* = 16.8 Hz, 2H), 5.24 (d, *J* = 1.0 Hz, 1H), 5.20 (s, 1H) 4.91 (s, 1H), 3.93 (m, 2H) 2.50 (ddd, *J* = 14.8, 8., 7.2, 1H), 2.23 (ddd, *J* = 13.6, 8.4, 6.4 Hz, 1H) 1.97 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.1, 159.2, 147.6, 138.3, 136.6, 132.1, 131.4, 122.4, 120.9, 119.1, 77.5, 63.5, 26.1, 20.8.
HRMS Calcd. for $C_{14}H_{17}NO_3$ (M): 247.1208, Found: 247.1211.
FTIR (NaCl Film): 3388, 3085, 3012, 2963, 1737, 1593, 1471, 1435, 1385, 1305, 1245, 1036, 993, 915, 763, 686 cm^{-1}.



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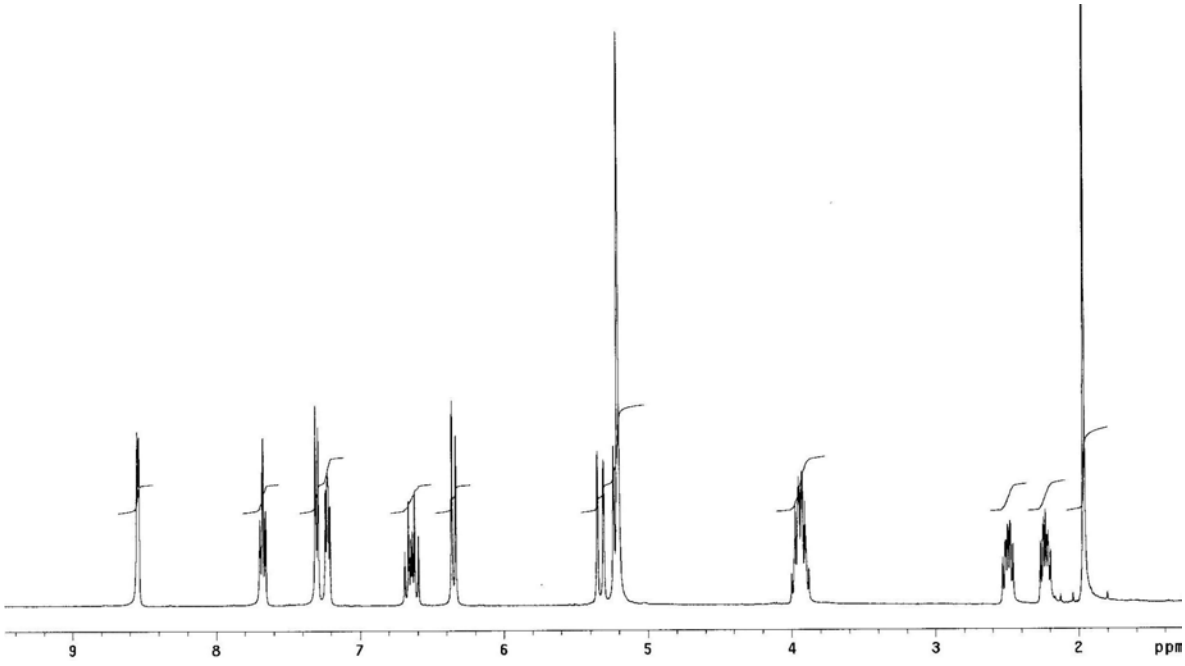
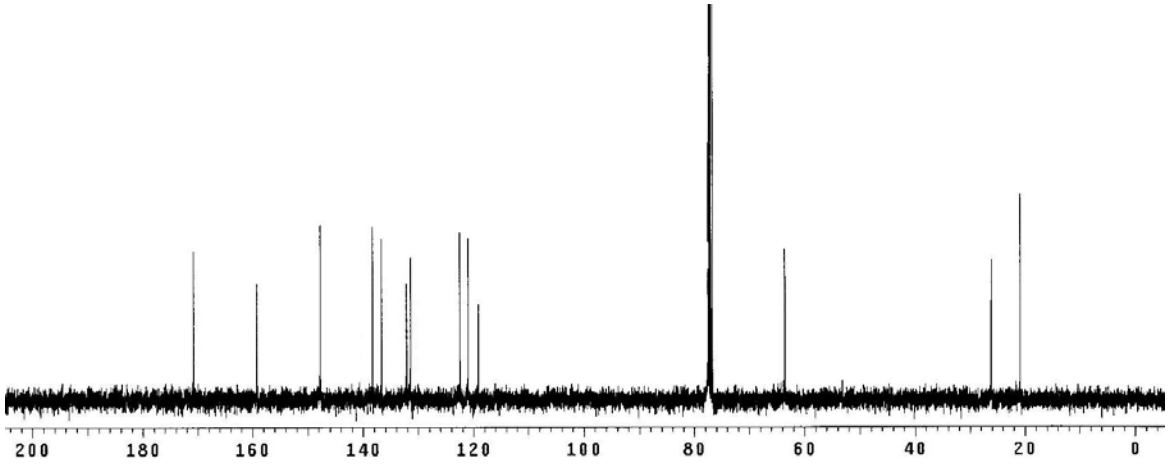
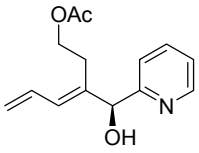
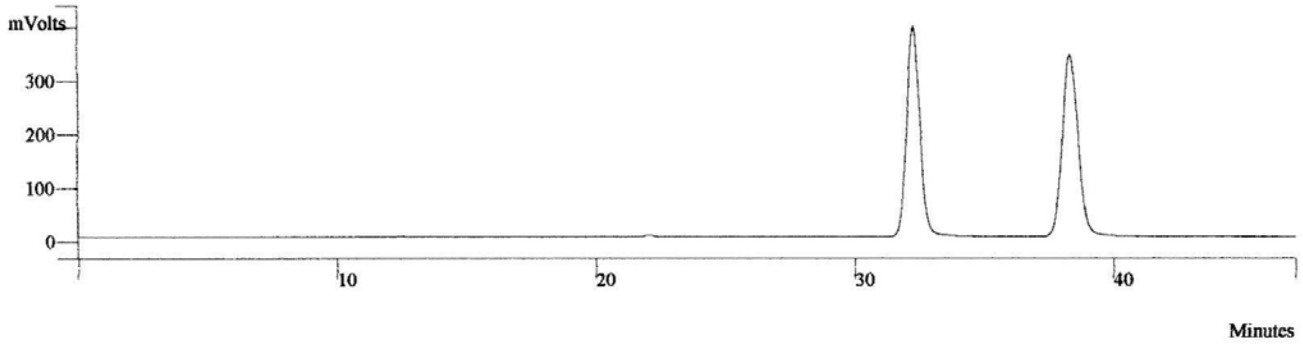






4

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 38.7 min, t_{major} = 32.4 min; ee = 94%.



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1		49.0338	32.250	0.000	13836061	0.00	BB	32.6		0
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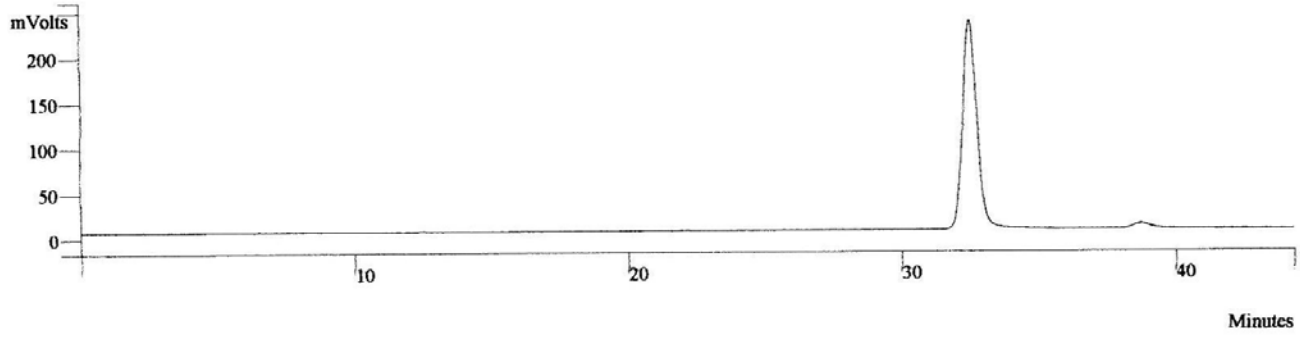

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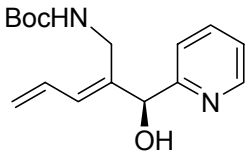
1		97.0072	32.488	0.000	8432441	0.00	BB	33.0		0
2		2.9928	38.727	0.000	260156	0.00	BB	41.1		0
	Totals	**100.0000**		**0.000**	**8692597**					

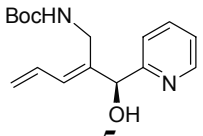
2-(Hydroxy-pyridin-2-yl-methyl)-penta-2,4-dienyl]-carbamic acid *tert*-butyl ester.



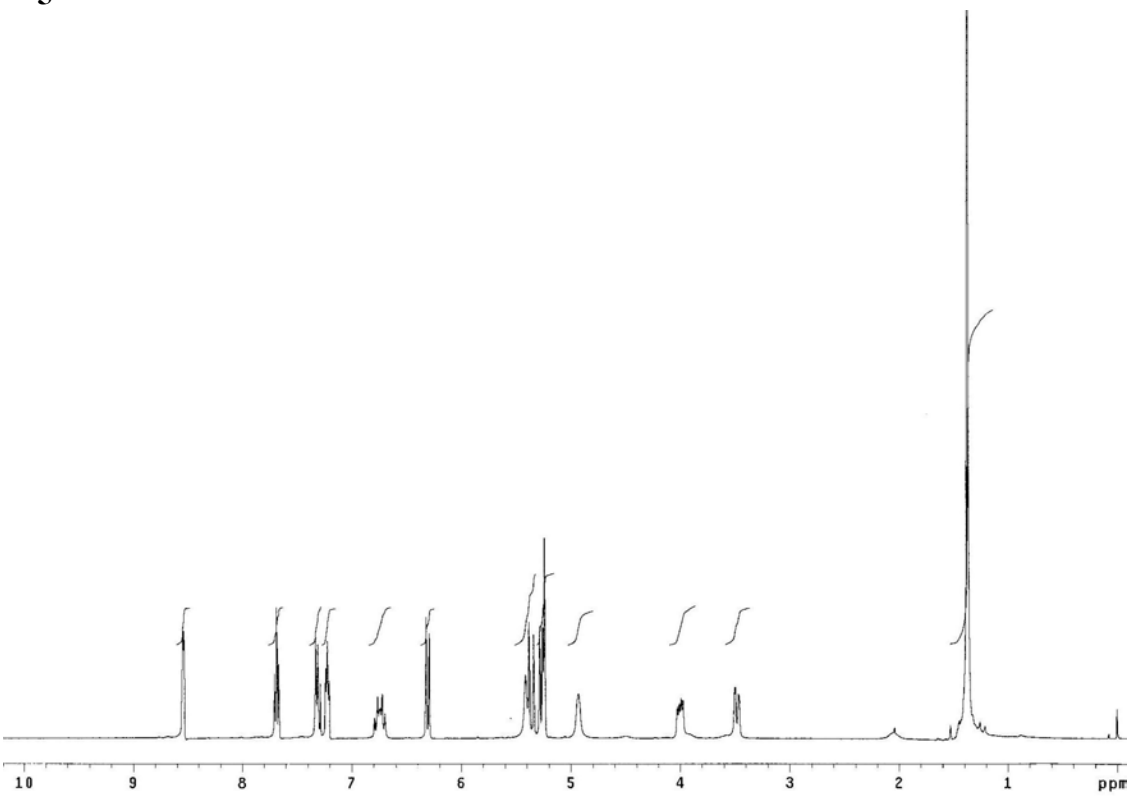
5

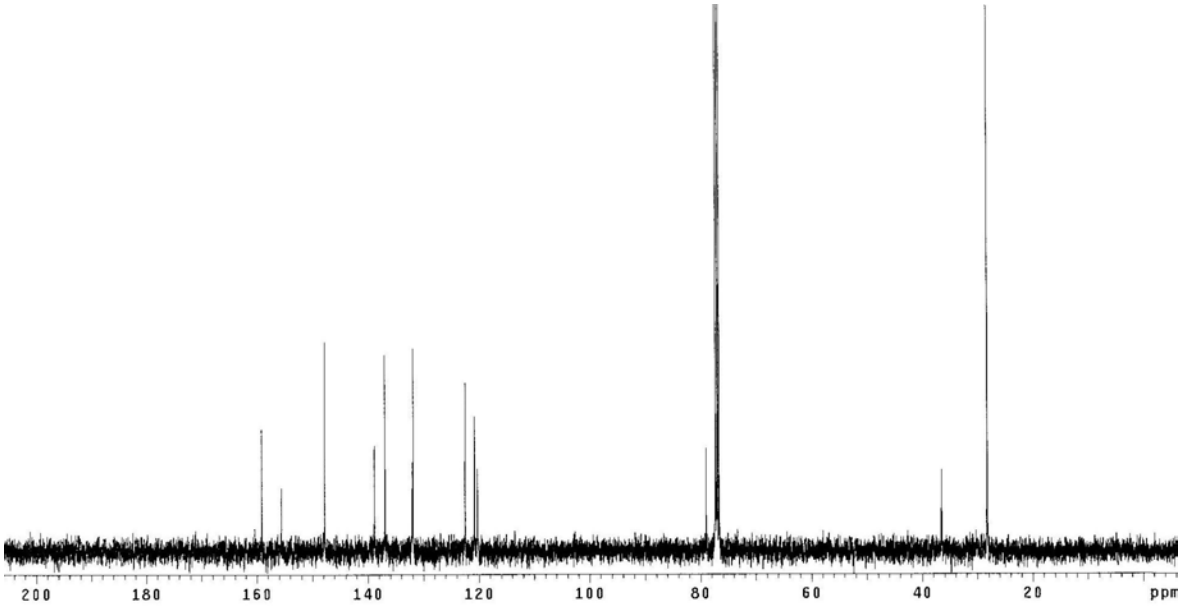
In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1c** (116.3 mg, 0.932 mmol, 200 mol%) was coupled to pyridine-2-carboxaldehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (113.0 mg, 0.389 mmol) as a thick syrup in 95% yield after purification by flash column chromatography (R_f = 0.22, 45% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 8.54 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.67 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.30 (dd, *J* = 7.6, 10.4 Hz, 1H), 7.22 (dd, *J* = 7.2, 5.2 Hz, 1H), 6.74 (dt, *J* = 16.4, 10.8 Hz, 1H), 6.31 (d, *J* = 10.8 Hz, 1H), 5.36 (dd, *J* = 16.4, 1.6 Hz, 2H), 5.27 (d, 10.4 Hz, 1H), 5.23 (s, 1H) 4.91 (s, 1H), 4.0 (dd, *J* = 7.2, 3.8 Hz 1H) 3.47 (dd, *J* = 14.0, 4.0, 1H) 1.40 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$): 159.1, 155.6, 147.8, 138.8, 136.9, 132.0, 131.8, 122.5, 120.8, 120.3, 79.0, 36.5, 28.3.
HRMS Calcd. for $C_{16}H_{22}N_2O_3$ (M): 290.1630, Found: 290.1631.
FTIR (NaCl Film): 3357, 3053, 2957, 2932, 1701, 1592, 1501, 1435, 1366, 1249, 1169, 1045, 995, 918, 755, 624 cm^{-1}.


BocHN
N
OH

5


10
9
8
7
6
5
4
3
2
1
ppm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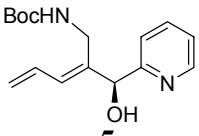
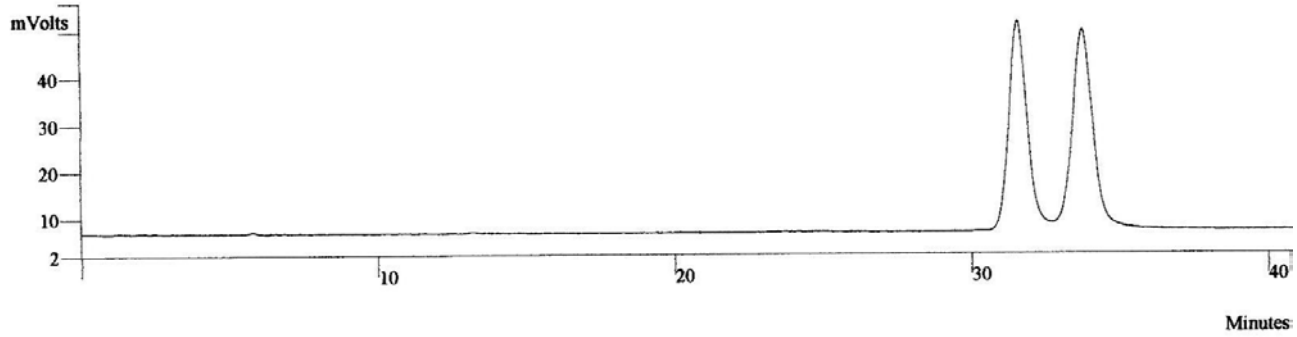
180
160
140
120
100
80
60
40
20
ppm

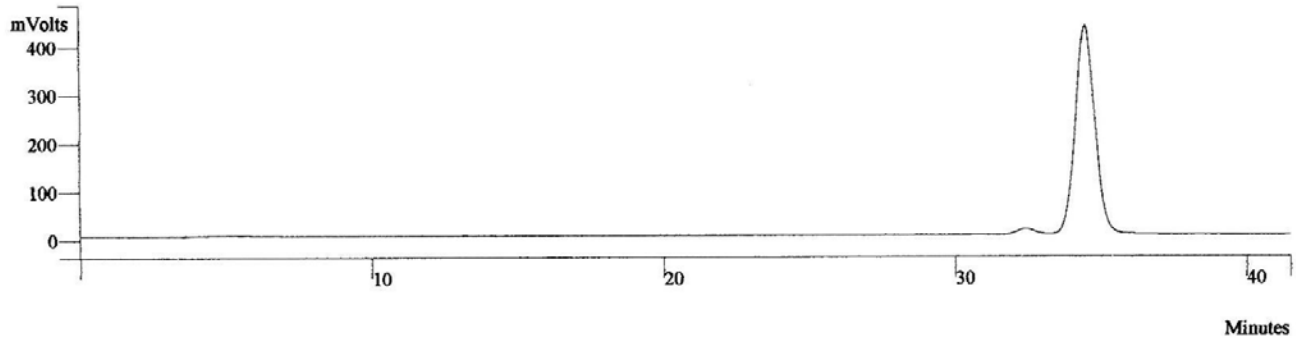


5

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 32.3 min, t_{major} = 34.4 min; ee = 95%

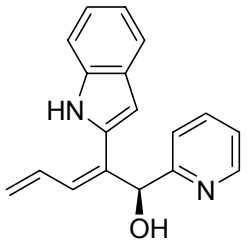


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.6771	31.609	0.000	1819531	0.00	BB	38.9		0
2		50.3229	33.771	0.000	1843184	0.00	BB	41.3		0
	Totals	**100.0000**		**0.000**	**3662715**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		2.4071	32.399	0.000	495490	0.00	BB	41.2		0
2		97.5929	34.482	0.000	20089394	0.00	BB	42.8		0
	Totals	**100.0000**		**0.000**	**20584884**					

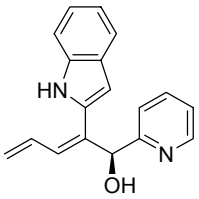
2-(1*H*-Indol-2-yl)-1-pyridin-2-yl-penta-2,4-dien-1-ol



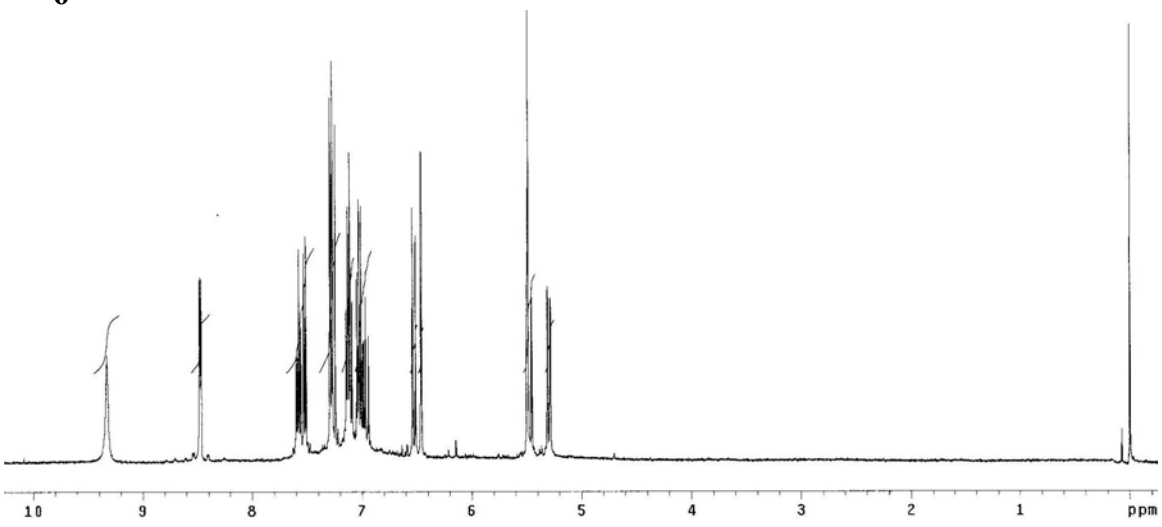
6

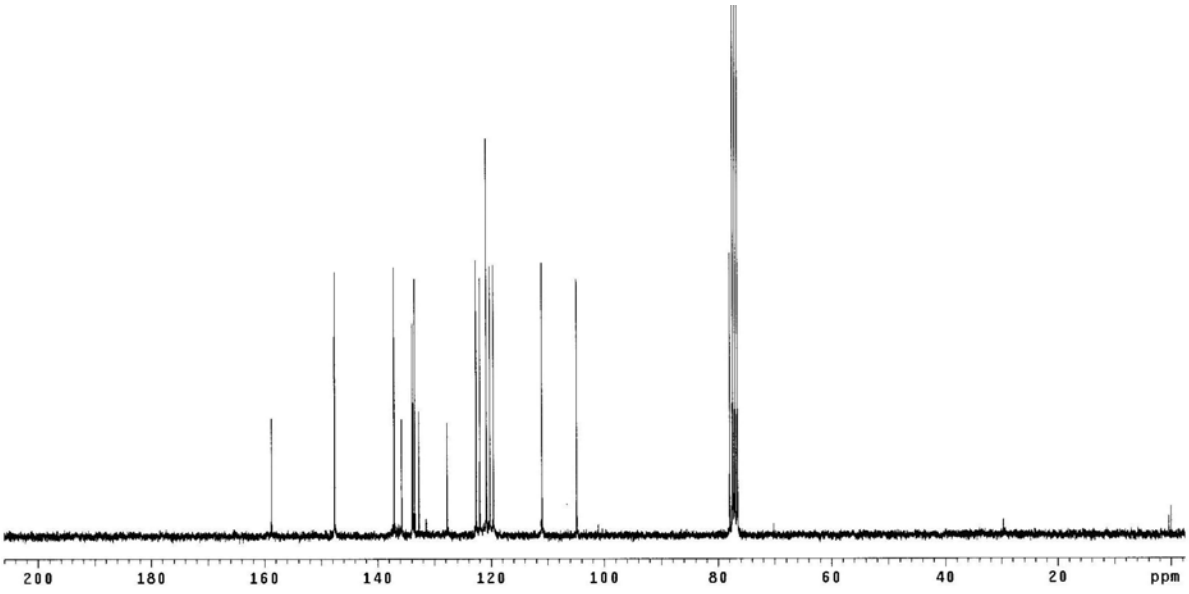
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1d** (120.0 mg, 0.932 mmol, 200 mol%) was coupled to pyridine-2-carboxaldehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (90.2 mg, 0.326 mmol) as an yellow solid in 72% yield after purification by flash column chromatography (R_f = 0.20, 45% EtOAc/hexanes).

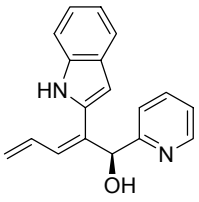
^{1}H NMR (400 MHz, $CDCl_3$): 9.40 (s, 1H), 8.44 (d, *J* = 4.8 Hz, 1H), 7.55 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.52 (t, *J* = 6.8 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.0 (m, 2H), 6.96 (m, 3H), 6.52 (d, *J* = 11.2 Hz, 1H), 6.45 (d, *J* = 1.0 Hz, 1H), 5.5 (s, 1H) 5.47 (d, *J* = 1.2 Hz, 1H), 5.43 (d, *J* = 1.2 Hz, 1H) 5.27 (dd, *J* = 10.4, 0.8., Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 158.8, 147.5, 137.0, 135.7, 133.8, 133.7, 133.2, 132.7, 127.7, 122.6, 122.0, 120.8, 120.1, 119.5, 111.0, 104.8, 77.8.
HRMS Calcd. for $C_{18}H_{16}N_2O$ (M): 276.1263, Found: 276.1261.
FTIR (NaCl Film): 3274, 3080, 3056, 2973, 2862, 1593, 1570, 1436, 1400, 1339, 1150, 1078, 1000, 913, 797, 749, 652 cm^{-1}.
MP 81 ^oC.



6

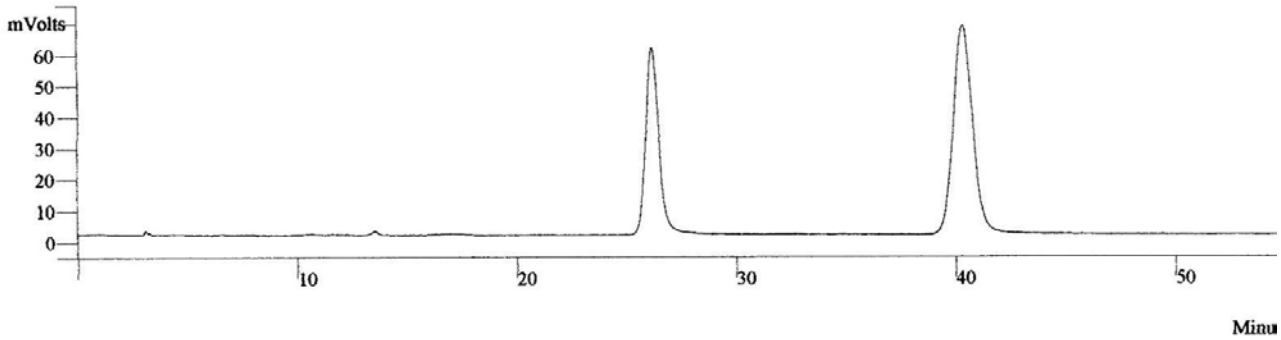




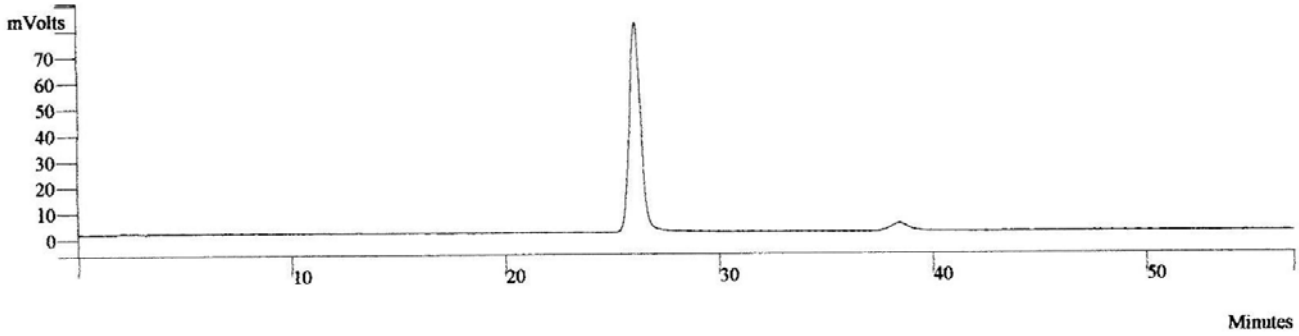


6

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 38.4 min, t_{major} = 26.0 min; ee = 90%.

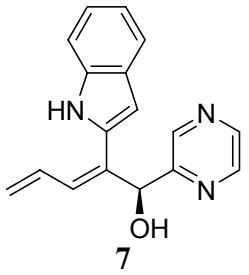


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		37.2739	26.175	0.000	2411647	0.00	BB	36.8		0
2		62.7261	40.347	0.000	4058421	0.00	BB	56.2		0
	Totals	**100.0000**		**0.000**	**6470068**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		94.9341	26.092	0.000	2982148	0.00	BB	33.2		0
2		5.0659	38.485	0.000	159134	0.00	BB	52.1		0
	Totals	**100.0000**		**0.000**	**3141282**					

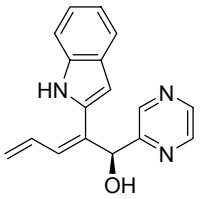
2-(1*H*-indol-2-yl)-1-pyrazin-2-yl-penta-2,4-dien-1-ol



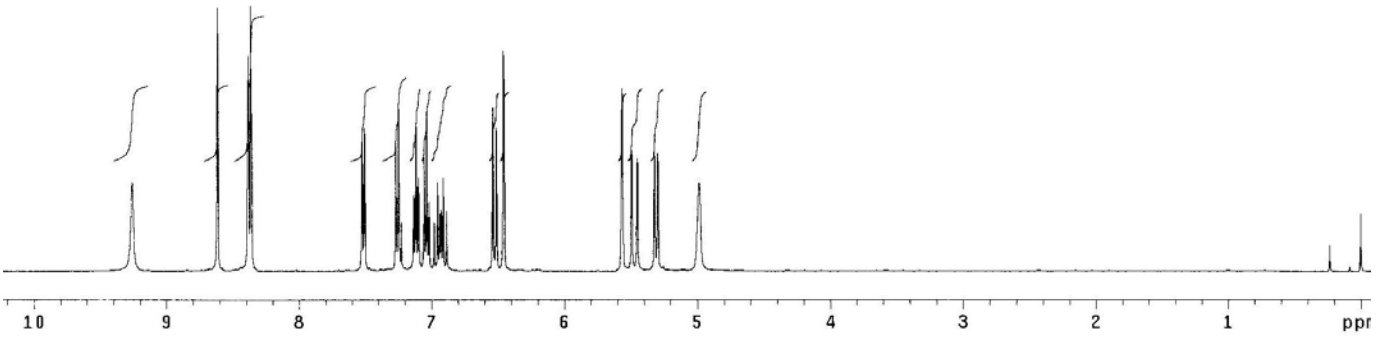
7

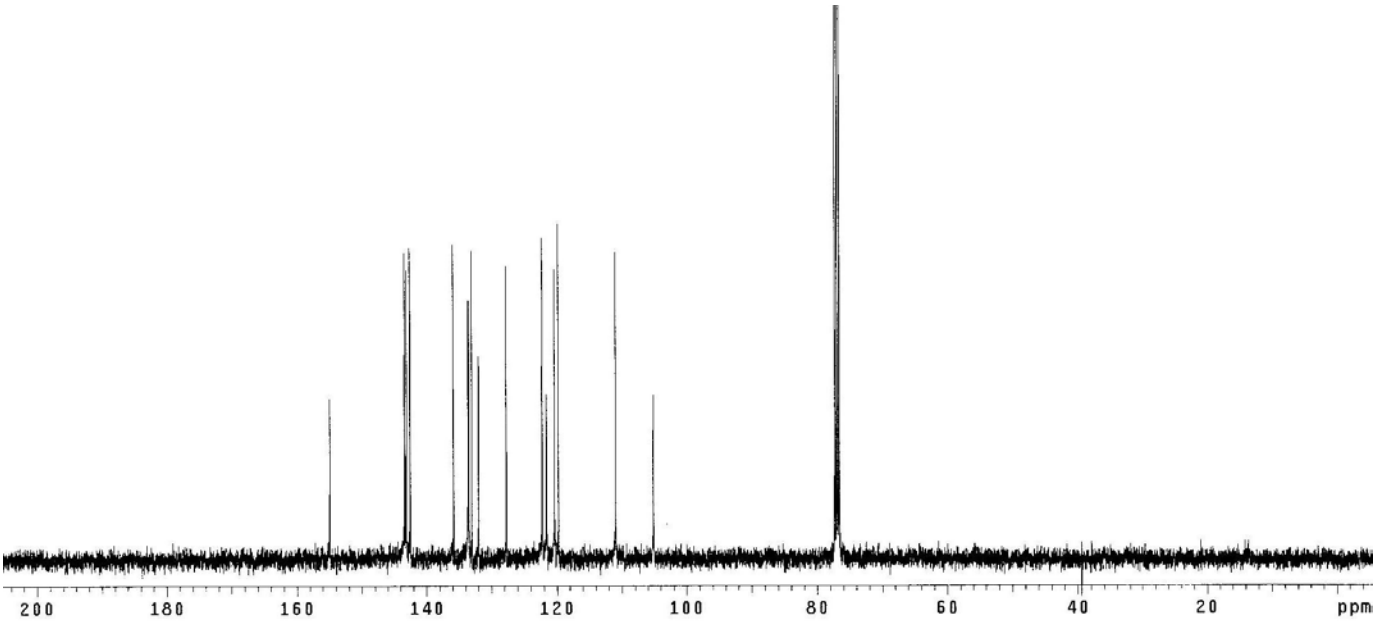
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1d** (154.0 mg, 0.925 mmol, 200 mol%) was coupled to pyrimidine-2-carbaxaldehyde (50.0 mg, 0.463 mmol, 100 mol%) to provide the title compound (120.0 mg, 0.433 mmol) as an yellow solid after purification by flash column chromatography (R_f = 0.25, 25% EtOAc/hexanes).

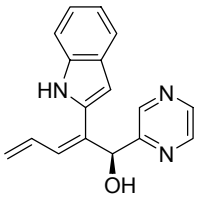
^{1}H NMR (400 MHz, $CDCl_3$): 9.30 (s, 1H), 8.60 (s, 1H), 8.34 (d, *J* = 9.2 Hz, 1H), 8.32 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 2H), 7.02 (d, *J* = 8 Hz, 1H), 6.91(dt, *J* = 17.2, 10.4 Hz, 1H), 6.50 (d, 10.8 Hz, 1H), 6.44 (s, 1H) 5.55 (s, 1H), 5.45 (d, *J* = 16.8 Hz, 1H), 5.30 (d, *J* = 10.0 Hz, 1H) 5.10 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 155.0, 143.2, 143.0, 142.5, 135.8, 133.4, 133.3, 133.0, 132.0, 127.7, 122.2, 121.5, 120.3, 119.7, 111.0, 105.0, 76.6.
HRMS Calcd. for $C_{17}H_{15}N_3O$ (M): 277.1215, Found: 277.1215.
FTIR (NaCl Film): 3400, 3082, 3056, 1454, 1403, 1339, 1265, 1150, 1084, 1001, 1020, 917, 1020, 917, 917, 824, 737, 657 cm^{-1}.
MP 68 ^oC.



7

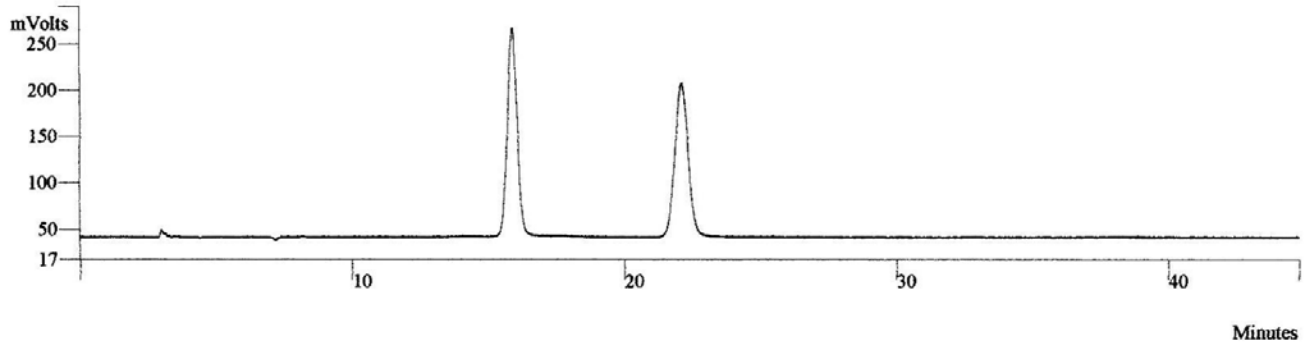




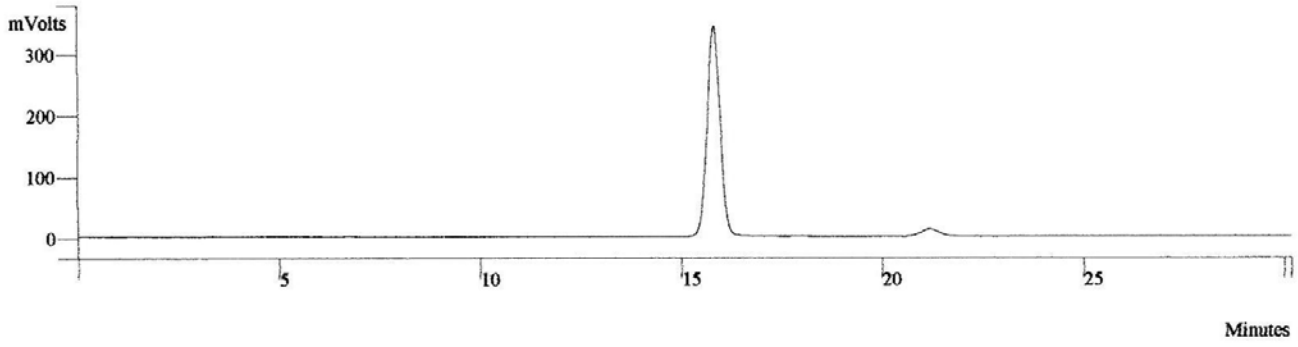


7

HPLC (Chiralcel AD-H column, 10% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm), t_{minor} = 21.2 min, t_{major} = 15.8 min; ee = 91%.

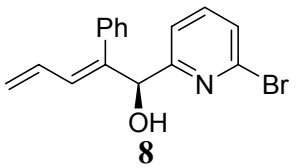


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.0611	15.890	0.000	5473537	0.00	BB	22.8		0
2		49.9388	22.119	0.000	5460165	0.00	BB	31.1		0
	Totals	**99.9999**		**0.000**	**10933702**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		95.6320	15.812	0.000	7644255	0.00	BB	20.7		0
2		4.3680	21.200	0.000	349151	0.00	BB	28.6		0
	Totals	**100.0000**		**0.000**	**7993406**					

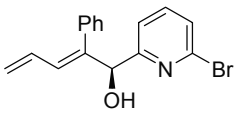
1-(6-Bromo-pyridin-2-yl)-2-phenyl-penta-2,4-dien-1-ol



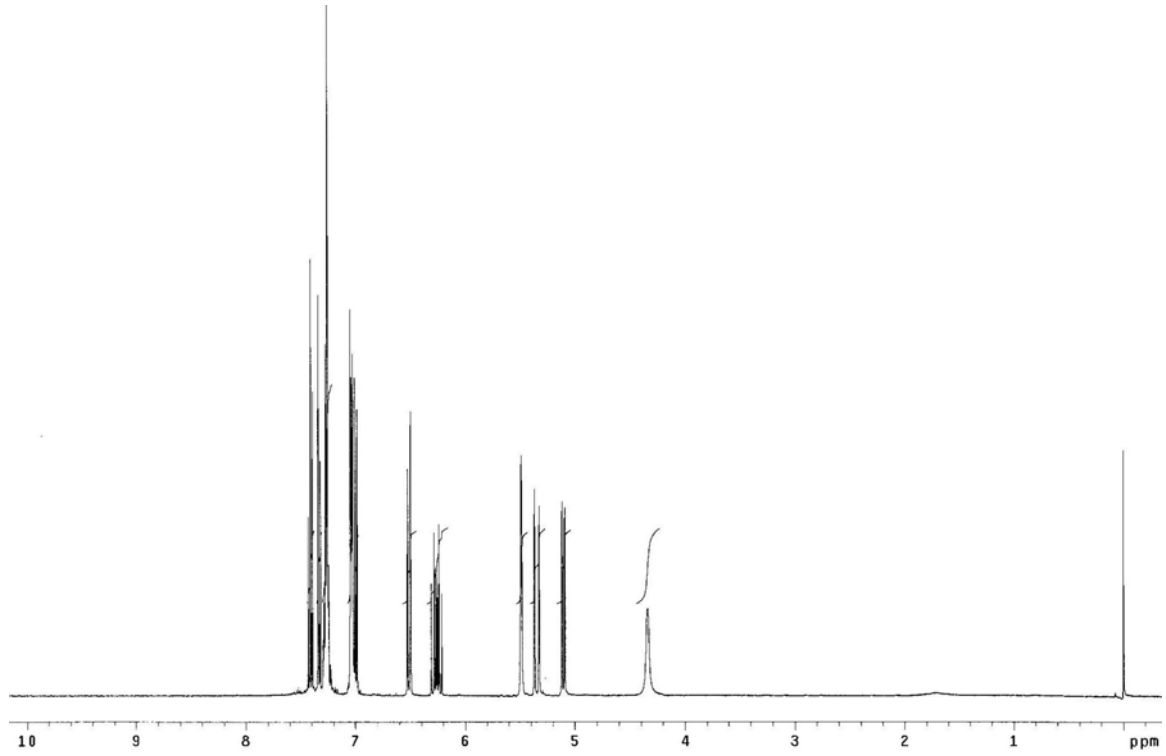
8

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1a** (274.0 mg, 2.14 mmol, 200 mol%) was coupled to 6-bromopyridine-2-carbaxaldehyde (200.0 mg, 1.070 mmol, 100 mol%) to provide the title compound (244.0 mg, 0.774 mmol) as a colorless oil in 71% yield after purification by flash column chromatography (R_f = 0.25, 10% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 7.40 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.25 (m, 3H), 7.03 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.21 (d, *J* = 11.2 Hz, 1H), 6.26 (dt, *J* = 16.8, 10.8 Hz, 1H), 5.49 (d, *J* = 5.2 Hz, 1H), 5.34 (d, *J* = 16.8 Hz, 1H) 5.10 (dd, *J* = 10.0, 0.8 Hz 1H), 4.35 (d, *J* = 5.6 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 161.0, 143.0, 140.6, 138.6, 137.0, 130.0, 129.5, 128.0, 127.4, 126.7, 120.0, 119.4, 76.8.
HRMS: Calcd. for $C_{16}H_{14}NOBr$ (M): 315.0259, Found: 315.0257.
FTIR (NaCl Film): 3413, 3079, 3051, 1580, 1553, 1434, 1407, 1158, 1123, 1072, 994, 915, 808, 705, 670 cm^{-1}.


Ph
N
Br
OH

8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9
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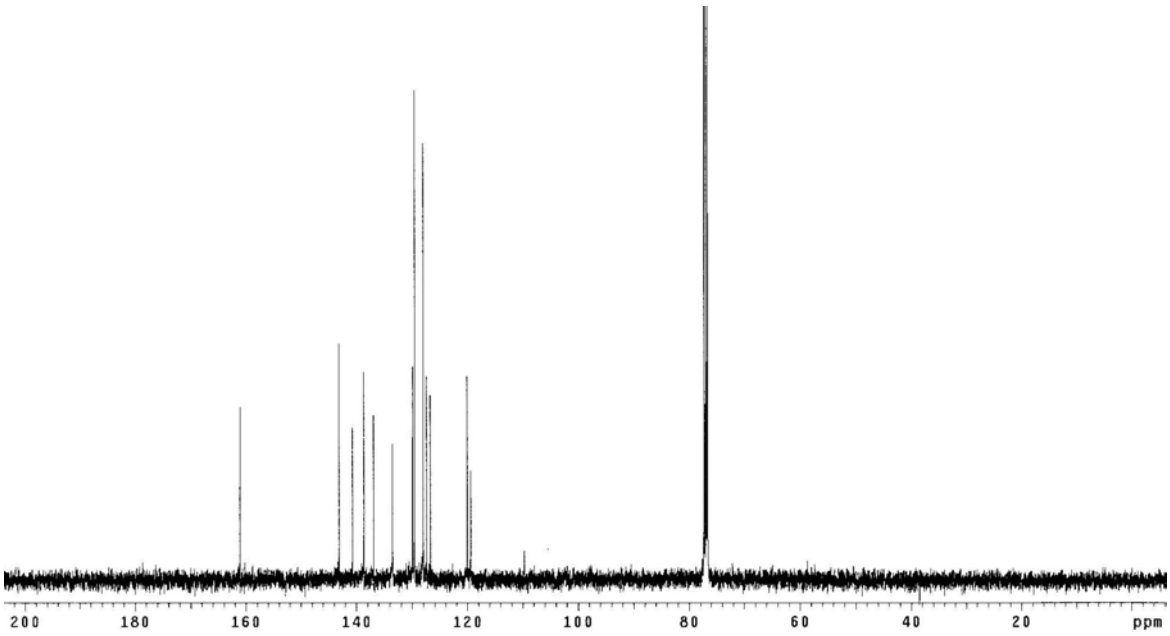
6
5
4
3
2
1
ppm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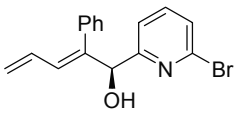
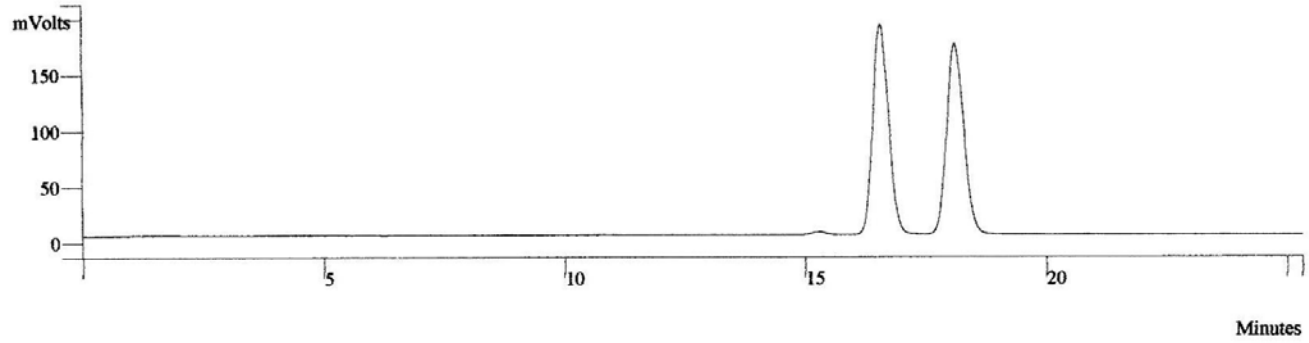
100
80
60
40
20
ppm

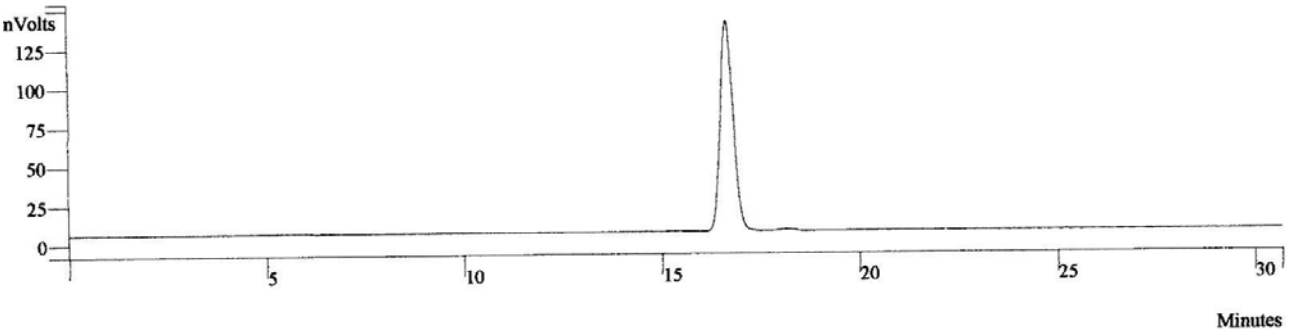


8

HPLC (Chiralcel OD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 18.1 min, t_{major} = 16.6 min; ee = 99%.

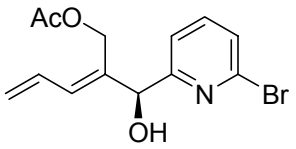


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.7002	16.564	0.000	4120798	0.00	BB	21.1		0
2		49.2998	18.126	0.000	4006982	0.00	BB	22.9		0
	Totals	**100.0000**		**0.000**	**8127780**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		99.4680	16.660	0.000	3049137	0.00	BB	21.3		0
2		0.5320	18.137	0.000	16307	0.00	BB	17.8		0
	Totals	**100.0000**		**0.000**	**3065444**					

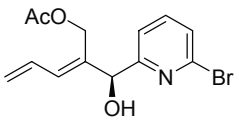
1-(6-Bromo-pyridin-2-yl)-2-phenyl-penta-2,4-dien-1-ol



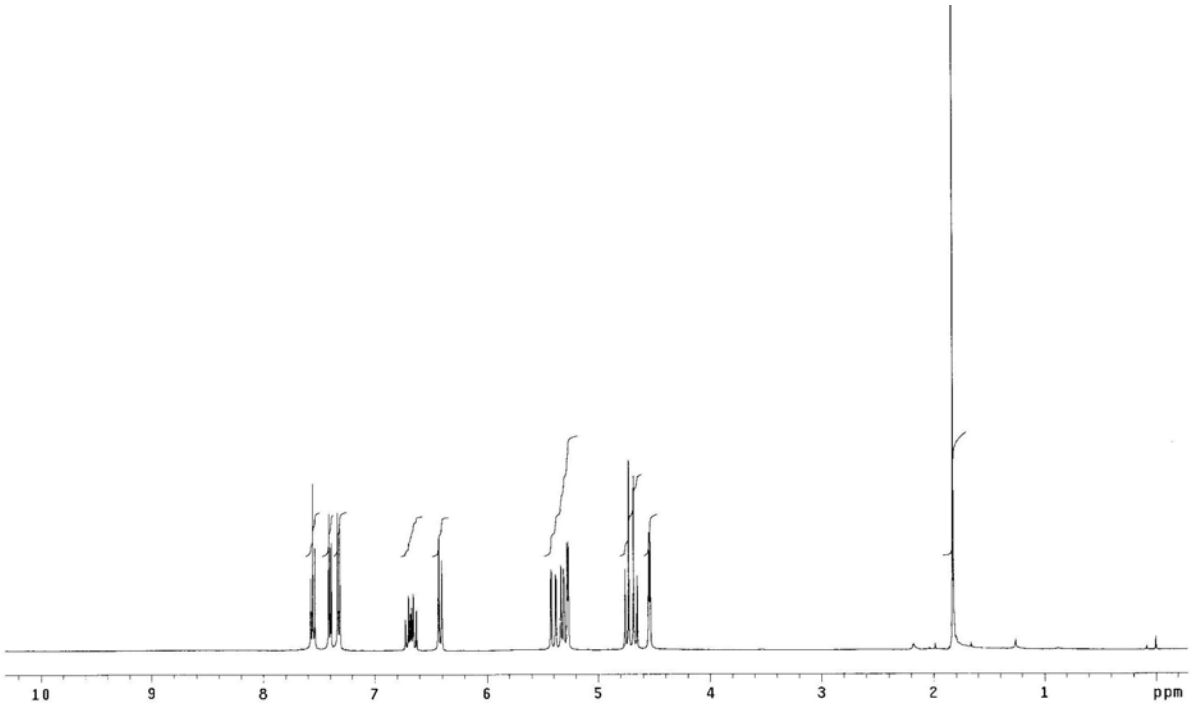
9

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1b** (130.0mg, 1.075 mmol, 200 mol%) was coupled to 6-bromopyridine-2-carbaxaldehyde (100.0 mg, 0.537 mmol, 100 mol%) to provide the title compound (124.0 mg, 0.397 mmol) as a colorless oil in 75% yield after purification by flash column chromatography (R_f = 0.24, 15% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 7.55 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0, Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 6.67 (dt, *J* = 16.4, 10.4 Hz, 1H), 5.41 (d, *J* = 10.8 Hz, 1H), 5.54 (m, 2H) 5.27 (d, *J* = 4.4 Hz 1H), 4.70 (q, *J* = 12.8 Hz, 2H), 4.54 (d, *J* = 4.8 Hz, 1H), 1.82 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.5, 161.5, 140.6, 138.8, 135.5, 133.8, 131.2, 126.6, 121.5, 119.7, 75.8, 58.6, 20.4.
HRMS: Calcd. for $C_{13}H_{14}NO_3Br$ (M) 311.0157, Found: 311.0157.
FTIR (NaCl Film): 3436, 2927, 1738, 1581, 1556, 1434, 1404, 1234, 1157, 1123, 1028, 986, 790, 742, 704 cm^{-1}.


AcO
N
Br
OH

9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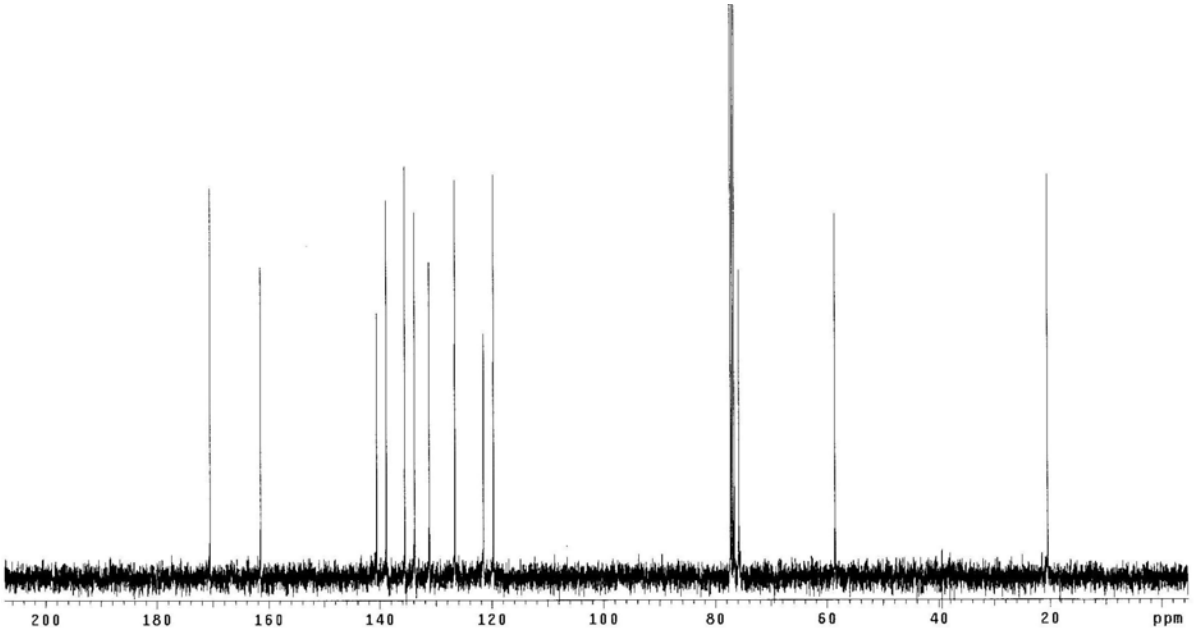
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100
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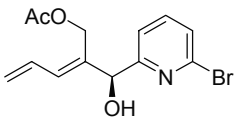
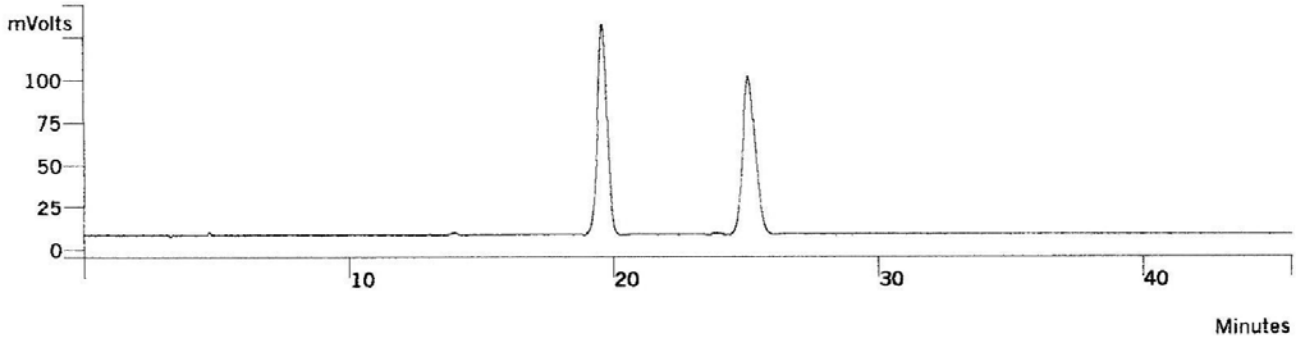
ppm

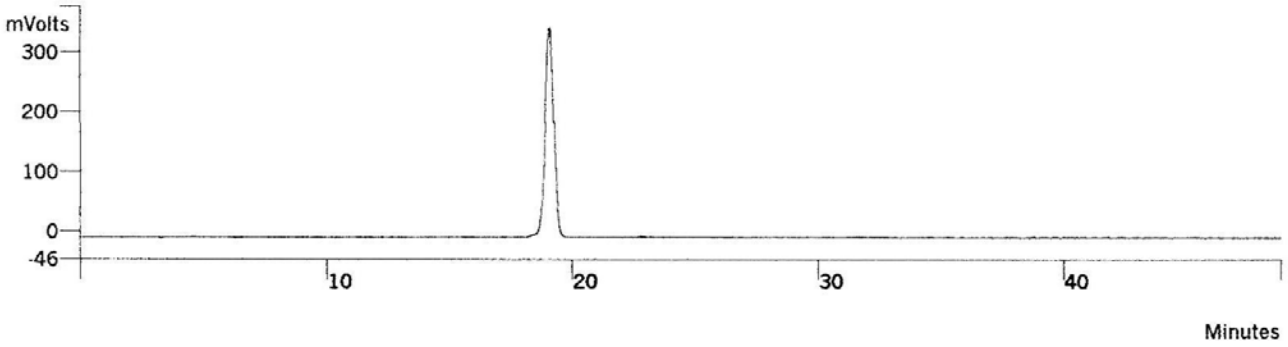


9

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 1 mL/min, 254 nm): t_{minor} = 22.6 min, t_{major} = 19.0 min; ee = > 99%.

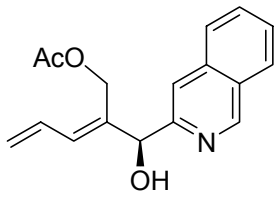


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.3470	19.562	0.000	3095687	0.00	BB	23.2		0
2		49.6530	25.079	0.000	3053010	0.00	BB	30.5		0
	Totals	**100.0000**		**0.000**	**6148697**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		99.7894	19.075	0.000	8642749	0.00	BB	22.7		0
2		0.2106	22.670	0.000	18240	0.00	BB	0.5		0
	Totals	**100.0000**		**0.000**	**8660989**					

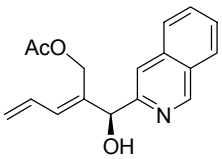
Acetic acid 2-(hydroxyl-isoquinolin-3-yl-methyl)-penta-2,4-dienyl ester



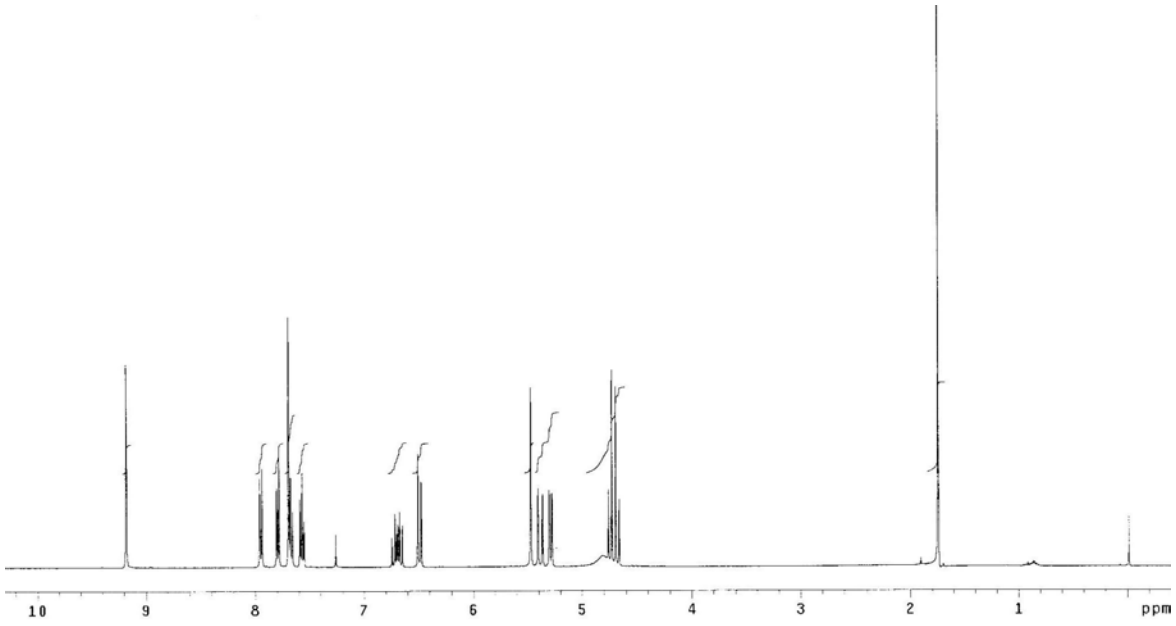
10

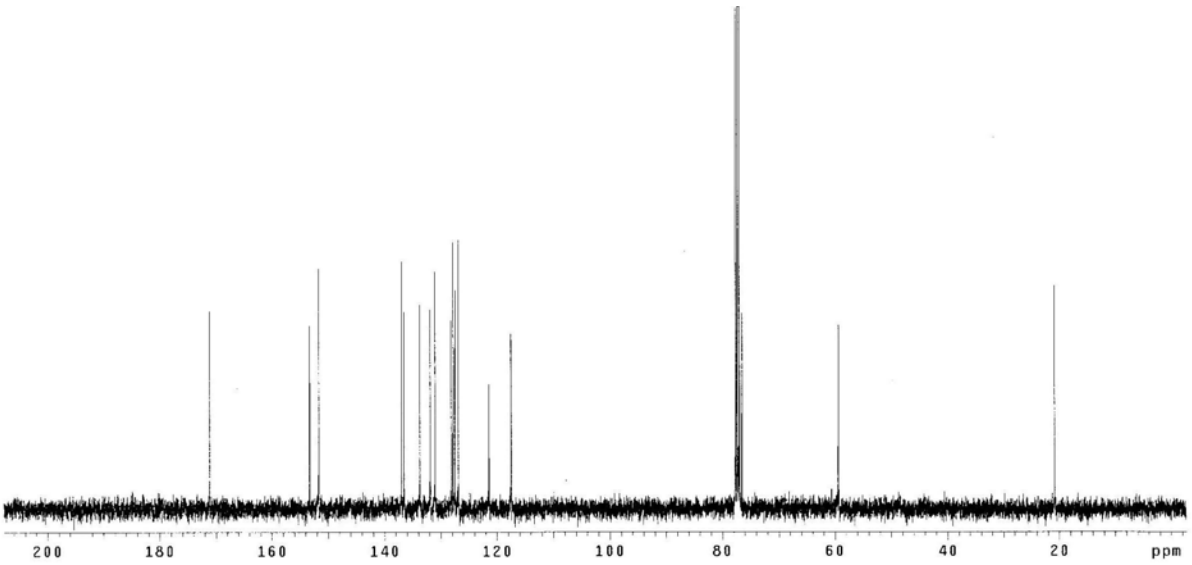
In accordance with the general procedure employing (*R*)- *tol*-BINAP as ligand, enyne **1b** (116.0 mg, 0.932 mmol, 200 mol%) was coupled to isoquinoline-2-carboxladehyde (50.0 mg, 0.466 mmol, 100 mol%) to provide the title compound (90.0 mg, 0.318 mmol) as an yellow solid in 96% yield after purification by flash column chromatography (R_f = 0.23, 30% EtOAc/hexanes).

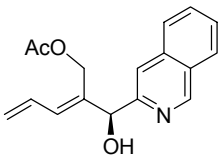
^{1}H NMR (400 MHz, $CDCl_3$): 9.20 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 4.0 Hz, 1H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 6.70 (dt, *J* = 16.8, 10.4 Hz, 1H), 6.49 (d, *J* = 11.2 Hz, 1H), 5.47 (s, 1H) 5.62 (s, 1H), 5.40 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.30 (d, *J* = 10.0 Hz, 1H), 4.71 (q, *J* = 12.4 Hz, 2H), 1.75 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.8, 153.0, 151.3, 136.7, 136.2, 133.4, 131.6, 130.7, 127.9, 127.5, 127.2, 126.6, 121.2, 117.2, 76.2, 59.0, 20.5.
HRMS Calcd. for $C_{17}17_2NO_3$ (M): 283.1208, Found: 283.1207.
FTIR (NaCl Film):3366, 3059, 2923, 1732, 1734, 1629, 1591, 1363, 1232, 1025, 962, 751, 667 cm^{-1}
MP 78 ^oC.



10

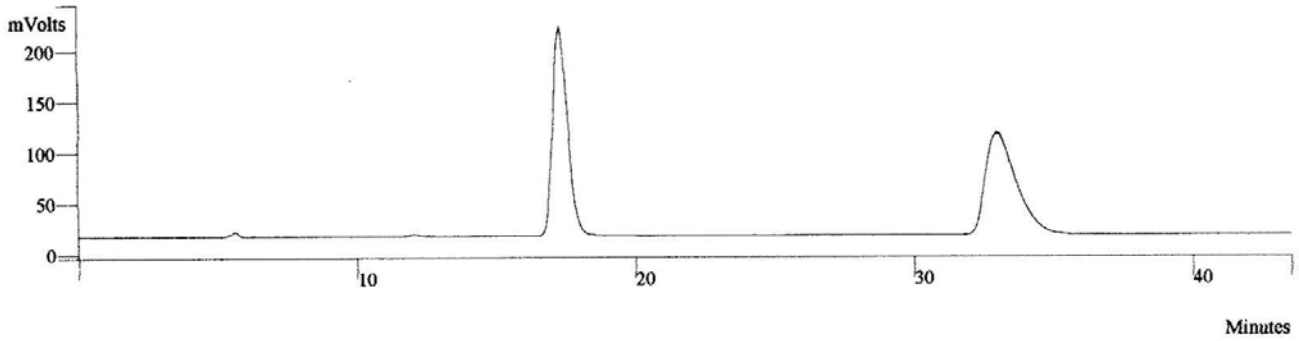




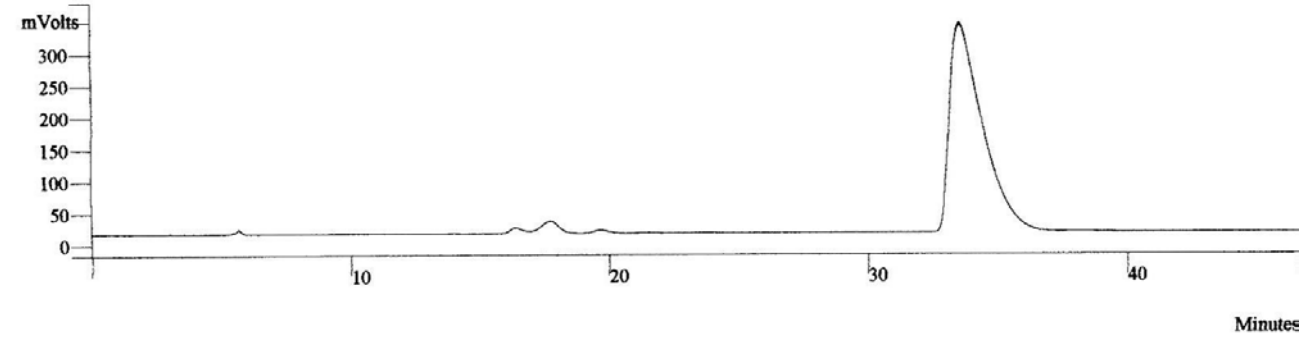


10

HPLC (Chiralcel OD-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 17.7 min, t_{major} = 33.5 min; ee = 95%.

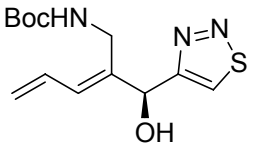


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.9765	17.281	0.000	7596762	0.00	BB	34.3		0
2		50.0235	32.938	0.000	7603896	0.00	BB	69.6		0
	Totals	**100.0000**		**0.000**	**15200658**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		2.4236	17.710	0.000	714057	0.00	BB	38.5		0
2		97.5764	33.582	0.000	28748082	0.00	BB	79.3		0
	Totals	**100.0000**		**0.000**	**29462140**					

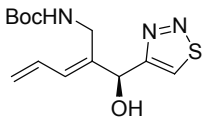
[2-(Hydroxy-[1,2,3]thiadiazol-4-yl-methyl)-penta-2,4-dienyl]-carbamic acid *tert*- butyl ester



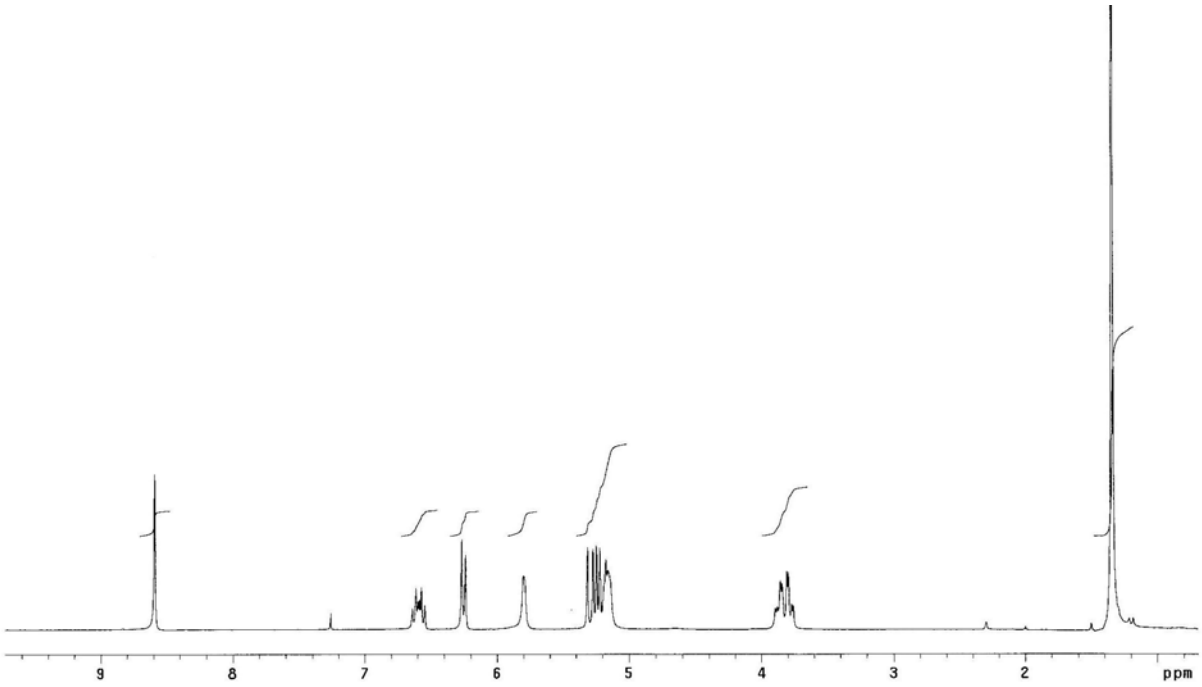
11

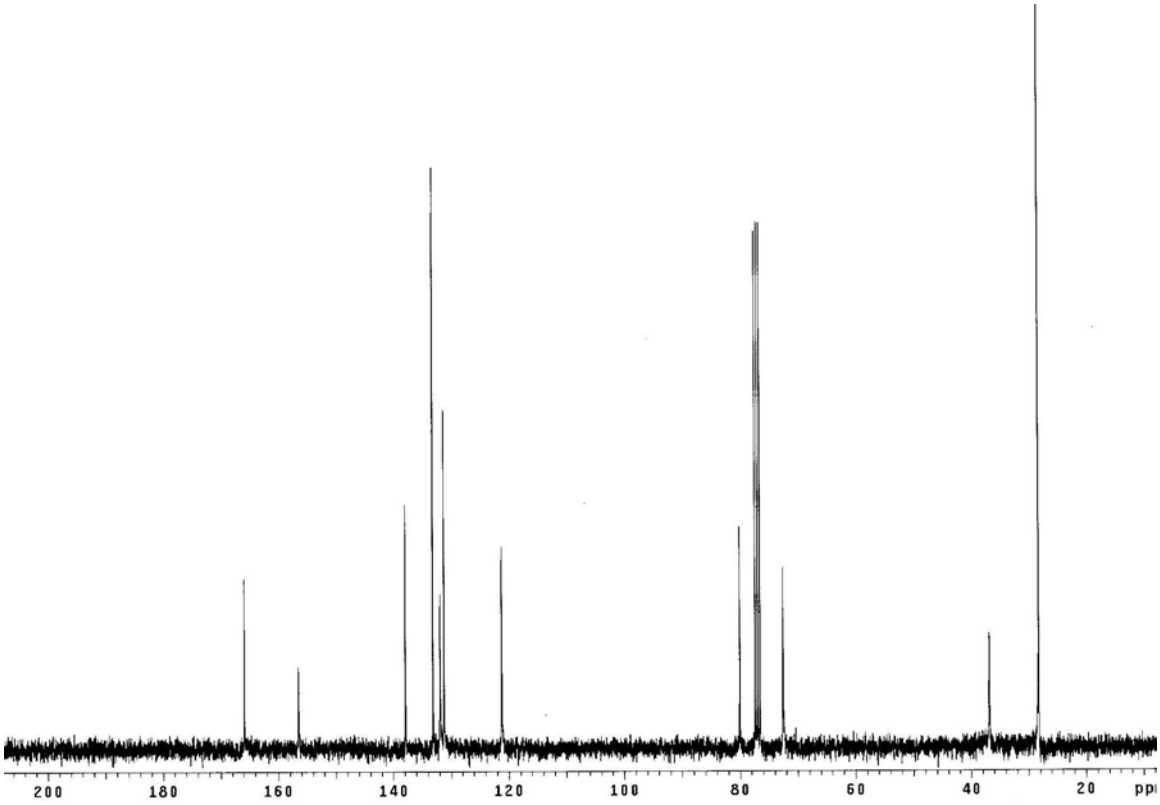
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1c** (158.0 mg, 0.876 mmol, 200 mol%) was coupled to 1,2,3-thiadiazole-4-carboxaldehyde (50.0 mg, 0.438 mmol, 100 mol%) to provide the title compound (90.0 mg, 0 303 mmol) as an yellow syrup in 71% yield after purification by flash column chromatography (R_f = 0.30, 25% EtOAc/hexanes).

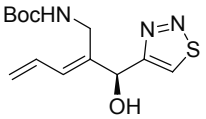
^{1}H NMR (400 MHz, $CDCl_3$): 8.60 (s, 1H), 6.60 (dt, *J* = 16.8, 10.4 Hz, 1H), 6.25 (d, *J* = 11.2 Hz, 1H), 5.80 (s, 1H), 5.30 (d, *J* = 16.8 Hz, 1H), 5.23 (d, *J* = 10.0, 1H), 5.16 (d, *J* = 6.4 Hz, 1H), 3.86 (dd, *J* = 15.2, 6.0, 1H), 3.78 (dd, *J* = 15.2, 5.6 Hz, 1H), 1.30 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$): 166.0, 156.5, 138.0, 133.1, 131.8, 121.2, 80.0, 72.5, 36.7, 28.2.
HRMS Calcd. for $C_{13}H_{19}N_3O_3S$ (M): 297.1147, Found: 297.1138.
FTIR (NaCl Film): 3361, 2977, 2931, 1690, 1682, 1515, 1367, 1251, 1166, 1046 cm^{-1}.



11

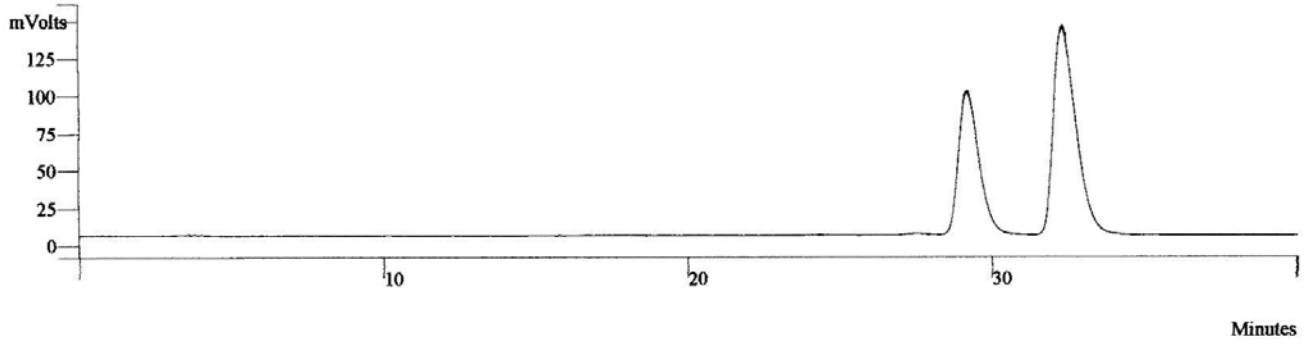




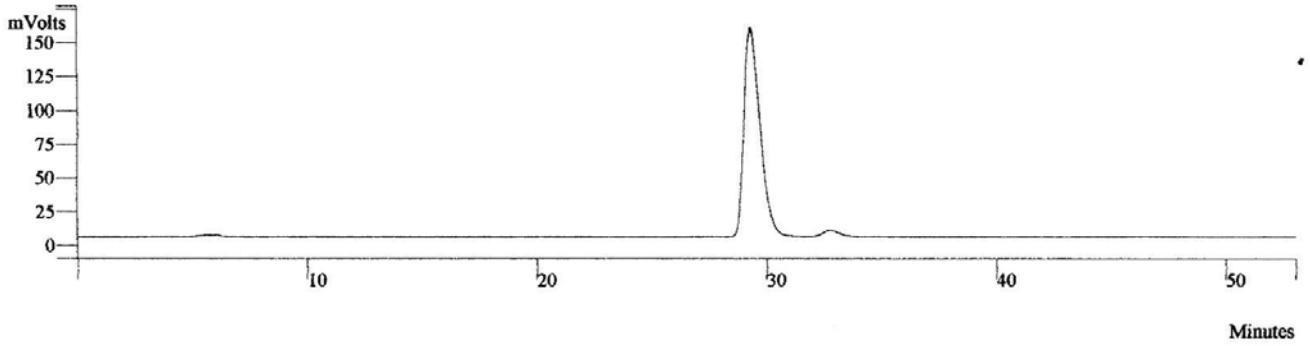


11

HPLC (Chiralcel OJ-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 32.7 min, t_{major} = 29.2 min; ee = 94%.

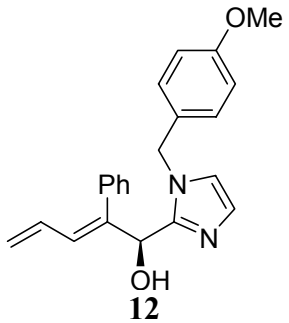


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		38.5643	29.214	0.000	4449225	0.00	BB	42.8		0
2		61.4357	32.328	0.000	7087926	0.00	BB	46.9		0
	Totals	**100.0000**		**0.000**	**11537151**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		97.0671	29.281	0.000	7519922	0.00	BB	45.0		0
2		2.9329	32.745	0.000	227218	0.00	BB	43.3		0
	Totals	**100.0000**		**0.000**	**7747140**					

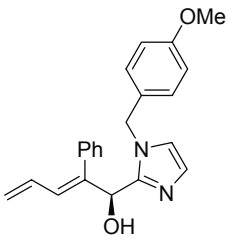
1-[1-(4-Methoxy-benzyl)-1*H*-imidazol-2-yl]-2-phenyl-penta-2,4-dien-1-ol



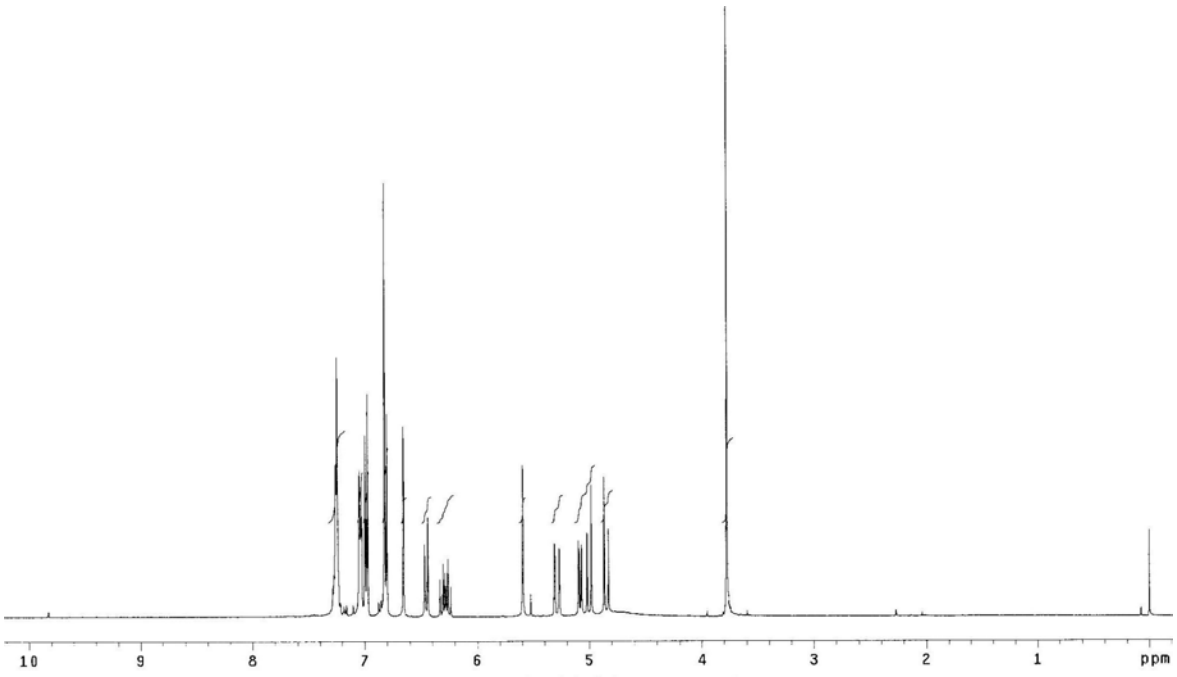
12

In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1a** (38.0 mg, 0.015 mmol, 200 mol%) was coupled to *N*-4-methoxybenzyl-2-imidazole carboxaldehyde (32.0 mg, 0.015 mmol, 100 mol%) to provide the title compound (37.0 mg, 0.106 mmol) as a white solid in 72% yield after purification by flash column chromatography (R_f = 0.18, 2% MeOH/ether).

^{1}H NMR (400 MHz, $CDCl_3$): 7.25 (m, 3H), 7.04 (dd, *J* = 7.2, 2.4 Hz, 3H), 7.0 (d, *J* = 8.8 Hz, 2H), 7.03 (dd, *J* = 7.6, 2.0 Hz, 3H), 7.05 (d, *J* = 8.8 Hz, 2H), 6.81 (dd, *J* = 4.8, 2.8 Hz, 3H), 6.63 (d, *J* = 1.2 Hz, 1H), 6.47 (d, *J* = 11.2 Hz, 1H), 6.29 (dt, *J* = 16.8 , 10.0 Hz, 1H) 5.62 (s, 1H), 5.28 (dd, *J* = 16.4, 1.6 Hz, 1H), 5.07 (dd, *J* = 10.0, 2.0, 1H), 5.02 (d, *J* = 14.8 Hz, 1H), 4.85 (d, *J* = 15.2 Hz, 1H), 3.85 (s, 3H).
^{13}C NMR(100 MHz, $CDCl_3$): 159.28, 147.5, 142.3, 135.7, 137.3, 133.5, 129.1, 129.0, 128.6, 128.0, 127.3, 126.8, 120.3, 119.1, 114.1, 70.7, 55.2, 49.0.
HRMS Calcd. for $C_{22}H_{22}N_2O_2$ (M): 346.1681, Found: 346.1687.
FTIR (NaCl Film): 3418, 3084, 2400, 1529, 1250, 1031, 7021 cm^{-1}.
MP 146 ^oC.


OMe
Ph
N
N
OH

12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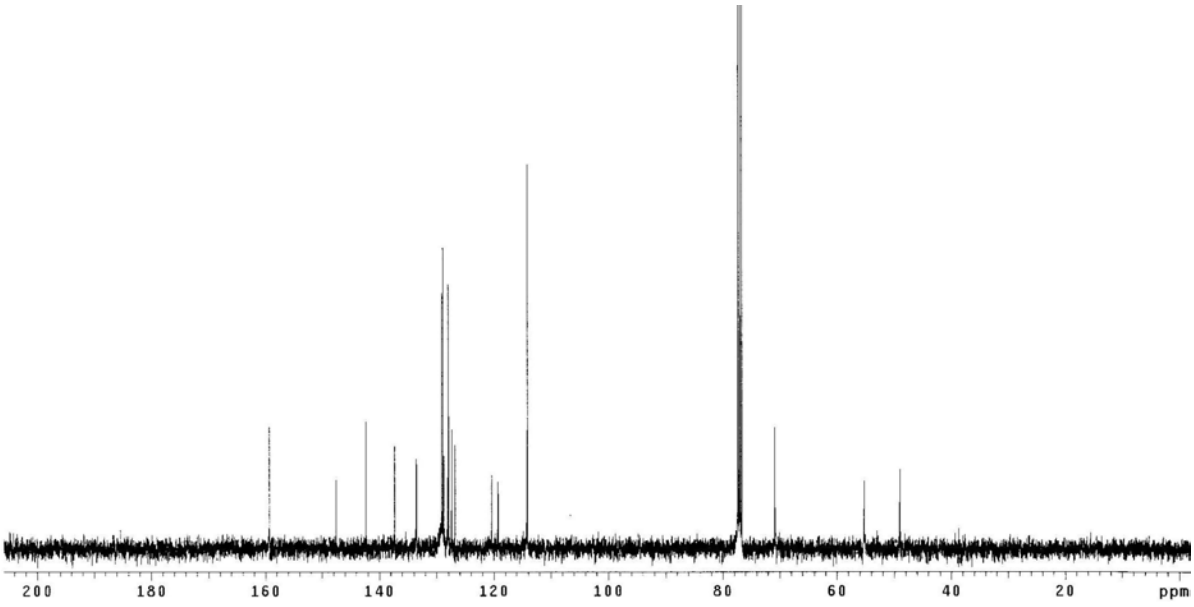
3
2
1
ppm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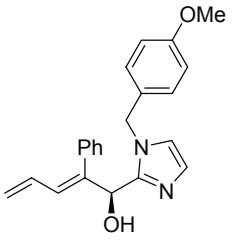
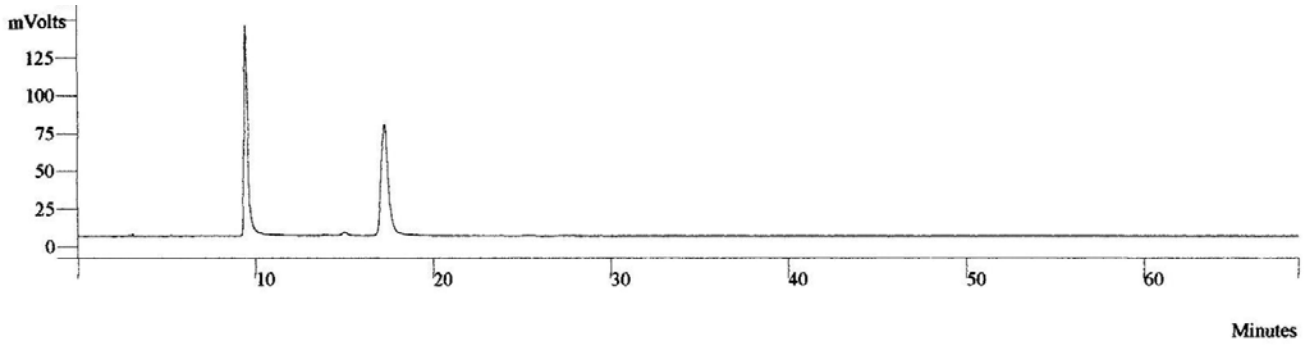
140
120
100
80
60
40
20
ppm

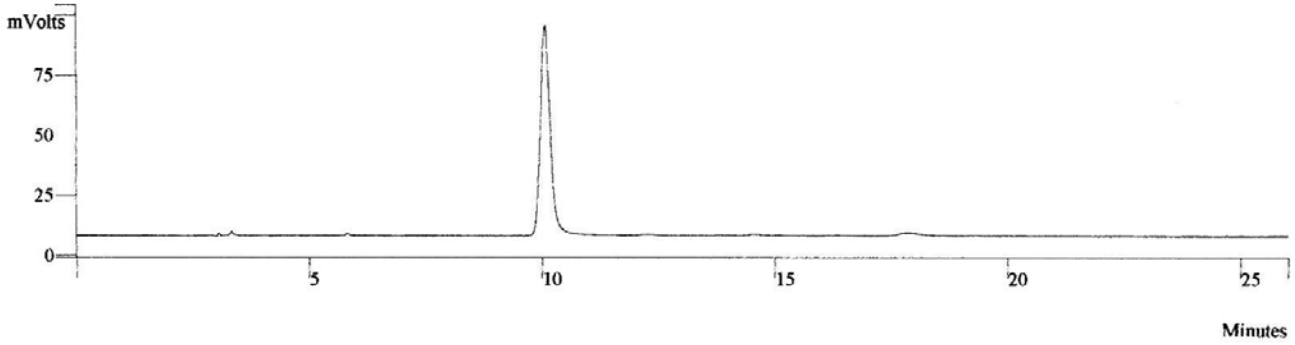


12

HPLC (Chiralcel AD-H column, 10% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm), t_{minor} = 17.1 min, t_{major} = 9.8 min; ee = 95%.

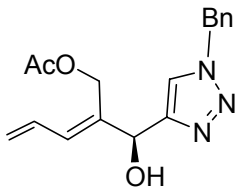


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.9734	9.462	0.000	1984939	0.00	BB	12.5		0
2		50.0266	17.251	0.000	1987051	0.00	BB	25.2		0
	Totals	**100.0000**		**0.000**	**3971990**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		97.3216	10.065	0.000	1300550	0.00	BB	13.2		0
2		2.6784	17.847	0.000	35793	0.00	BB	24.9		0
	Totals	**100.0000**		**0.000**	**1336343**					

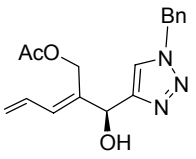
1-(Benzyl-1*H*-[1,2,3]-triazol-4-yl)-penta-2,4-dien-1-ol



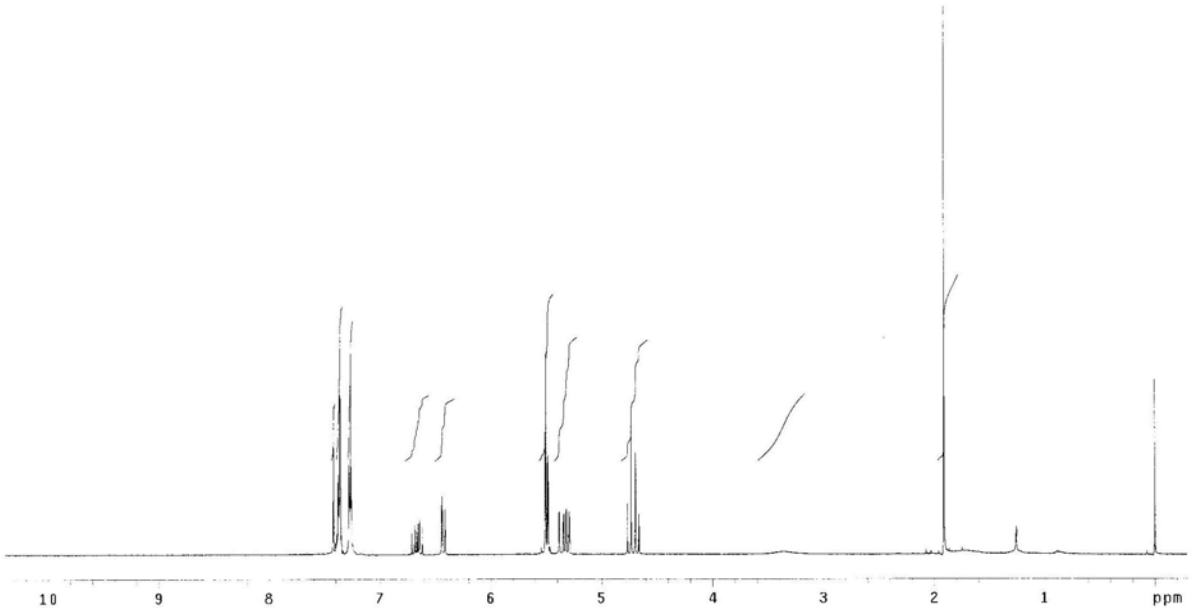
13

In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1b** (66.0 mg, 0.534 mmol, 200 mol%) was coupled to *N*-benzyltriazene-4-carboxaldehyde (50.0 mg, 0.267 mmol, 100 mol%) to provide the title compound (56.0 mg, 0.179 mmol) as a colorless syrup in 68% yield after purification by flash column chromatography (R_f = 0.30, 50% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 7.42 (s, 1H), 7.36 (m, 3H), 7.27 (m, 2H), 6.66 (ddd, *J* = 16.8, 10.8, 10.0 Hz, 1H), 6.42 (d, *J* = 11.2 Hz, 1H), 5.50 (s, 2H), 5.48 (s, 1H), 5.33 (m, 2H), 4.71 (q, *J* = 12.4 Hz, 2H), 3.39 (s, 1H), 3.98 (dd, *J* = 15.2, 5.6 Hz, 1H) 1.91 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 149.7, 135.3, 134.4, 133.1, 131.4, 129.1, 128.8, 128.1, 121.6, 121.2, 70.2, 59.6, 54.2, 20.7.
HRMS Calcd. for $C_{18}H_{23}N_2O_4$ (M): 13.1658, Found: 313.1659.
FTIR (NaCl Film): 3368, 3142, 2925, 1731, 1455, 1367, 1239, 1047, 724 cm^{-1}.


Bn
AcO
N
N
N
OH

13


10
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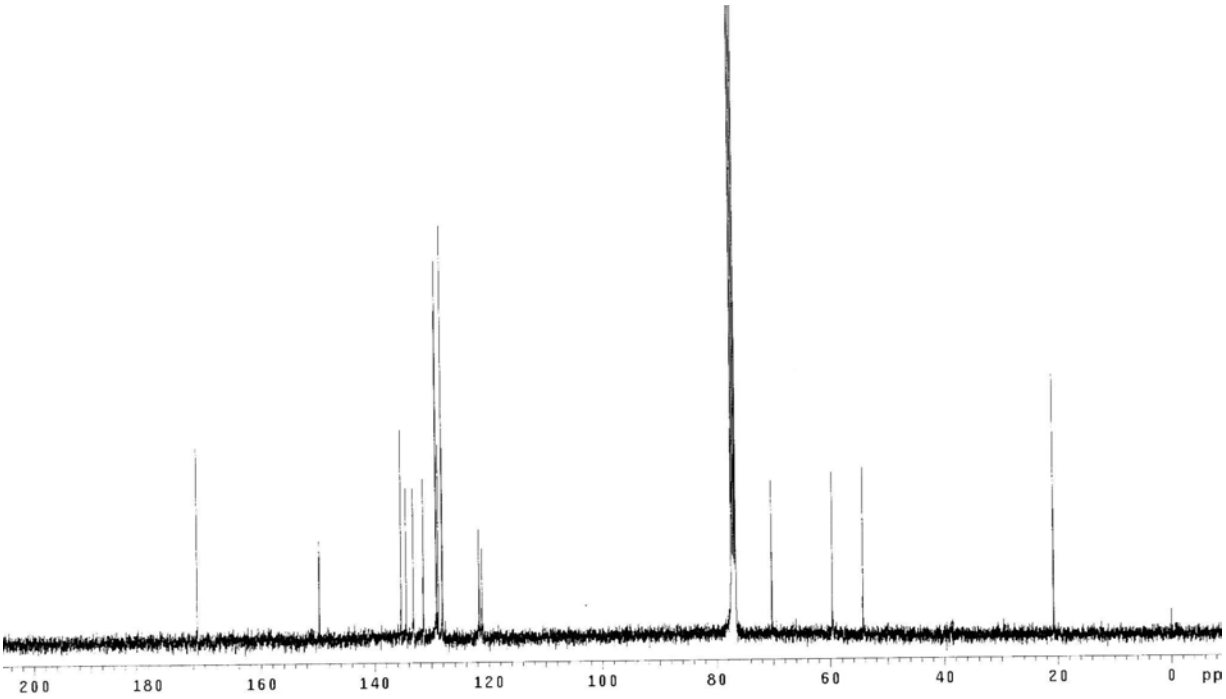
ppm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80
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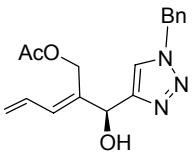
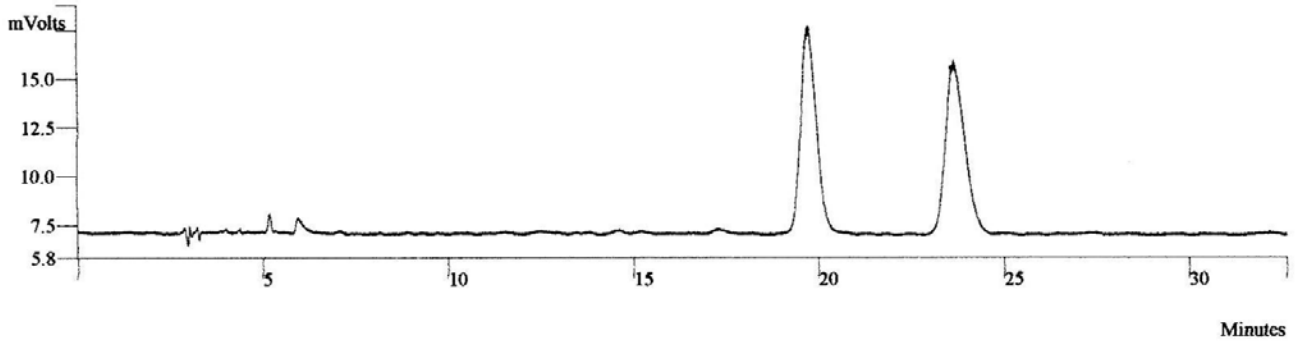
40
20
0
pp

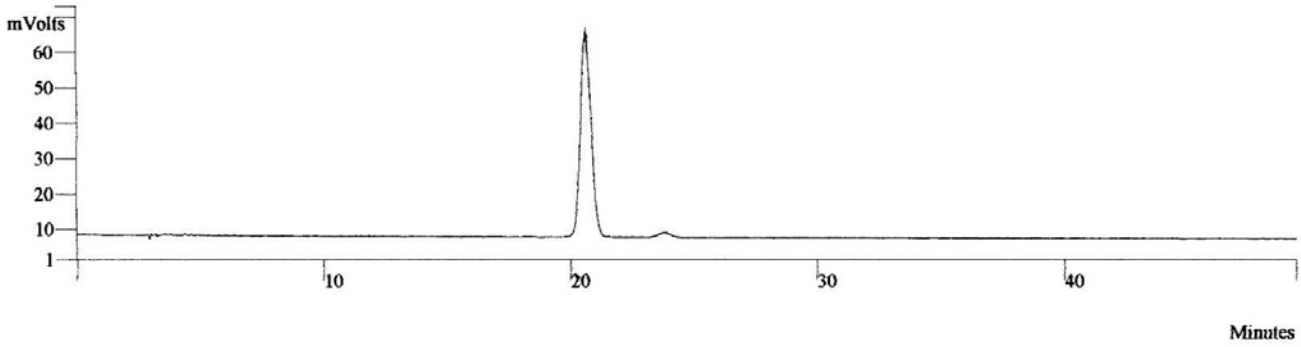


13

HPLC (Chiralcel AD-H column, 10% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 23.8 min, t_{major} = 20.6 min; ee = 95%.

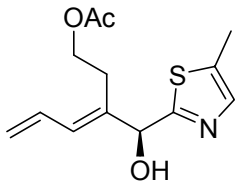


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.5678	19.719	0.000	306055	0.00	BB	26.7		0
2		50.4322	23.658	0.000	311393	0.00	BB	32.3		0
	Totals	**100.0000**		**0.000**	**617448**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		97.5129	20.611	0.000	1754134	0.00	BB	27.4		0
2		2.4871	23.876	0.000	44740	0.00	BB	27.6		0
	Totals	**100.0000**		**0.000**	**1798874**					

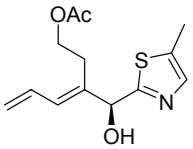
Acetic acid 3-[hydroxy-(5-methyl-thiazol-2-yl)-methyl]-hexa-3,5-dienyl ester



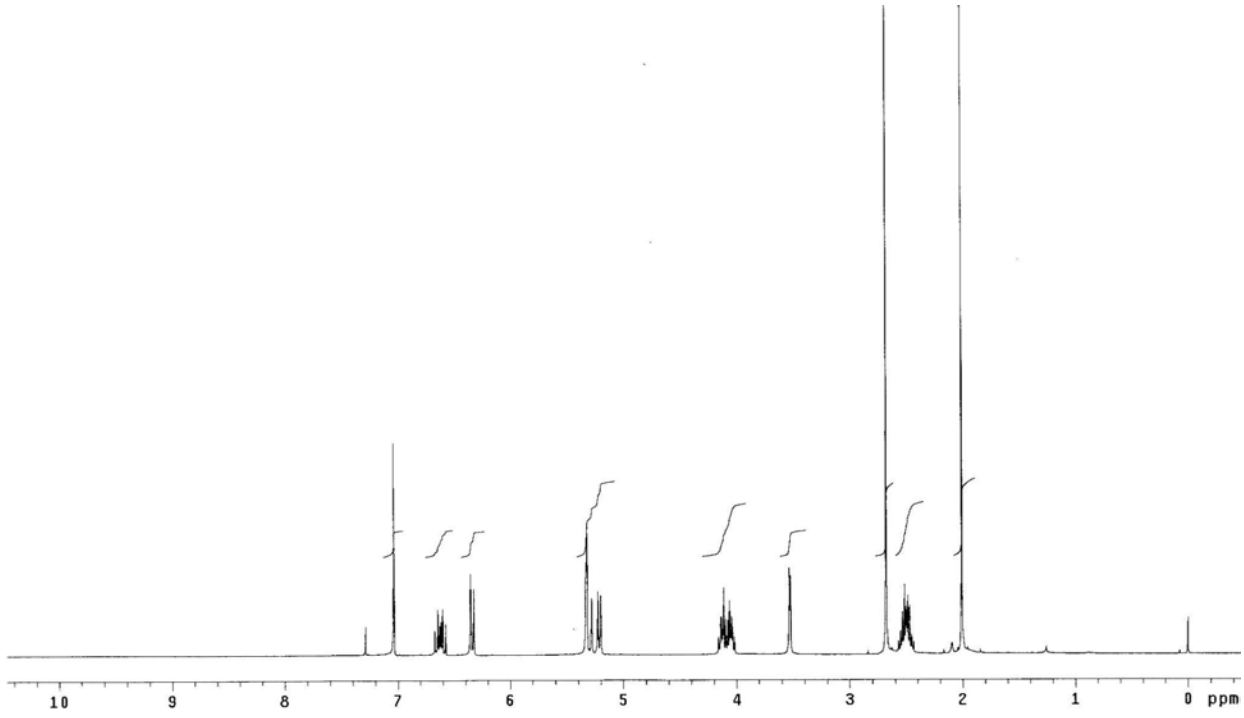
14

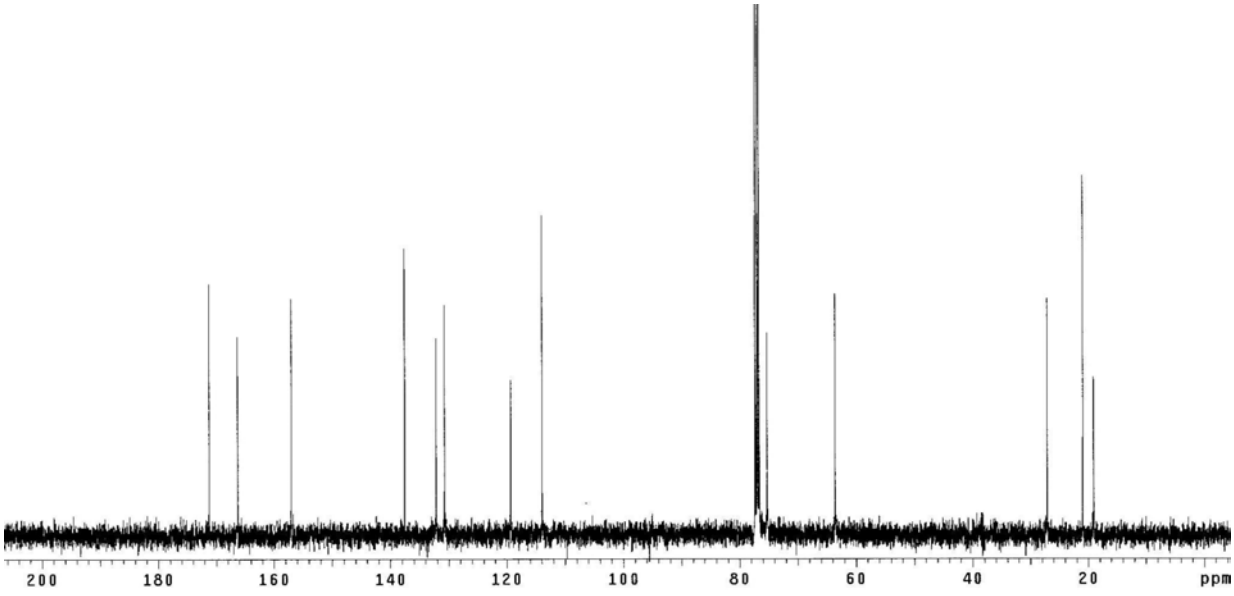
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1e** (130.0 mg, 0.943 mmol, 200 mol%) was coupled to 5-Methyl-2-thiazocarbaldehyde (60.0 mg, 0.471 mmol, 100 mol%) to provide the title compound (89.0 mg, 0.333 mmol) as a colorless oil in 71% yield after purification by flash column chromatography (R_f = 0.30, 30% EtOAc/hexanes).

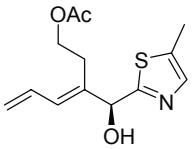
^{1}H NMR (400 MHz, $CDCl_3$): 7.0 (s, 1H), 6.42 (dt, *J* = 17.2, 10.4 Hz, 1H), 6.33 (d, *J* = 10.3 Hz, 1H), 5.32 (s, 1H), 5.28 (d, *J* = 2.0 Hz, 1H), 5.22 (dd, *J* = 10.4, 2.0 Hz, 1H), 4.14 (ddd, *J* = 14.4, 10.4, 7.2 Hz, 1H), 4.05 (ddd, *J* = 17.2, 10.8, 7.6 Hz, 1H), 2.68 (s, 1H) 2.51 (m, 2H), 2.10 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 171.3, 166.3, 157, 137.5, 132.1, 130.8, 119.3, 113.0, 75.3, 63.6, 27.1, 21.0, 19.1.
HRMS Calcd. for $C_{13}H_{17}NO_3S$ (M): 267.0929, Found: 267.0927.
FTIR (NaCl Film): 3500, 3117, 2960, 1732, 1738, 1470, 1385, 1245, 1187, 1036, 991, 915, 736, 666 cm^{-1}.


OAc
S
N
OH

14

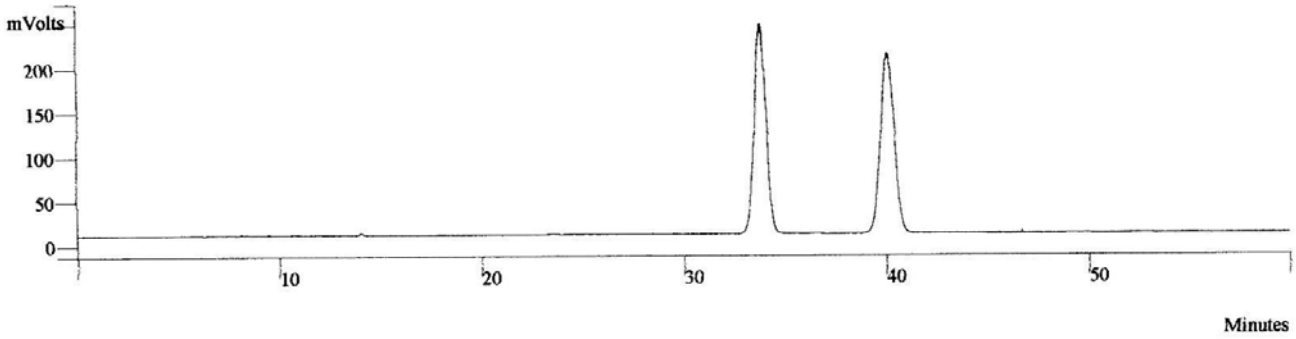

10
9
8
7
6
5
4
3
2
1
0 ppm


200
180
160
140
120
100
80
60
40
20
ppm

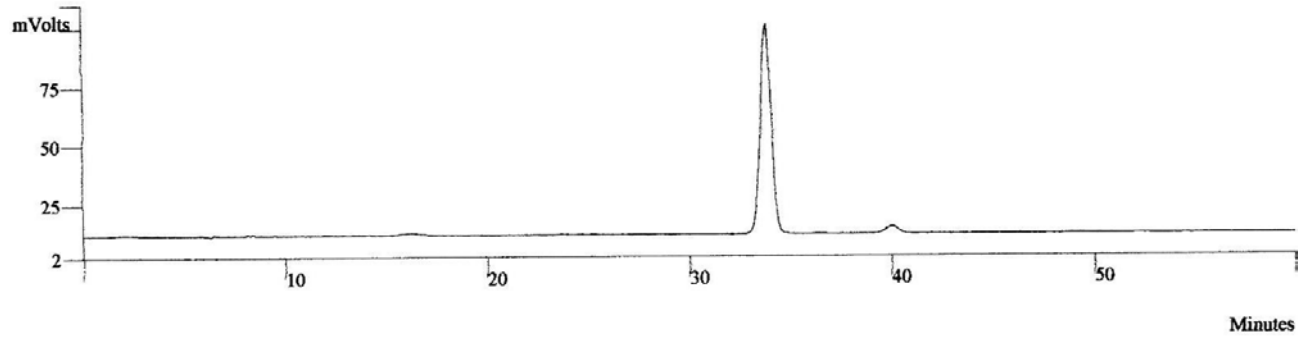


14

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 40.0 min, t_{major} = 33.8 min; ee = 92%.

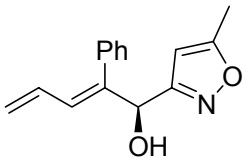


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.6330	33.796	0.000	9420205	0.00	BB	37.4		0
2		50.3670	40.096	0.000	9559518	0.00	BB	44.3		0
	Totals	**100.0000**		**0.000**	**18979724**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		96.1891	33.810	0.000	3354155	0.00	BB	35.2		0
2		3.8109	40.026	0.000	132887	0.00	BB	38.5		0
	Totals	**100.0000**		**0.000**	**3487042**					

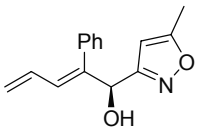
1-(5-Methyl-isoxazol-2-yl)-2-phenyl-penta-2,4-dien-1-ol



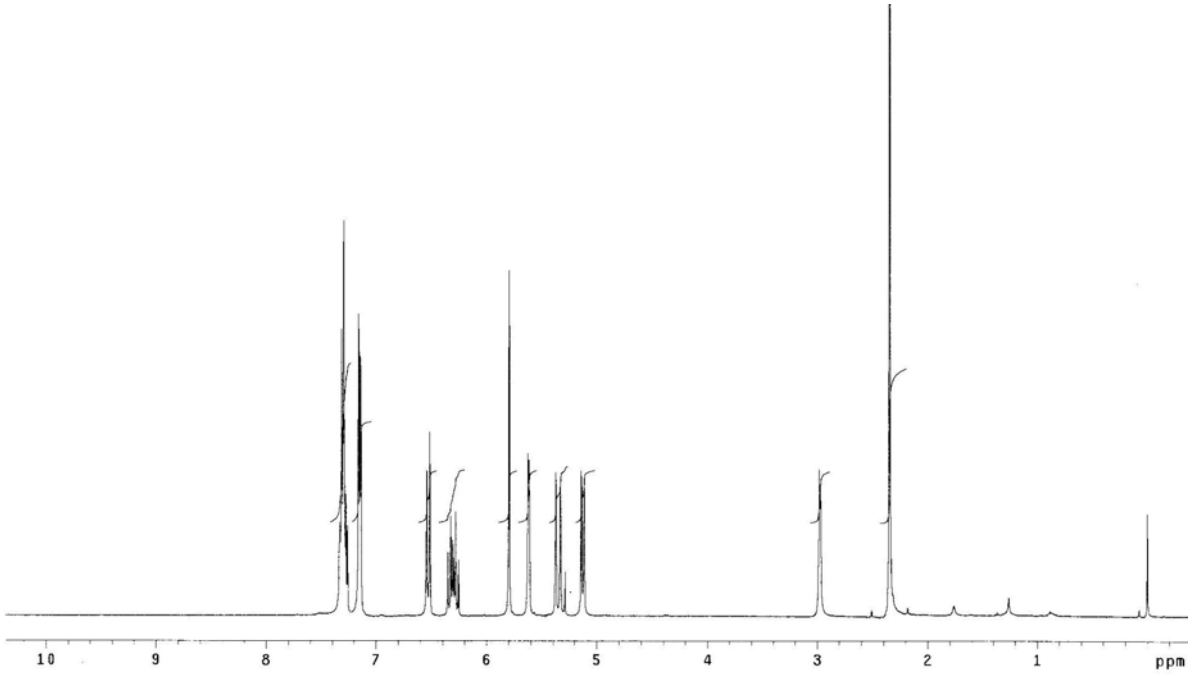
15

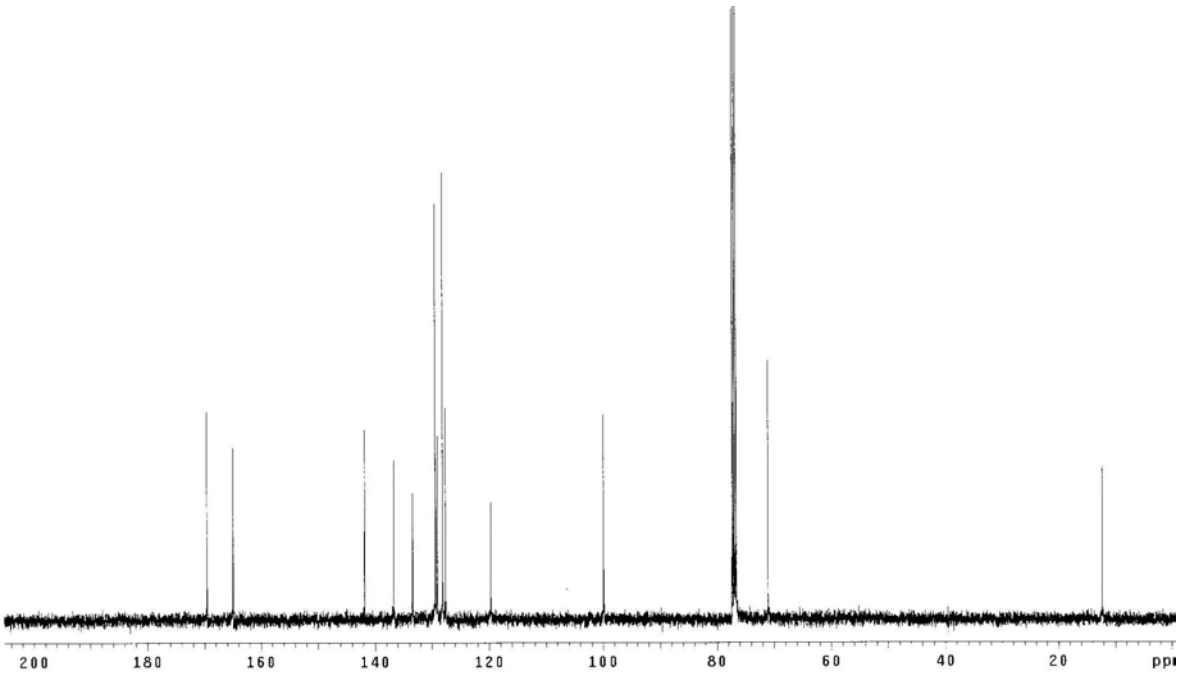
In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1a** (138 mg, 1.08 mmol, 200 mol%) was coupled to 5-methyl-isoxazol-2-carbaxaldehyde (60.0 mg, 0.540 mmol, 100 mol%) to provide the title compound (94.0 mg, 0.390 mmol) as a white solid in 73% yield after purification by flash column chromatography (R_f = 0.25, 25% EtOAc/hexanes).

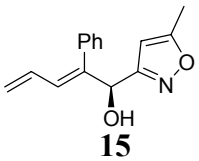
^{1}H NMR (400 MHz, $CDCl_3$): 7.29 (m, 3H), 7.15 (d, *J* = 1.6 Hz, 1H), 7.13 (s, 1H), 6.52 (d, *J* = 10.8, 1H), 6.66 (dt, *J* = 16.8, 10.4 Hz, 1H), 5.80 (s, 1H), 5.61 (d, *J* = 4.8 Hz, 1H), 5.34 (dd, *J* = 16.8, 1.8 Hz, 1H), 5.12 (dd, *J* = 10.4, 2.0 Hz, 1H), 3.06 (d, *J* = 4.4 Hz, 1H), 2.35 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 166.5, 165.0, 141.8, 136.6, 133.3, 129.3, 129.0, 128.1, 127.6, 119.6, 99.9, 70.9, 12.2.
HRMS Calcd. for $C_{15}H_{15}NO_2$ (M): 241.1103, Found: 241.1100.
FTIR (NaCl Film): 3368, 3081, 1603, 1480, 1442, 1295, 1258, 1088, 1026, 997, 915, 788, 688 cm^{-1}.
MP 88 ^oC.



15

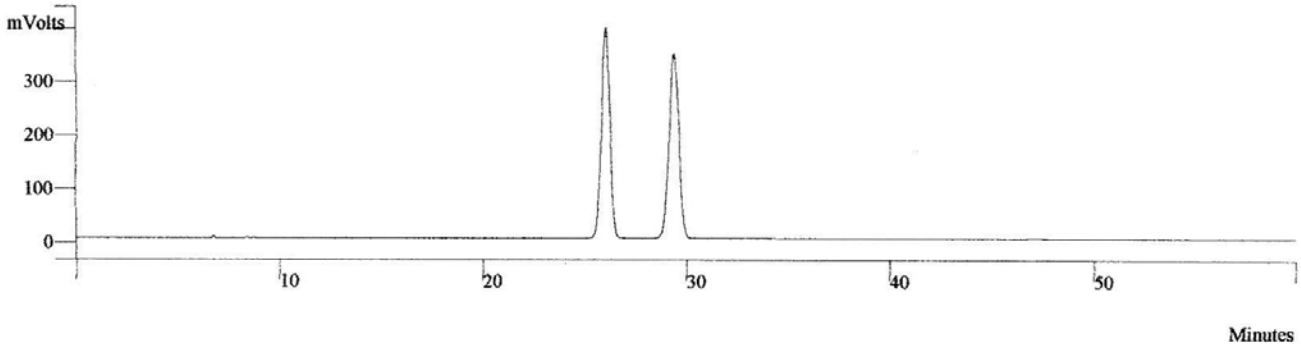




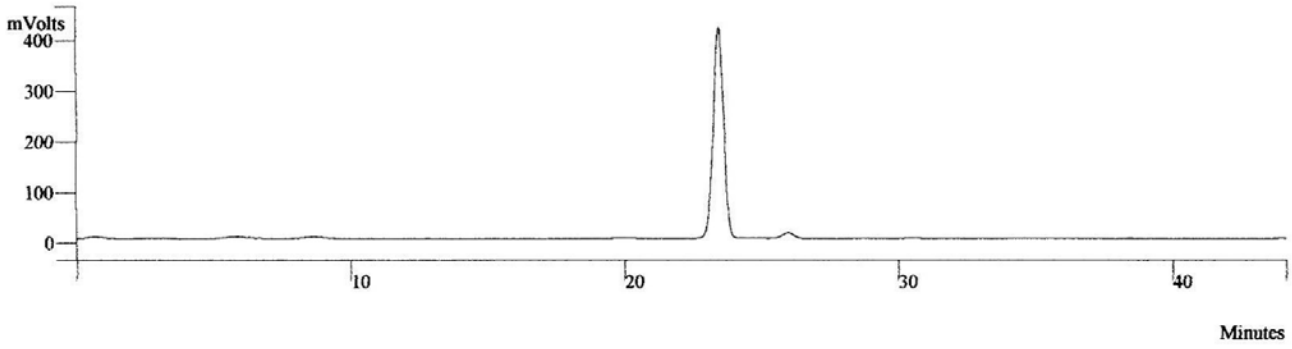


15

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 25.9 min, t_{major} = 23.4 min; ee = 94%.

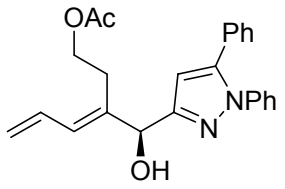


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.7583	26.051	0.000	11380999	0.00	BB	27.0		0
2		50.2417	29.393	0.000	11491580	0.00	BB	31.1		0
	Totals	**100.0000**		**0.000**	**22872580**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		97.2750	23.442	0.000	10950510	0.00	BB	24.5		0
2		2.7250	25.954	0.000	306756	0.00	BB	26.8		0
	Totals	**100.0000**		**0.000**	**11257266**					

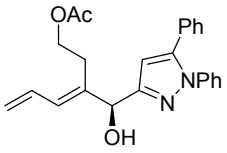
Acetic acid 3-[(1,5-diphenyl-1*H*-pyrazol-3-yl)-hydroxy-methyl]-hexa-3,5-dienyl ester



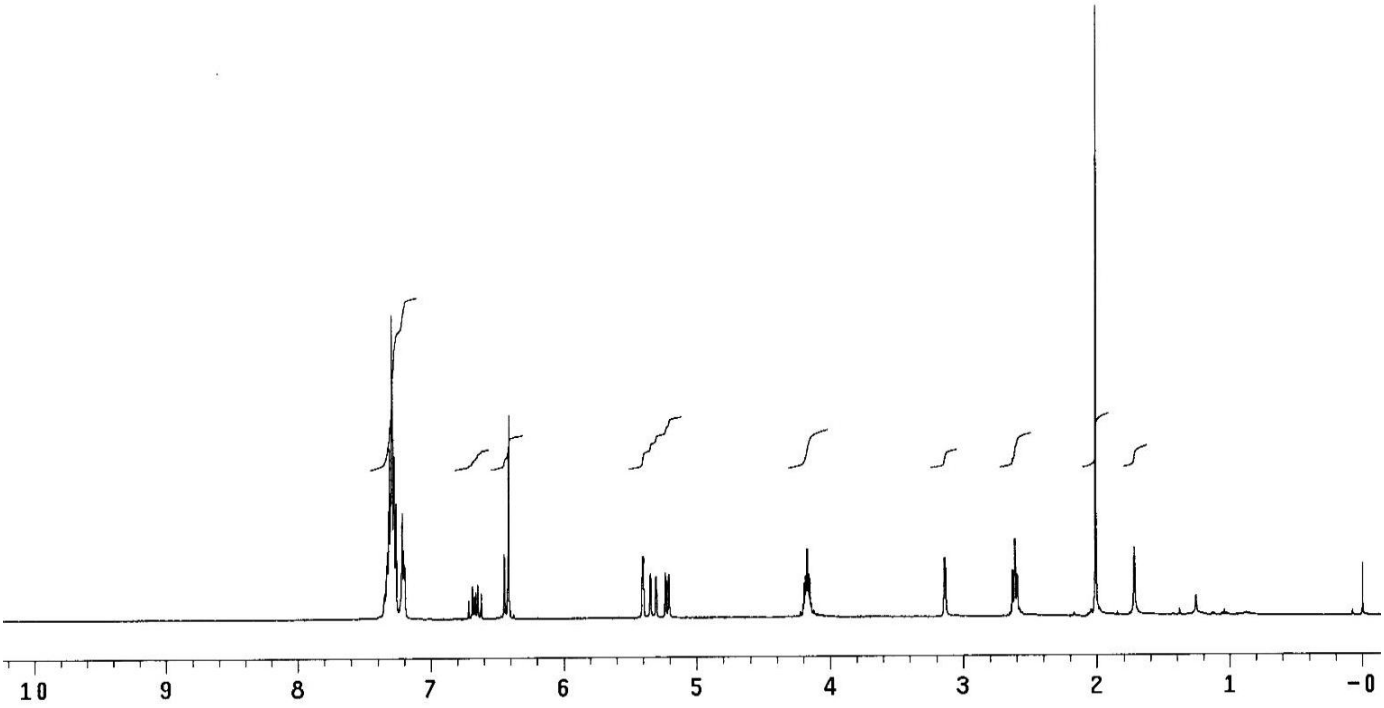
16

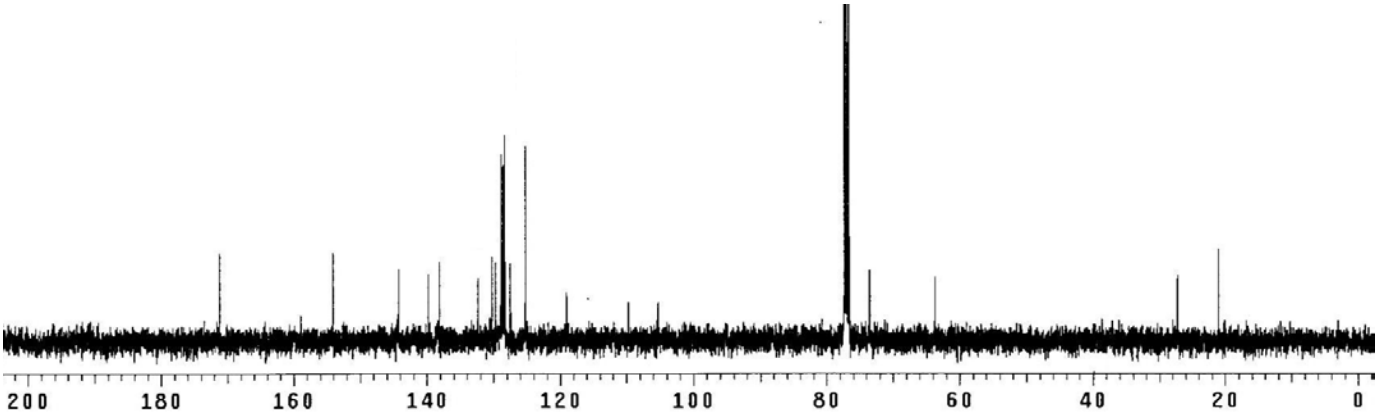
In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1b** (55.0 mg, 0.402 mmol, 200 mol%) was coupled to *N*-phenyl-5-pyrazine-2-carboxaldehyde (50.0 mg, 0.201 mmol, 100 mol%) to provide the title compound (59.0 mg, 0.152 mmol) as a white solid in 76% yield after purification by flash column chromatography (R_f = 0.25, 25% EtOAc/hexane).

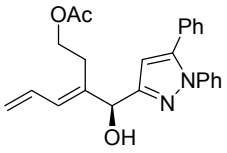
^{1}H NMR (400 MHz, $CDCl_3$): 7.28 (m, 10H), 6.66 (dt, *J* = 16.8, 10.8 Hz, 1H), 6.43 (d, *J* = 10.8 Hz, 1H), 6.41 (s, 1H), 5.40 (d, *J* = 3.2 Hz, 1H), 5.32 (dd, *J* = 16.8, 2 Hz, 1H), 5.21 (dd, *J* = 10.4, 2.0 Hz, 1H), 4.17 (m, 2H), 3.13 (d, *J* = 3.2 Hz, 1H), 2.61 (dt, *J* = 6.8, 1.6, 2H), 2.0 (s, 3H) 1.72 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 154.0, 144.2, 139.8, 138.1, 132.3, 130.2, 129.7, 128.9, 128.6, 128.4, 128.3, 127.4, 125.2, 119.0, 109.6, 105.2, 73.5, 63.7, 39.8, 38.5, 27.2, 21.0.
HRMS Calcd. for $C_{24}H_{24}N_2O_3$ (M): 388.1787, Found: 388.1786.
FTIR (NaCl Film): 3500, 3293, 3039, 2928, 1604, 1489, 1440, 1256, 1101, 1000, 919, 905, 781, 703 cm^{-1}.
MP 149 ^oC.


OAc
Ph
NPh
N
OH

16

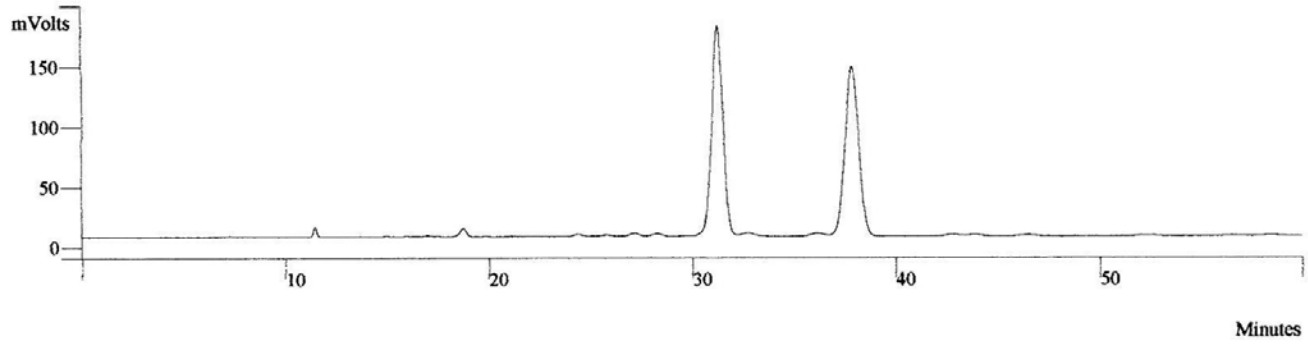

10
9
8
7
6
5
4
3
2
1
-0


200
180
160
140
120
100
80
60
40
20
0

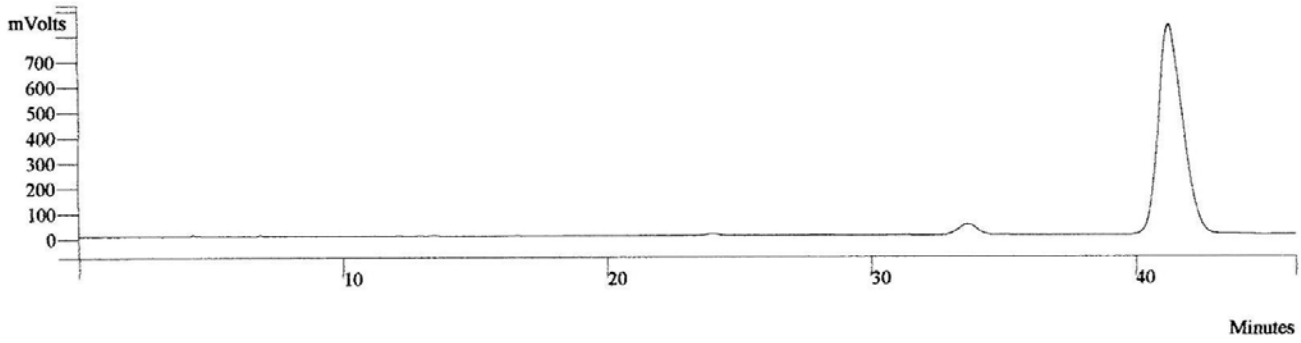


16

HPLC (Chiralcel AD-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 33.6 min, t_{major} = 41.2 min; ee = 92%.

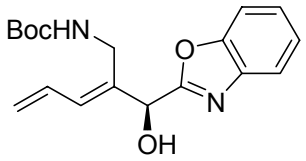


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.2746	31.244	0.000	6590806	0.00	BB	35.2		0
2		49.7254	37.855	0.000	6518804	0.00	BB	43.4		0
	Totals	**100.0000**		**0.000**	**13109610**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		3.6403	33.658	0.000	2012941	0.00	BB	45.9		0
2		96.3597	41.270	0.000	53283716	0.00	BB	59.6		0
	Totals	**100.0000**		**0.000**	**55296656**					

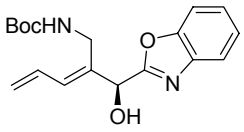
[2-(Benzooxazol-2-yl-hydroxy-methyl)-penta-2,4-dienyl]-carbamic acid *tert*-butyl ester



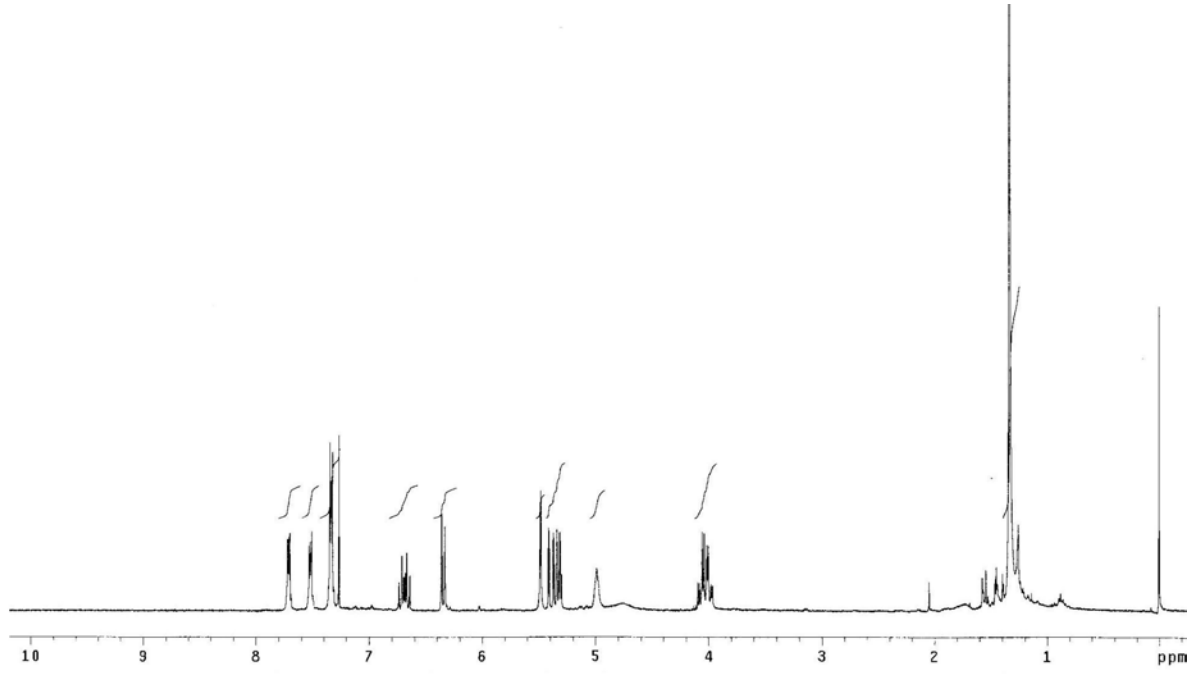
17

In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1c** (147.0 mg, 0.932 mmol, 200 mol%) was coupled to benzaxazol-2-carboxaldehyde (60.0 mg, 0.407 mmol, 100 mol%) to provide the title compound (89.0 mg, 0.269 mmol) as a colorless oil in 65% yield after purification by flash column chromatography (R_f = 0.29, 40% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 7.71 (m, 1H), 7.51 (m, 1H), 7.33 (m, 2H), 6.69 (ddd, *J* = 16.8, 10.8, 10.0 Hz, 1H), 6.34 (d, *J* = 10.8 Hz, 1H), 5.49 (s, 1H), 5.40 (dd, *J* = 16.8, 1.6 Hz, 2H), 5.32 (dd, *J* = 10.0, 1.6 Hz, 1H), 5.01 (s, 1H), 4.06 (dd, *J* = 15.2, 6.8 Hz, 1H), 3.98 (dd, *J* = 15.2, 5.6 Hz, 1H) 1.45 (s, 3H) 1.33 (s, 9H), 5.45 (d, *J* = 16.8 Hz, 1H), 5.30 (d, *J* = 10.0 Hz, 1H) 5.10 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 159.1, 147.6, 144.0, 137.1, 136.3, 133.6, 129.4, 127.7, 127.0, 122.2, 118.8, 76.7.
HRMS Calcd. for $C_{18}H_{23}N_2O_4$ (M): 313.1658, Found: 313.1654.
FTIR (NaCl Film): 3321, 2976, 2929, 1734, 1611, 1507, 1455, 1367, 1243, 1167, 1047, 916, 746, 646 cm^{-1}.


BocHN
O
N
OH

17


10
9
8
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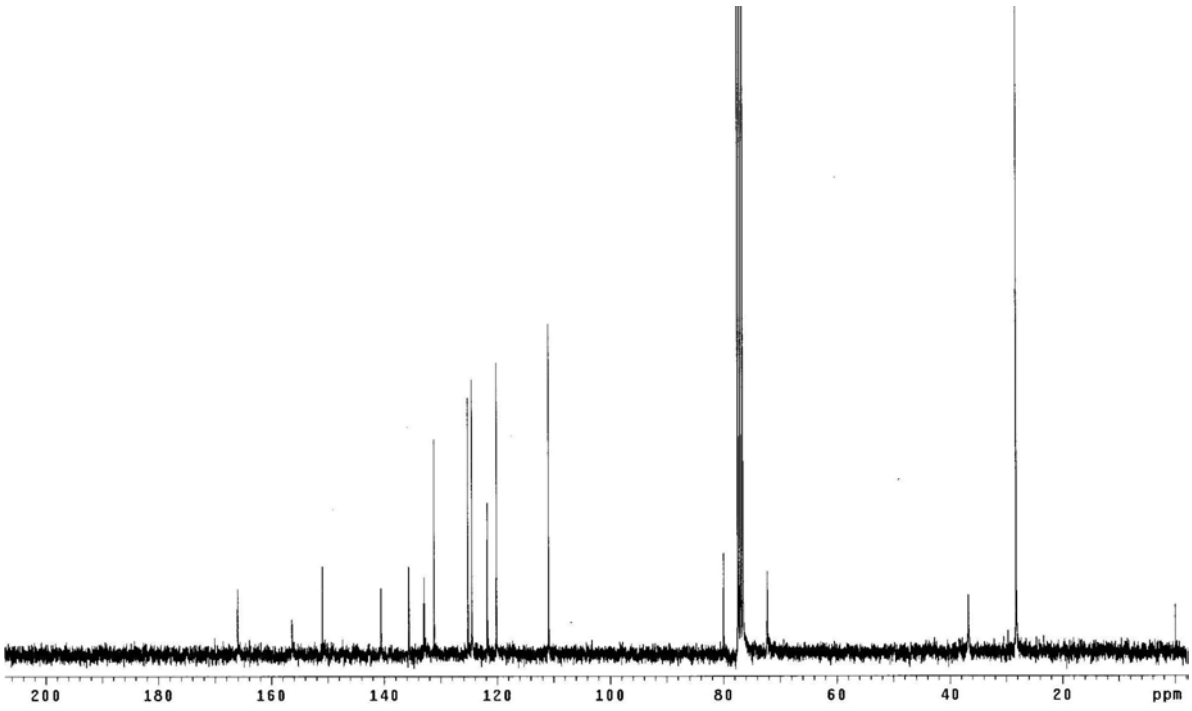
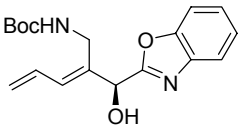
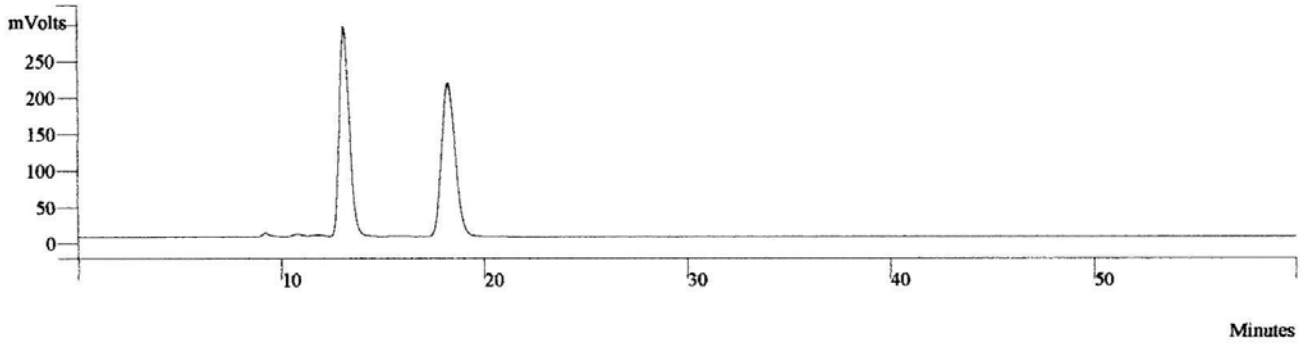
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

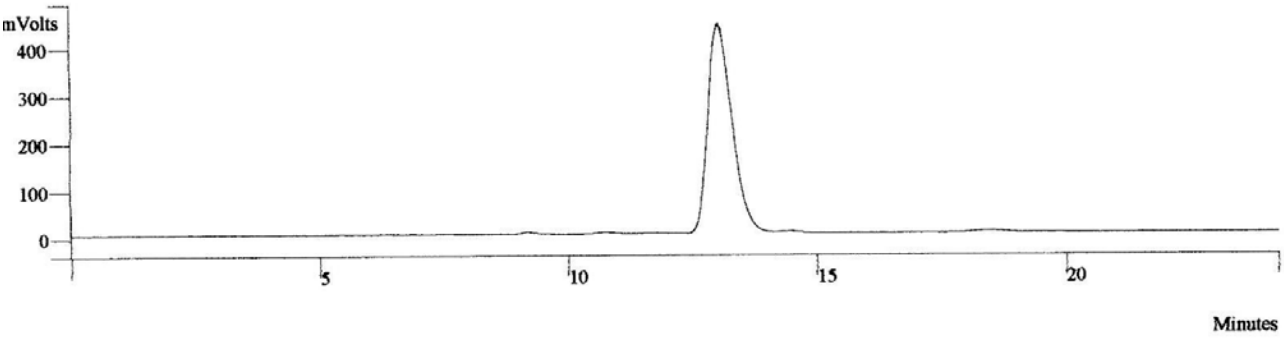


17

HPLC (Chiralcel OD-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 18.0 min, t_{major} = 12.9 min; ee = 96%.

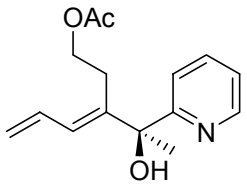


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.6683	13.065	0.000	9780852	0.00	BB	31.6		0
2		50.3317	18.220	0.000	9911494	0.00	BB	43.8		0
	Totals	**100.0000**		**0.000**	**19692346**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		98.7842	13.039	0.000	14693796	0.00	BB	31.6		0
2		1.2158	18.411	0.000	180850	0.00	BB	39.8		0
	Totals	**100.0000**		**0.000**	**14874646**					

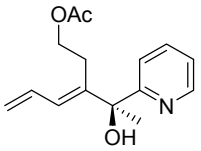
Acetic acid 3-(1-hydroxy-1-pyridin-2-yl-ethyl)-hexa-3, 5-dienyl ester



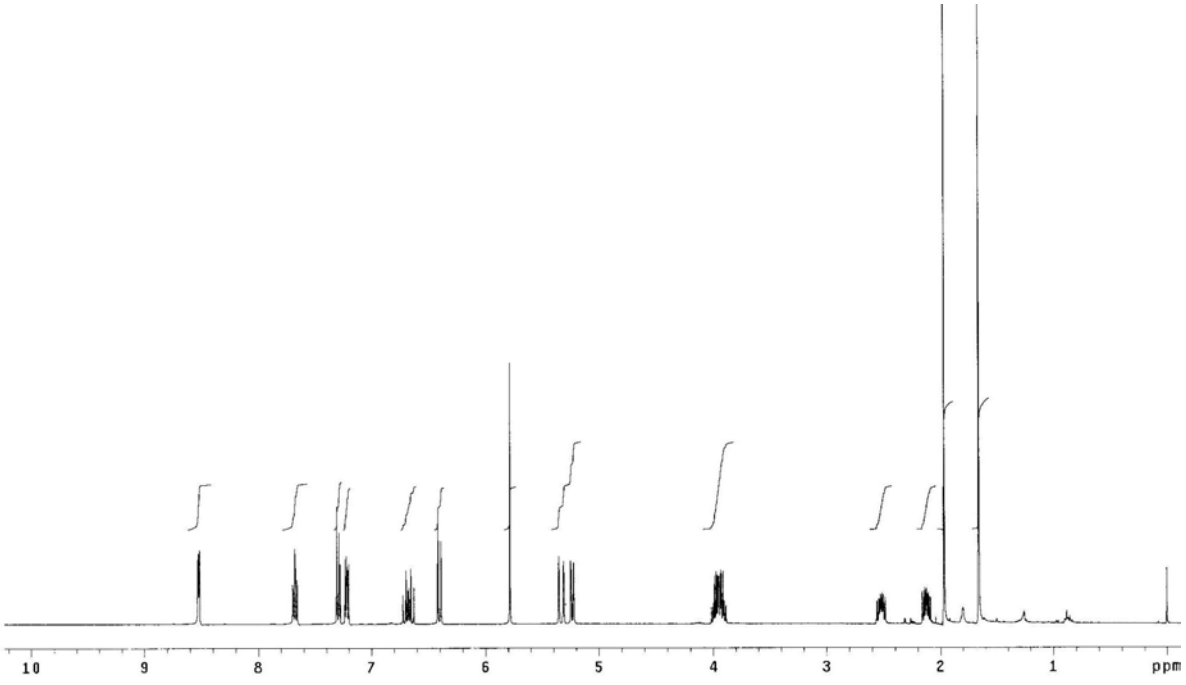
18

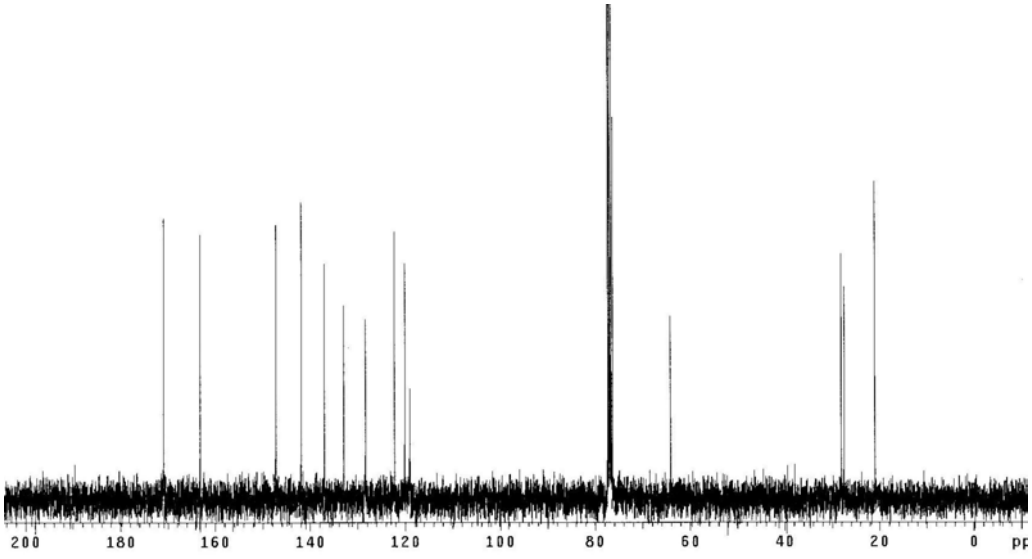
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1e** (100.0 mg, 0.825 mmol, 200 mol%) was coupled to 2-acetylpyridine (50.0 mg, 0.412 mmol, 100 mol%) to provide the title compound (95.0 mg, 0.363 mmol) as a colorless oil in 95% yield after purification by flash column chromatography (R_f = 0.23, 25% EtOAc/hexanes).

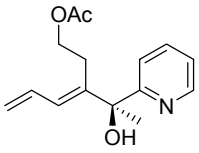
^{1}H NMR (400 MHz, $CDCl_3$): 8.52 (m, 1H), 7.67 (dt, *J* = 7.6, 2.0 Hz, 1H), 7.29 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.22 (m, 1H), 6.64 (dt, *J* = 16.8, 10.8 Hz, 1H), 6.67 (dt, *J* = 16.8, 10.0 Hz, 1H), 6.40 (d, *J* = 10.8 Hz, 1H), 5.70 (s, 1H), 5.33 (dd, *J* = 16.8, 2.0 Hz, 1H) 5.23 (d, *J* = 10.0, 1.6 Hz, 1H), 3.94 (m, 2H), 2.52 (ddd, *J* = 12.8, 9.6, 6.0 Hz, 1H), 2.12 (ddd, *J* = 12.8, 9.6, 5.6 Hz, 1H), 1.97 (s, 3H), 1.66 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.9, 163.1, 147.2, 141.8, 137.0, 132.9, 128.3, 122.2, 120.0, 119.0, 76.3, 64.1, 28.1, 27.4, 20.9.
HRMS Calcd. for $C_{15}H_{19}NO_3$ (M): 261.1365, Found: 261.1366.
FTIR (NaCl Film): 3388, 2976, 2360, 1735, 1672, 1591, 1470, 1432, 1365, 1244, 1033, 786 cm^{-1}.



18

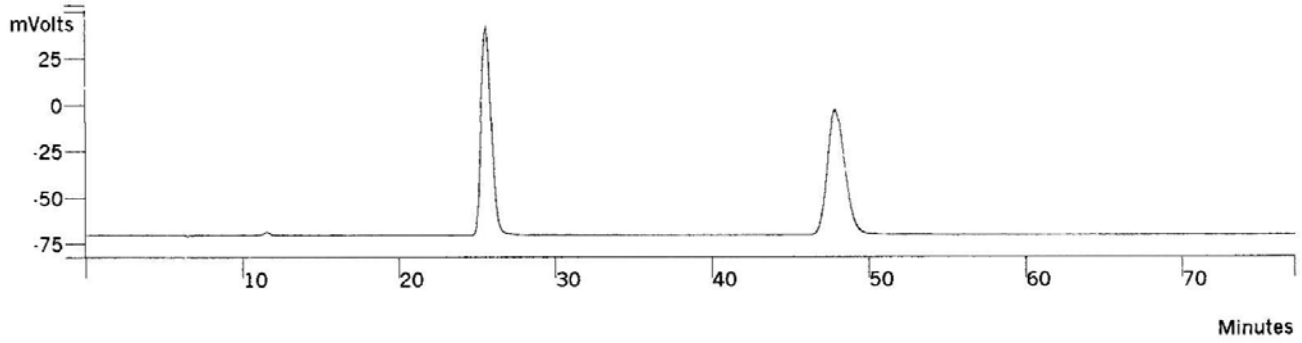




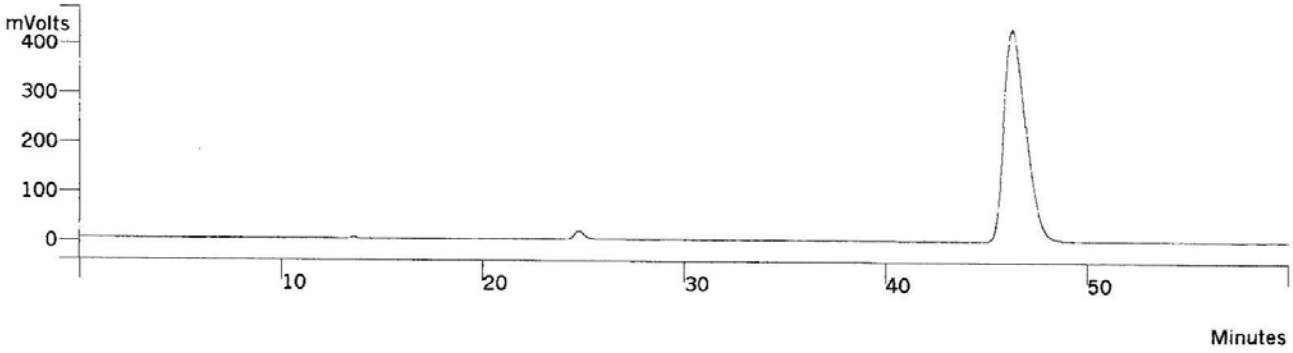


18

HPLC (Chiralcel OJ-H column, 5% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm): t_{minor} = 46.2 min, t_{major} = 24.7 min; ee = 97%.

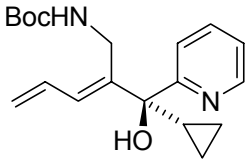


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.6414	25.595	0.000	5117409	0.00	BB	42.8		0
2		50.3586	47.870	0.000	5191340	0.00	BB	71.9		0
	Totals	**100.0000**		**0.000**	**10308749**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		1.7326	24.751	0.000	567886	0.00	BB	32.4		0
2		98.2674	46.239	0.000	32208052	0.00	BB	70.9		0
	Totals	**100.0000**		**0.000**	**32775938**					

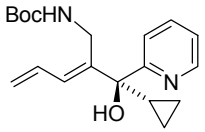
[2-(Cyclopropyl-hydroxy-pyridin-2-yl-methyl)-penta-2,4-dienyl]-carbamic acid *tert*-butyl ester



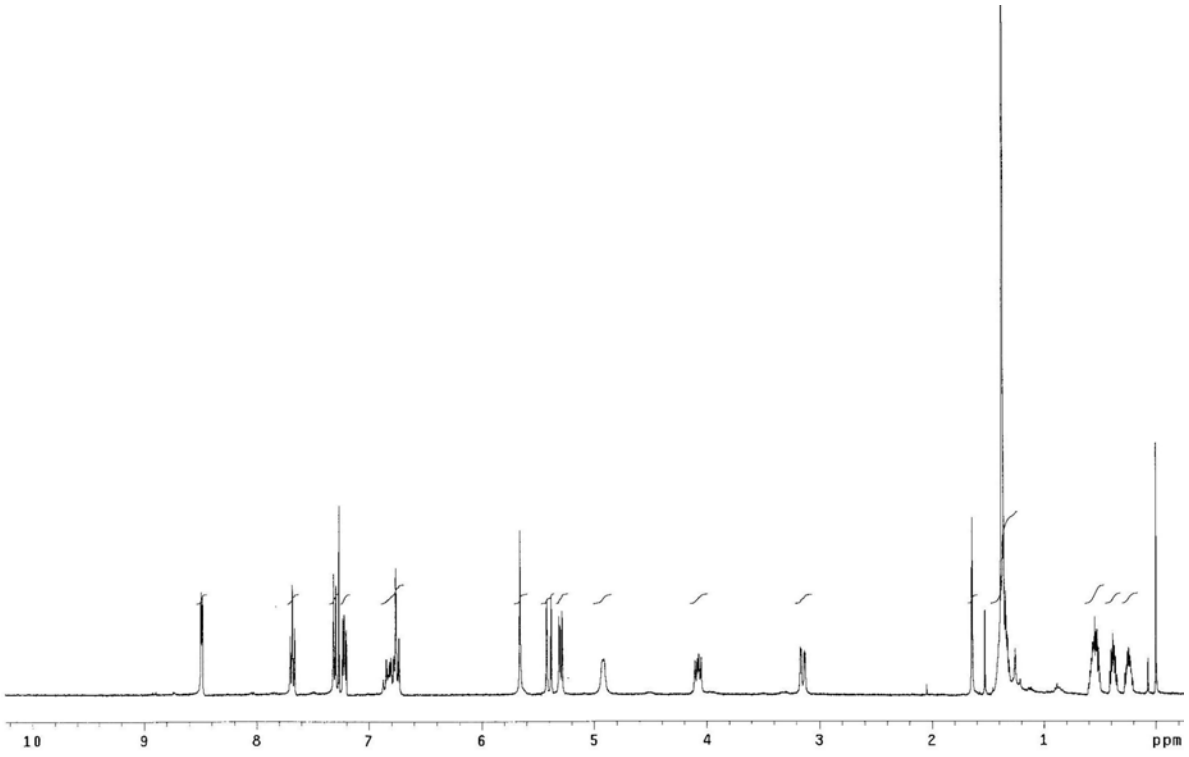
19

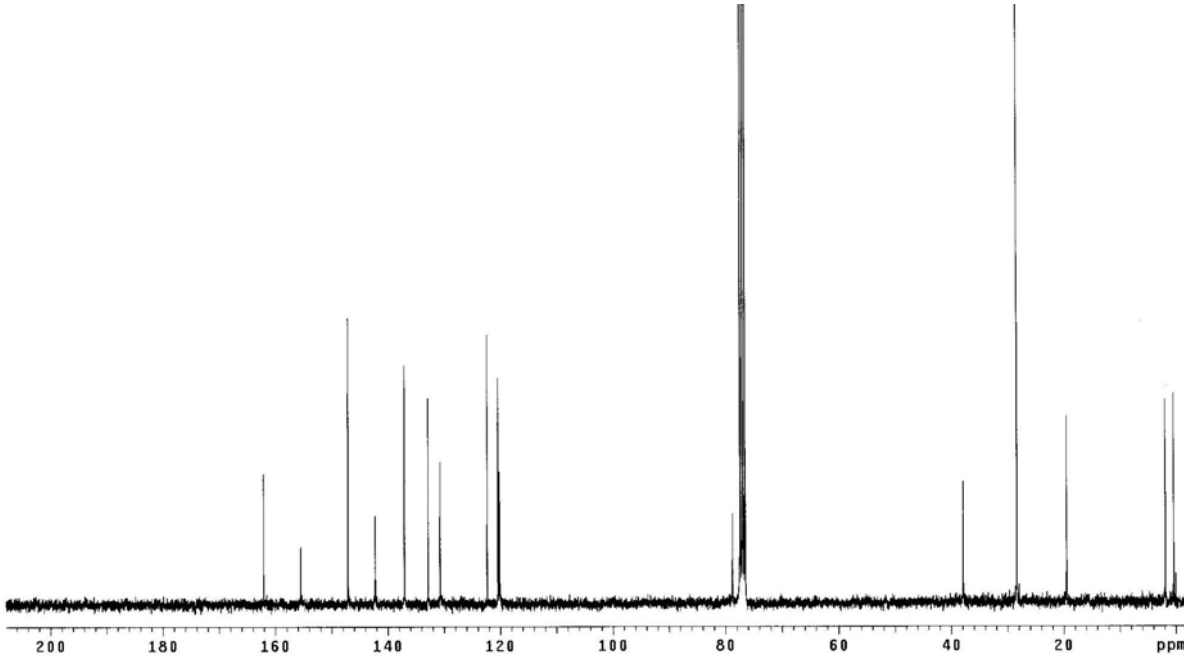
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1c** (120.0 mg, 0.825 mmol, 200 mol%) was coupled to cyclopropyl-2-pyridyl ketone (50.0 mg, 0.335 mmol, 100 mol%) to provide the title compound (104.0 mg, 0.315 mmol) as a pale yellow oil in 89% yield after purification by flash column chromatography (R_f = 0.22, 30% EtOAc/hexanes).

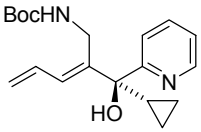
^{1}H NMR (400 MHz, $CDCl_3$): 8.49 (d, *J* = 4.8 Hz, 1H), 7.68 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.21 (m, 1H), 6.78 (m, 2H), 6.66 (s, 1H), 5.40 (dd, *J* = 16.4, 2.4 Hz, 1H), 5.29 (d, *J* = 10.0, 1.6 Hz, 1H), 4.91 (s, 1H) 4.91 (s, 1H), 4.08 (dd, *J* = 13.2, 7.6 Hz 1H) 3.15 (dd, *J* = 13.6, 2.8 Hz, 1H) 1.64 (s, 1H), 1.37 (s, 9H), 0.54 (m, 2H), 0.38 (m, 1H), 0.24 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): 162.1, 155.4, 147.0, 142.2, 137.0, 132.8, 130.6, 122.3, 120.1, 78.7, 77.4, 76.5, 37.9, 28.3, 19.5, 1.8, 0.3.
HRMS Calcd. for $C_{19}H_{26}N_2O_3$ (M): 330.1943, Found: 330.1939.
FTIR (NaCl Film): 3521, 3342, 1709, 1592, 1503, 1469, 1433, 1391, 1366, 1251, 1168, 1049, 996, 914, 753 cm^{-1}.


BocHN
N
HO

19

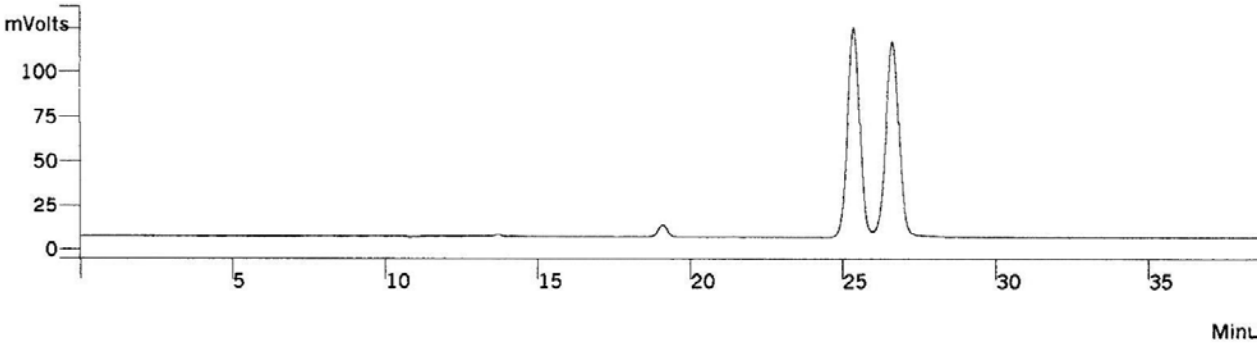

10
9
8
7
6
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

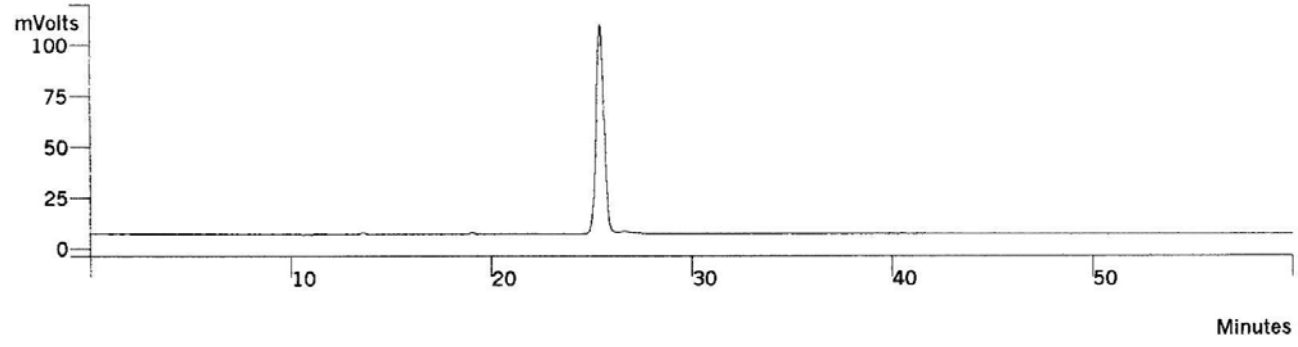


19

HPLC (Chiralcel AD-H column, 3% *i*-PrOH/hexanes, 0.5 mL/min, 254 nm), t_{minor} = 25.0 min, t_{major} = 26.2 min; ee = 97%.

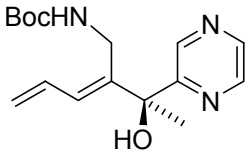


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.2153	25.339	0.000	3132386	0.00	BB	25.8		0
2		49.7847	26.613	0.000	3105523	0.00	BB	26.8		0
	Totals	**100.0000**		**0.000**	**6237909**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		99.2796	25.410	0.000	2781752	0.00	BB	25.3		0
2		0.7204	26.605	0.000	20185	0.00	BB	15.4		0
	Totals	**100.0000**		**0.000**	**2801937**					

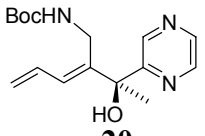
[2-(1-hydroxy-1-pyrazin-2-yl-ethyl)-penta-2,4-dienyl]-carbamic acid *tert*-butyl ester



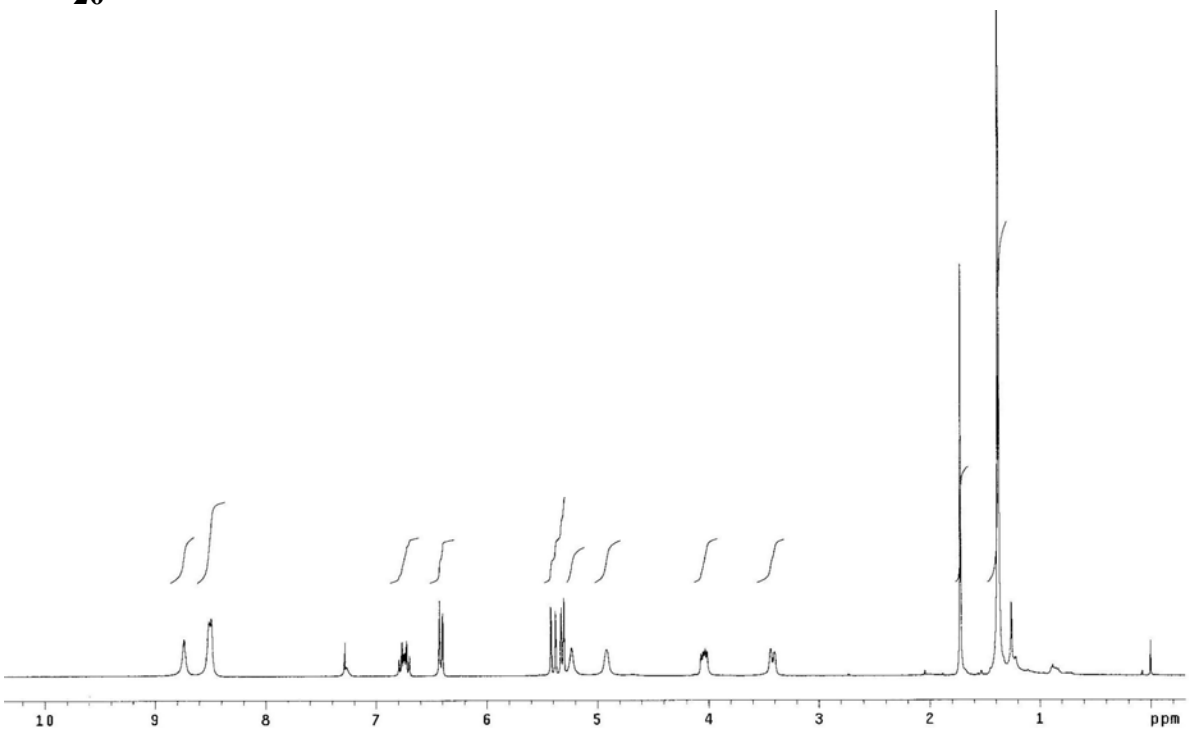
20

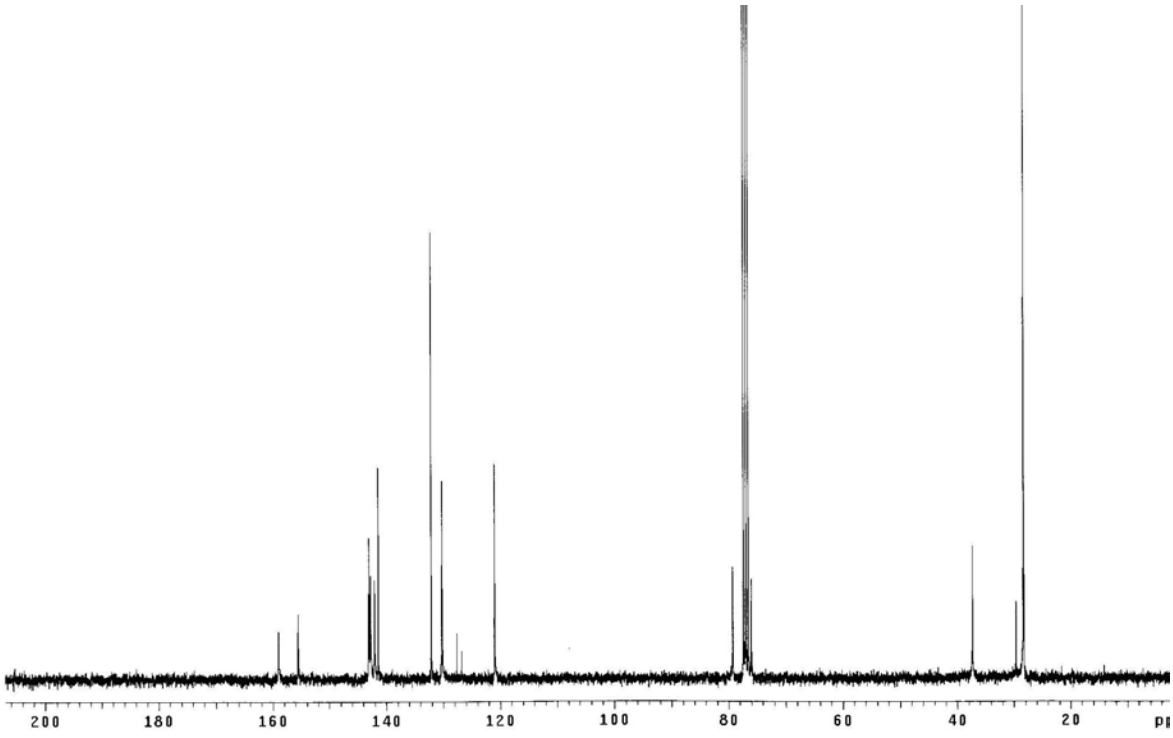
In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1c** (75.0 mg, 0.400 mmol, 200 mol%) was coupled to 2-acetylpyrazine (25.0 mg, 0.200 mmol, 100 mol%) to provide the title compound (57.0 mg, 0.186 mmol) as a white solid in 92% yield after purification by flash column chromatography (R_f = 0.22, 30% EtOAc/hexanes).

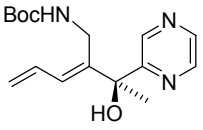
^{1}H NMR (400 MHz, $CDCl_3$): 8.70 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.30 (dd, *J* = 7.6, 10.4 Hz, 1H), 6.74 (dt, *J* = 16.4, 10.0 Hz, 1H), 6.41 (d, *J* = 11.2 Hz, 1H), 5.40 (d, *J* = 16.8 Hz, 1H), 5.31 (d, *J* = 10.8 Hz, 1H), 5.23 (bs, 1H) 4.91 (s, 1H), 4.0 (dd, *J* = 14.0, 7.2 Hz ,1H) 3.42 (d, *J* = 13.6 Hz, 1H) 1.72 (s, 3H), 1.37 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$): 159.0, 155.5, 143.0, 142.7, 142.0, 141.4, 132.1, 130.2, 127.6, 121.0, 79.3, 77.4, 76.0, 37.3, 29.6, 28.2.
HRMS Calcd. for $C_{16}H_{23}N_3O_3$ (M): 305.1739, Found: 307.1745.
FTIR (NaCl Film): 3342, 2977, 2930, 1688, 1503, 1392, 1366, 1250, 1167, 1016, 915 cm^{-1}.
MP 152 ^oC.



20

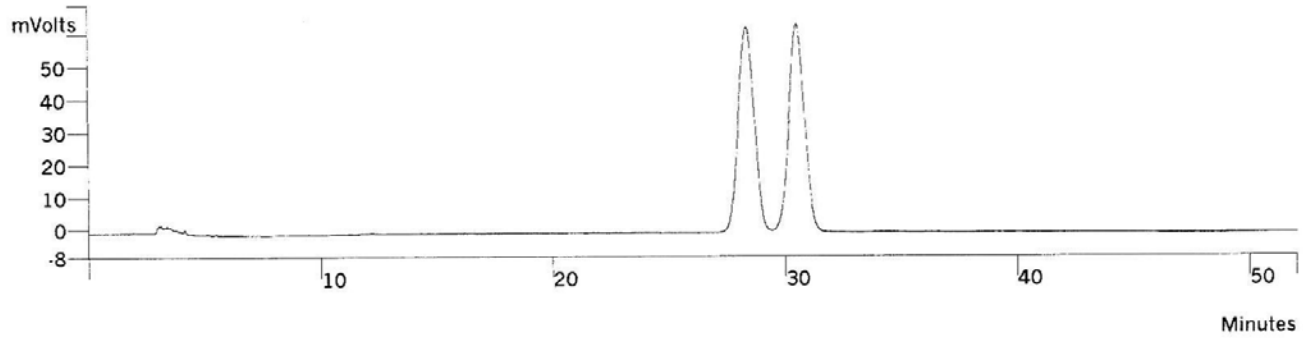




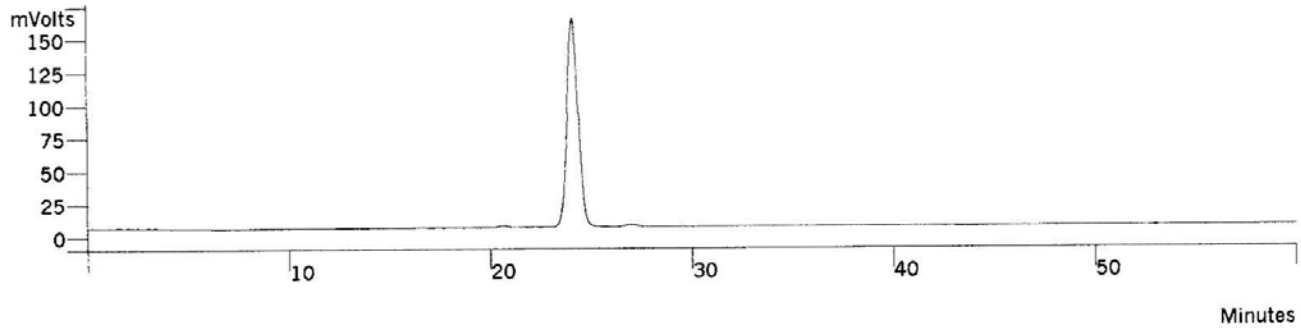


20

HPLC (Chiralcel AD-H column, 3% *i*-PrOH:hexanes, 1.0 mL/min, 254 nm): t_{major} = 24.0 min, t_{minor} = 26.9 min; ee = 98%.

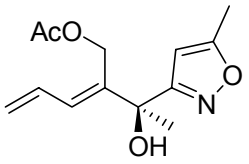


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.2026	28.343	0.000	2962094	0.00	BB	45.4		0
2		49.7974	30.499	0.000	2938186	0.00	BB	43.8		0
	Totals	**100.0000**		**0.000**	**5900280**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		99.1299	24.080	0.000	6104905	0.00	BB	35.7		0
2		0.8701	26.971	0.000	53586	0.00	BB	33.3		0
	Totals	**100.0000**		**0.000**	**6158491**					

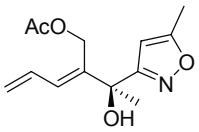
Acetic acid 2-[1-hydroxy-1-(5-methyl-isoxazol-3-yl)-ethyl]-penta-2,4-dienyl ester



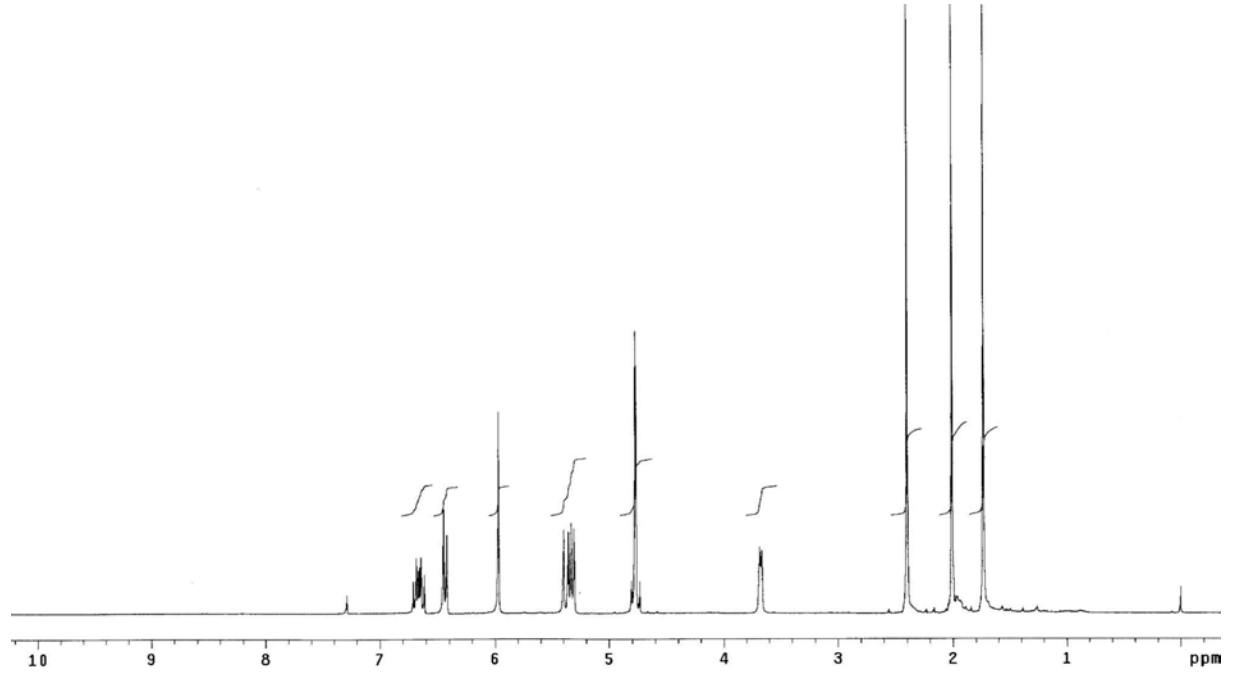
21

In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1c** (100.0 mg, 0.800 mmol, 200 mol%) was coupled to 3-acetyl-5-methylisoxazole (50.0 mg, 0.400 mmol, 100 mol%) to provide the title compound (74.0 mg, 0.294 mmol) as a colorless syrup in 74% yield after purification by flash column chromatography (R_f = 0.27, 30% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 6.65 (ddd, *J* = 16.8, 11.2, 10.4 Hz, 1H), 6.43 (d, *J* = 11.2 Hz, 1H), 5.96 (s, 1H), 5.37 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.31 (dd, *J* = 10.0, 1.6 Hz, 1H), 4.76 (dd, *J* = 15.6, 12.4 Hz, 1H), 3.67 (d, *J* = 7.2 Hz, 1H), 2.39 (d, *J* = 0.4 Hz, 3H), 2.0 (s, 3H), 1.73 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 169.5, 168.7, 138.1, 131.8, 131.7, 121.7, 121.6, 100.1, 73.0, 59.4, 27.2, 20.7, 12.2.
HRMS Calcd. for $C_{15}H_{15}NO_2$ (M): 241.1103, Found: 241.1101.
FTIR (NaCl Film): 3432, 2983, 2933, 1737, 1605, 1452, 1364, 1236, 1136, 1025, 961, 918 cm^{-1}.


AcO
O
N
OH

21


10
9
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7
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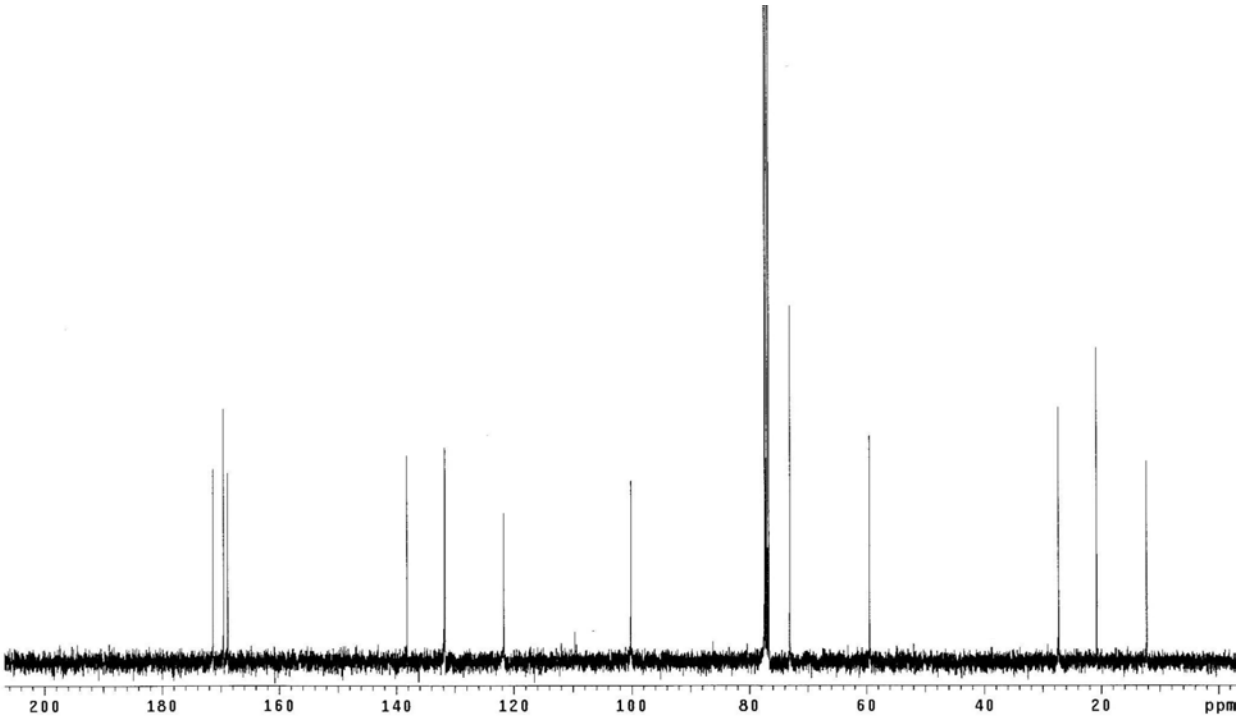
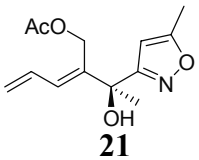
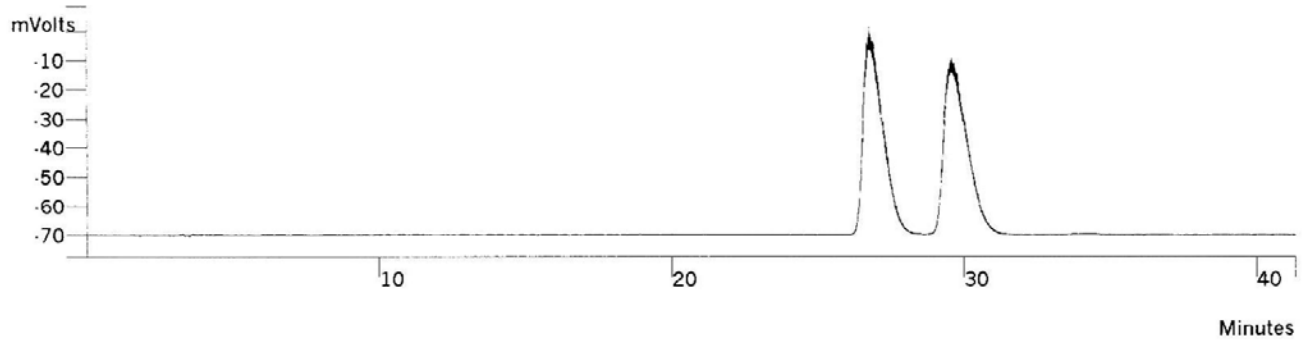
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

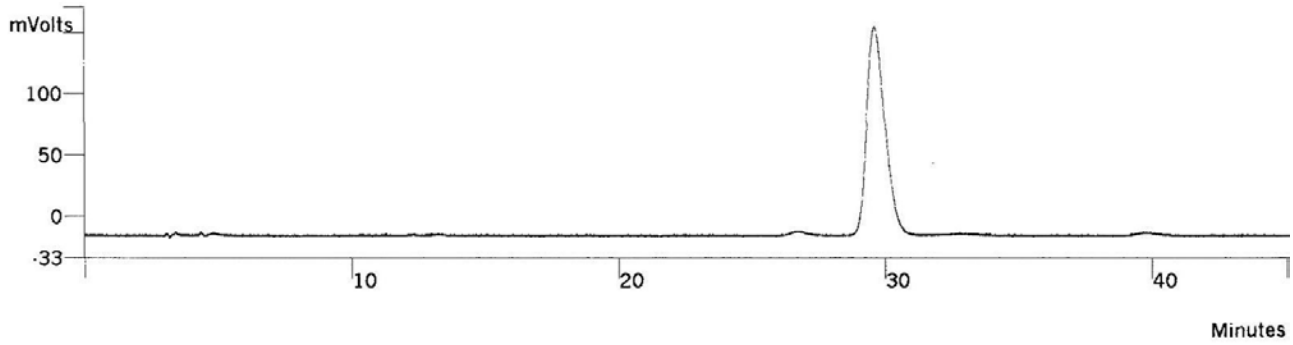


21

HPLC (Chiralcel OJ-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 26.8 min, t_{major} = 29.5 min; ee = 97%

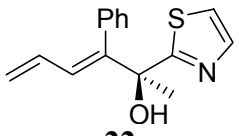


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		49.6377	26.762	0.000	3154413	0.00	BB	41.7		0
2		50.3623	29.575	0.000	3200460	0.00	BB	50.5		0
	Totals	**100.0000**		**0.000**	**6354873**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		1.5434	26.870	0.000	125056	0.00	BB	29.8		0
2		98.4566	29.575	0.000	7977510	0.00	BB	43.9		0
	Totals	**100.0000**		**0.000**	**8102566**					

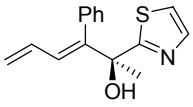
3-Phenyl-2-thiazol-2-yl-hexa-3,5-dien-2-ol



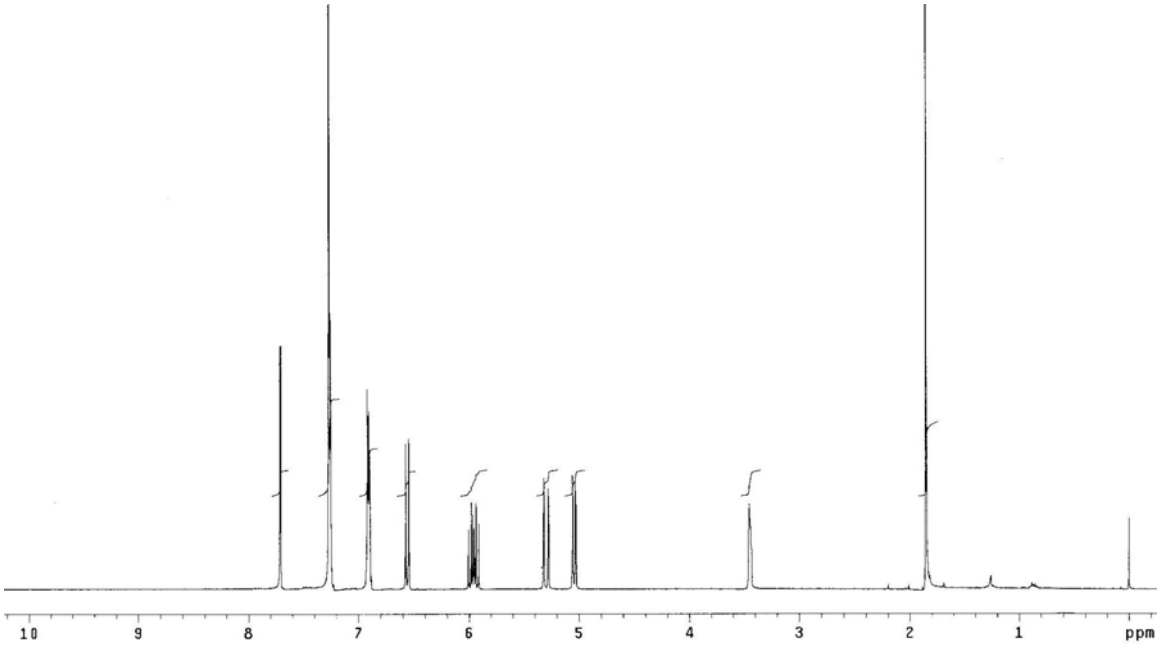
22

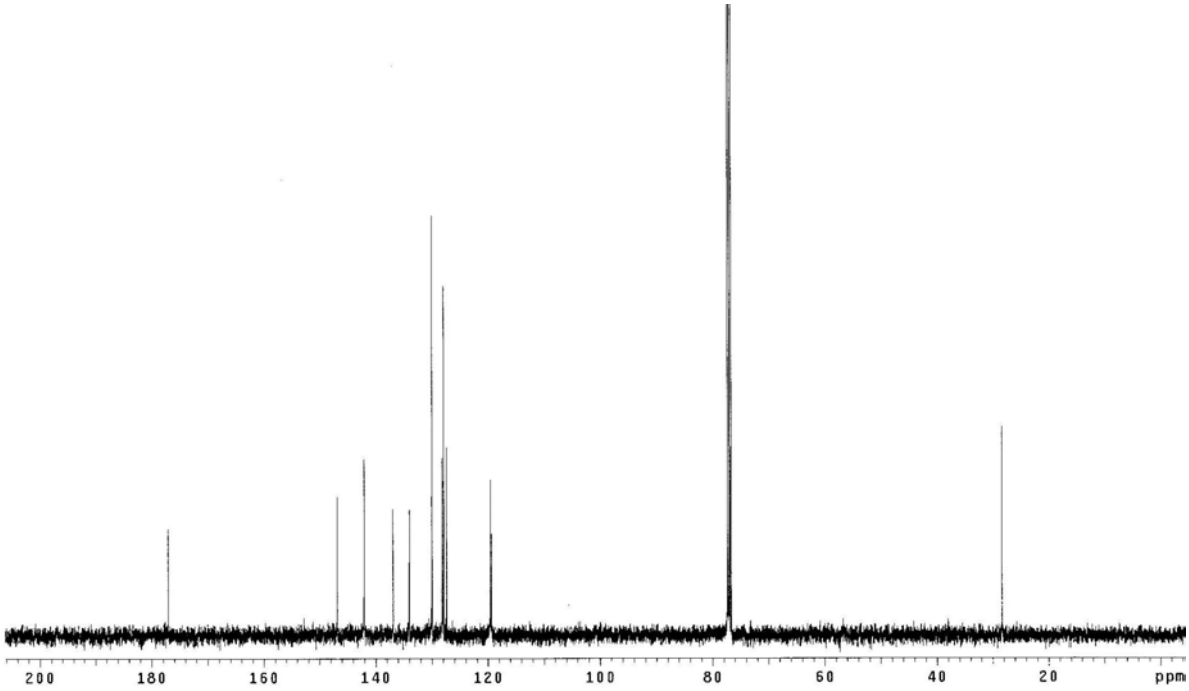
In accordance with the general procedure employing (*R*)-*tol*-BINAP as ligand, enyne **1a** (190.0 mg, 1.574 mmol, 200 mol%) was coupled to 2-acetylthiazole (100.0 mg, 0.787 mmol, 100 mol%) to provide the title compound (165.0 mg,0.642 mmol) as a white solid in 82% yield after purification by flash column chromatography (R_f = 0.27, 30% EtOAc/hexanes).

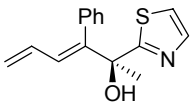
^{1}H NMR (400 MHz, $CDCl_3$): 7.71 (d, *J* = 3.2 Hz, 1H), 7.25 (m, 4H), 6.90 (m, 2H), 6.55 (d, *J* = 10.4 Hz, 1H), 5.95 (dt, *J* = 17.2, 10.4 Hz, 1H), 5.32 (dd, *J* = 17.2, 2.0.Hz, 1H), 5.04 (dd, *J* = 9.6, 1.6 Hz, 1H), 3.45 (bs, 1H) 1.85 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 177.0, 146.8, 142.0, 136.8, 134.0, 130.0, 128.1, 127.9, 127.4, 119.5, 119.3, 28.3.
HRMS Calcd. for $C_{15}H_{15}NOS$ (M): 257.0874, Found: 257.0876.
FTIR (NaCl Film): 3279, 3080, 2979, 2930, 1601, 1497, 1441, 1367, 1122, 1058, 996, 912, 773, 708 cm^{-1}.
MP 115 ^oC**.**



22

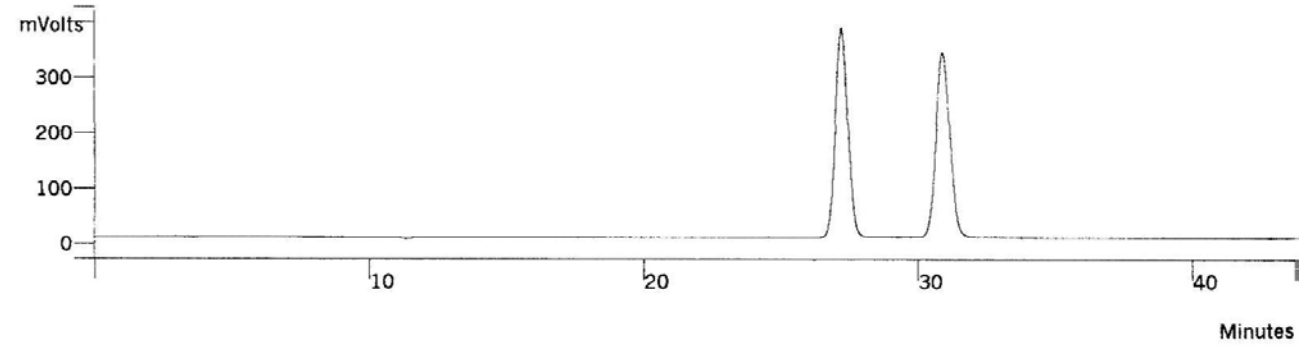




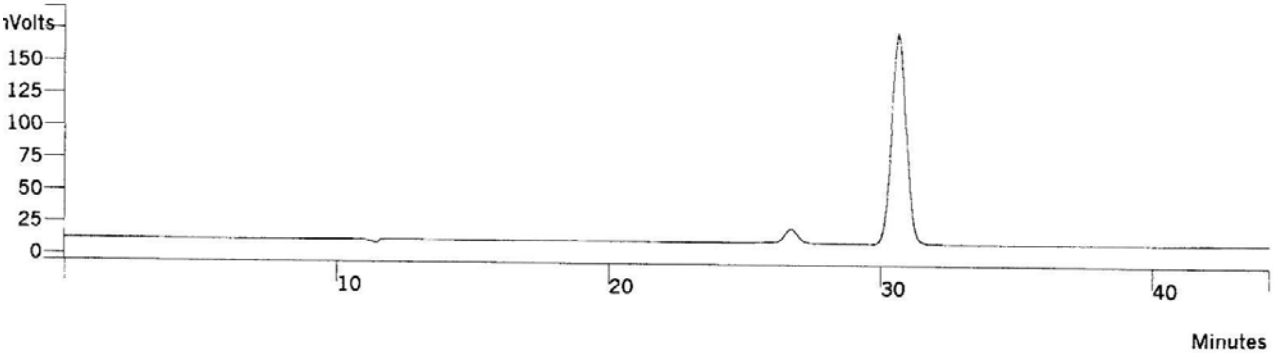


22

HPLC (Chiralcel OD-H column, 5% *i*-PrOH/hexanes, 0.3 mL/min, 254 nm): t_{minor} = 26.6 min, t_{major} = 30.6 min; ee = 90%.

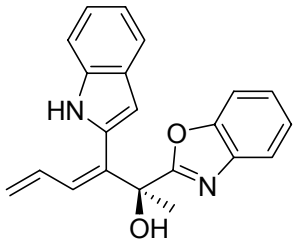


Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		50.3455	27.194	0.000	11898070	0.00	BB	29.5		0
2		49.6545	30.885	0.000	11734784	0.00	BB	32.9		0
	Totals	**100.0000**		**0.000**	**23632854**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		4.9944	26.699	0.000	316163	0.00	BB	30.1		0
2		95.0057	30.611	0.000	6014250	0.00	BB	34.5		0
	Totals	**100.0001**		**0.000**	**6330413**					

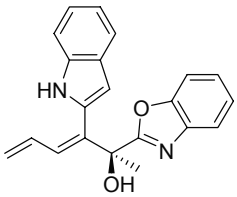
2-Benzaxazol-2-yl-3-(1*H*-indol-2-yl)-hexa-3,5-dien-2-ol



23

In accordance with the general procedure employing (*R*)-*xylyl*-WALPHOS as ligand, enyne **1c** (52.0 mg, 0.310 mmol, 200 mol%) was coupled to 2-acetylbenzaxazole (25.0 mg, 0.155 mmol, 100 mol%) to provide the title compound (37.0 mg, 0.172 mmol) as an yellow thick syrup in 71% yield after purification by flash column chromatography (R_f = 0.24, 20% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): 9.32 (bs, 1H), 7.67 (dd, *J* = 7.6, 2.4 Hz, 1H), 7. 58 (d, *J* = 8.0 Hz, 1H), 7.54 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.34 (m, 3H), 7.17 (dt, *J* = 6.8, 1.2 Hz, 1H), 7.09 (dt, *J* = 8.0, 1.2 Hz, 2H), 6.73 (dt, *J* = 15.2, 10.0 Hz, 1H), 6.49 (d, *J* = 1.2 Hz, 1H), 6.18 (d, *J*= 10.8 Hz, 1H), 5.32 (dd, *J* = 17.2, 0.8 Hz, 1H), 5.19 (d, *J* = 10.0, 1.2 Hz, 1H), 4.75 (bs, 1H), 1.87 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 169.5, 150.9, 140.0, 136.0, 135.4, 134.0, 132.5, 131.0, 127.7, 125.4, 124.7, 122.2, 121.4, 120.3, 120.1, 119.7, 111.1, 111.0, 105.8, 75.5, 26.2.
HRMS Calcd. for $C_{21}H_{18}N_2O_2$ (M): 330.1368, Found: 330.1369.
FTIR (NaCl Film): 3416, 3058, 2245, 1609, 1563, 1454, 1319, 1241, 1090, 909, 736 cm^{-1}.



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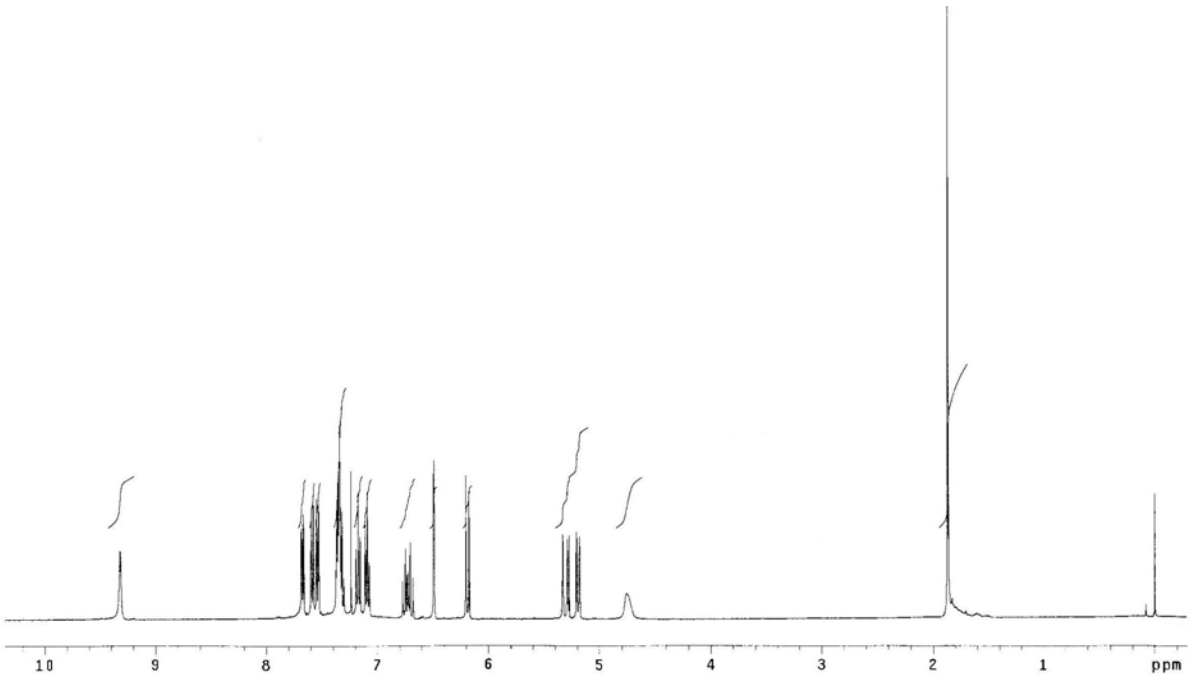
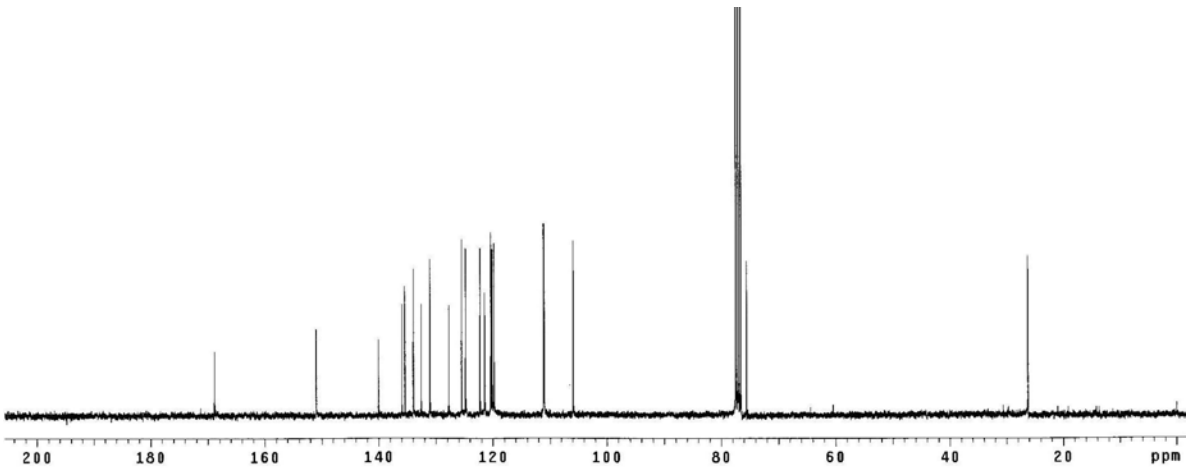
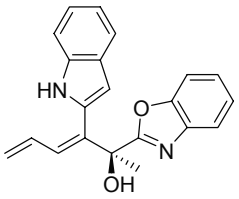
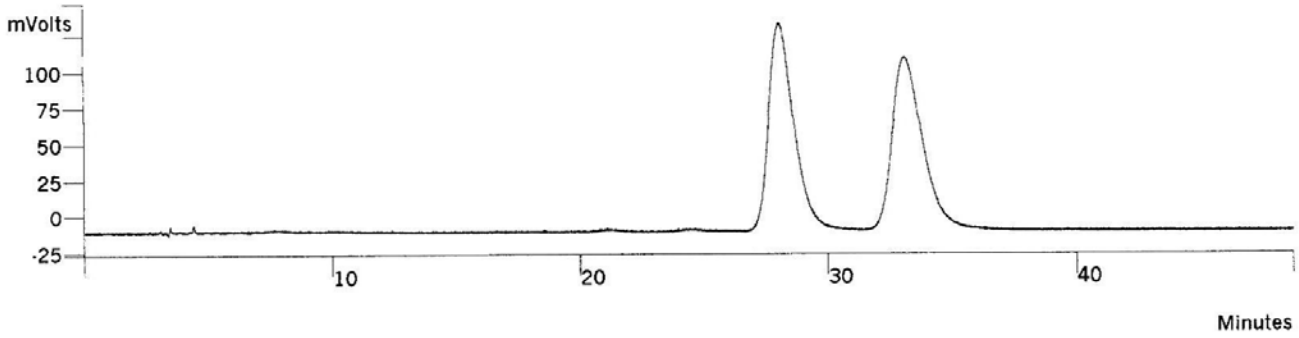






23

HPLC (Chiralcel OJ-H column, 5% *i*-PrOH/hexanes, 1.0 mL/min, 254 nm): t_{minor} = 29.7 min, t_{major} = 34.2 min; ee = 97%.



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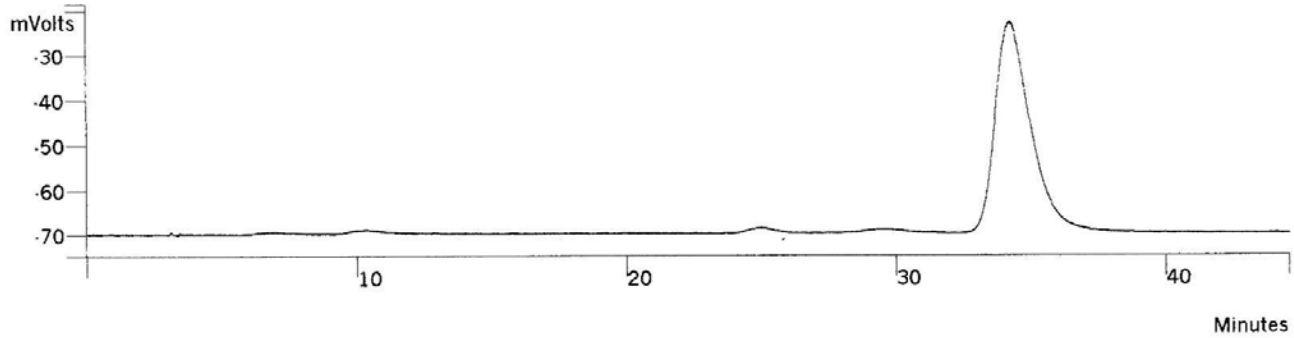
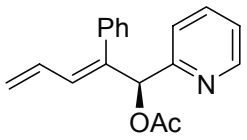
2		49.6994	33.113	0.000	10036442	0.00	BB	76.9		0
	Totals	**100.0000**		**0.000**	**20194312**					



Peak No	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Rel Ret Time	Sep. Code	Width 1/2 (sec)	Status Codes	Group
1		1.5745	29.502	0.000	69082	0.00	BB	62.8		0
2		98.4255	34.225	0.000	4318504	0.00	BB	82.5		0
	Totals	**100.0000**		**0.000**	**4387586**					

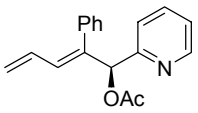
Acetic acid 2-phenyl-1-pyridin-2-yl-penta-2,4-dienyl ester



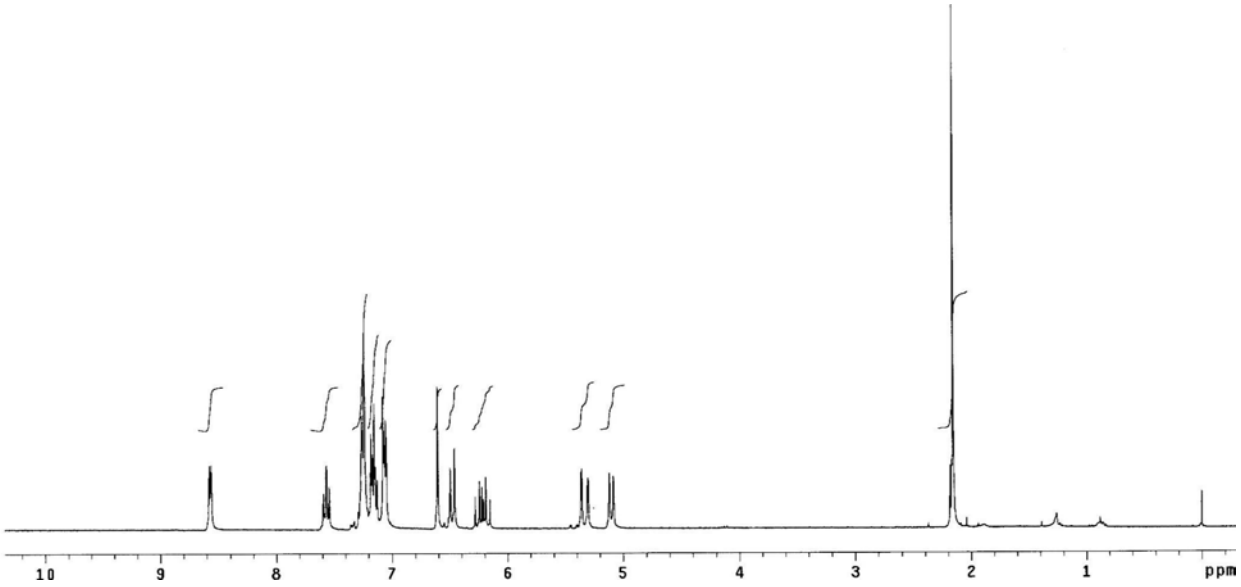
2a

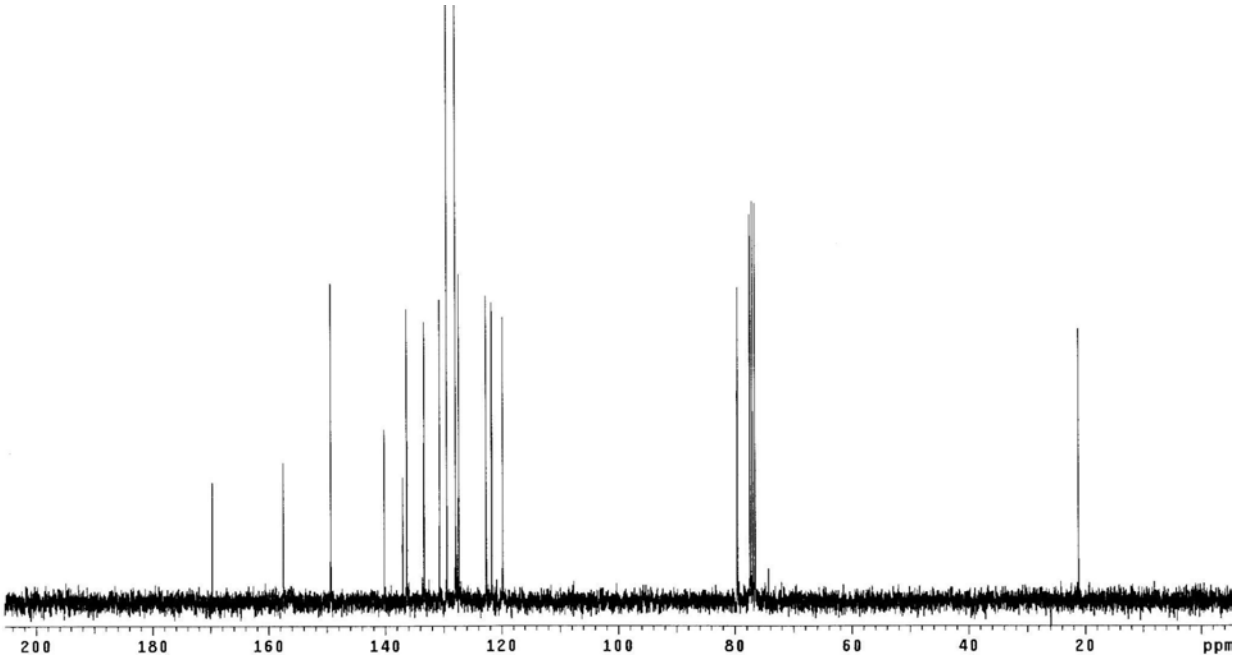
To a solution of 2-Phenyl-1-pyridin-2-yl-penta-2,4-dien-1-ol (**2**) (200.0 mg, 0.858 mmol) and triethylamine (1.0 mL) in freshly distilled dichloromethane (2.0 mL, 0.42 M) in a 10 mL RB, acetic anhydride (0.32 mL, 1.710 mmol) and catalytic amount of DMAP were added and stirred at ambient temperature for 1 hour. The reaction mixture was quenched with water and extracted with dichloromethane (2 x 20.0 mL) and washed with brine solution (10.0 mL). The crude was purified by flash silical chromatography (R_f = 0.30, 15% EtOAc/hexanse) to afford (221.0 mg, 0.792 mmol) as an yellow oil (94% yield).

^{1}H NMR (300 MHz, $CDCl_3$): 8.35 (ddd, *J* = 4.8, 1.5, 1.2 Hz, 1H), 7.56 (dt, *J* = 7.5, 1.8 Hz, 1H), 7.24 (m,, 3H), 7.15 (m, 2H), 7.05 (m, 2H), 6.61 (s,1H), 6.48 (d, *J* = 11.1 Hz, 1H), 6.21 (dt, *J* = 16.8, 10.2 Hz, 1H), 5.33 (dd, *J* = 16.8, 1.8 Hz, 1H), 2.05 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$): 169.7, 157.4, 149.3, 140.1, 137.0, 136.3, 133.3, 130.6, 129.4, 129.9, 127.3, 122.6, 121.7, 119.8, 79.5, 21.1.
HRMS Calcd. for $C_{18}H_{17}NO_2$ (M): 279.1259, Found: 279.1257.
FTIR (NaCl Film): 3054, 2335, 1748, 1589, 1572, 1470, 1370, 1228, 1022, 995, 914, 705 cm^{-1}.

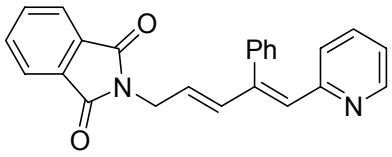


2a





2-(2-phenyl-3-pyridin-2-yl-1-vinyl-allyl)-isoindole-1,3-dione

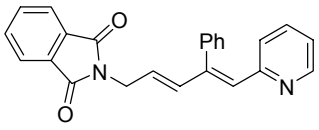


24

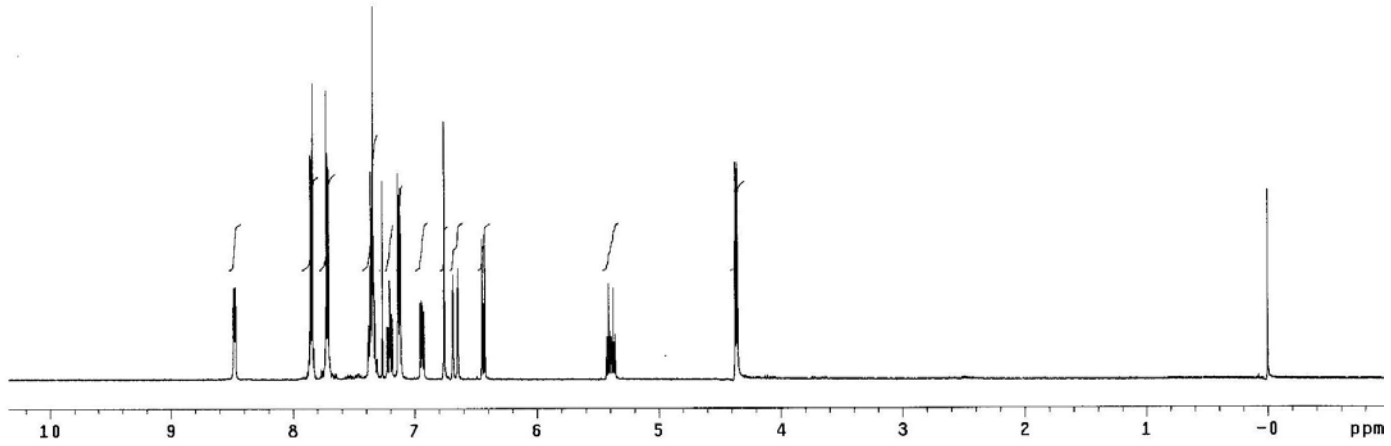
A solution of acetic acid 2-phenyl-1-pyridin-2-yl-penta-2,4-dienyl ester (**2a**) (100 mg, 0.358 mmol, 100 mol%), potassium phthalimide (132.0 mg, 0.716 mmol, 200 mol%) and triphenylphosphine (18.0 mg, 0.071 mmol, 20 mol%) in freshly distilled THF (3.6 mL, 0.1 M) in 10 mL RB flask was degassed and tetrakis(triphenylphosphino) palladium (0) catalyst (41.0 mg, 0.035 mmol, 10 mol%) was added. The reaction vessel was sparged with argon gas and the reaction mixture was allowed to stir at reflux under an argon atmosphere for 14 hours.[1] Upon complete consumption of starting material, as revealed by TLC analysis, the reaction mixture was concentrated *in vacuo* and the resulting residue was subjected to flash column chromatography (R_f = 0.25, 25% EtOAc/hexanes) to furnish the title compound (99.0 mg, 0.270 mmol) as a white solid in 76% yield.

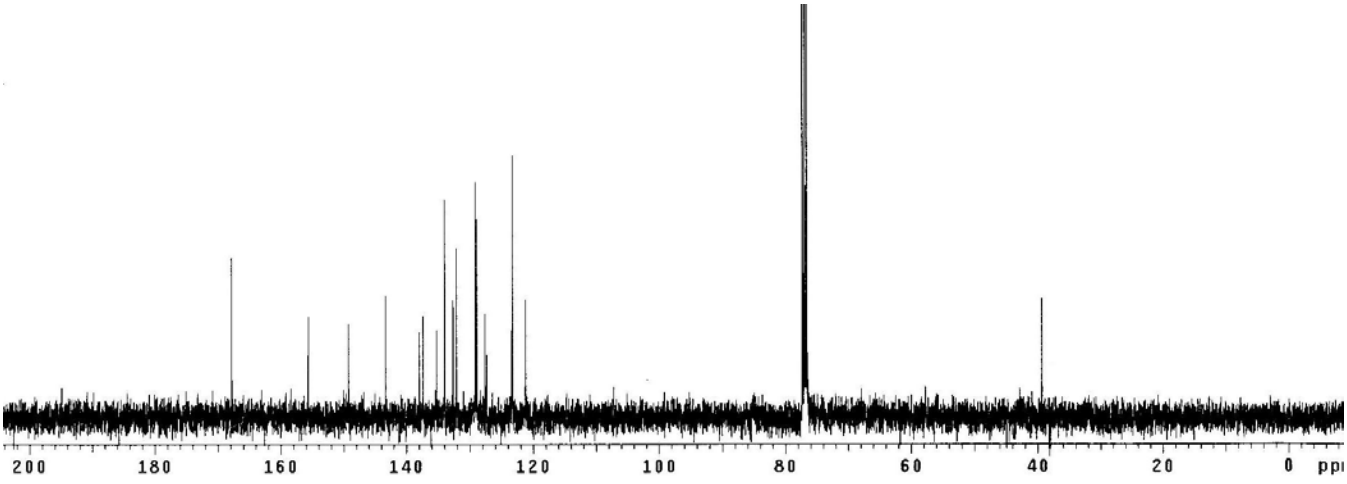
^{1}H NMR (400 MHz, $CDCl_3$): 8.48 (d, *J* = 4.4 Hz, 1H), 7.84 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.15 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.35 (m, 4H), 7.20 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.11 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.94 (ddd, *J* = 7.2, 4.8, 0.8 Hz, 1H), 6.75 (s, 1H) 6.66 (d, *J* = 15.2 Hz, 1H), 6.43 (d, *J* = 8.0 Hz, 1H), 5.39 (dt, *J* = 15.6, 6.4 Hz, 1H), 4.36 (d, *J* = 6.0, Hz, 2H).
^{13}C NMR (100 MHz, $CDCl_3$): 167.8, 155.6, 149.1, 143.2, 137.9, 137.3, 135.2, 133.9, 132.6, 132.0, 129.1, 128.9, 127.6, 127.3, 123.4, 123.3, 121.2, 39.3.
HRMS Calcd. for $C_{24}H_{18}N_2O_2$ (M): 366.1368, Found: 366.1366.
FTIR (NaCl Film): 2923, 2852, 1770, 1712, 1580, 1458, 1392, 1347, 954, 711 cm^{-1}.
MP 178 ^{0}C.

(6) Kang, S-K., Kim, S-G., Lee, J-S. *Tetrahedron Asymm*., **1992**, *3*, 1139.

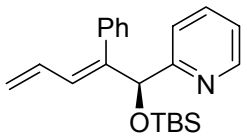


24





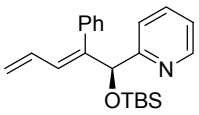
2-[1-(*tert*-Butyl-dimethyl-silanyloxy)-2-phenyl-penta-2,4-dienyl-pyridine



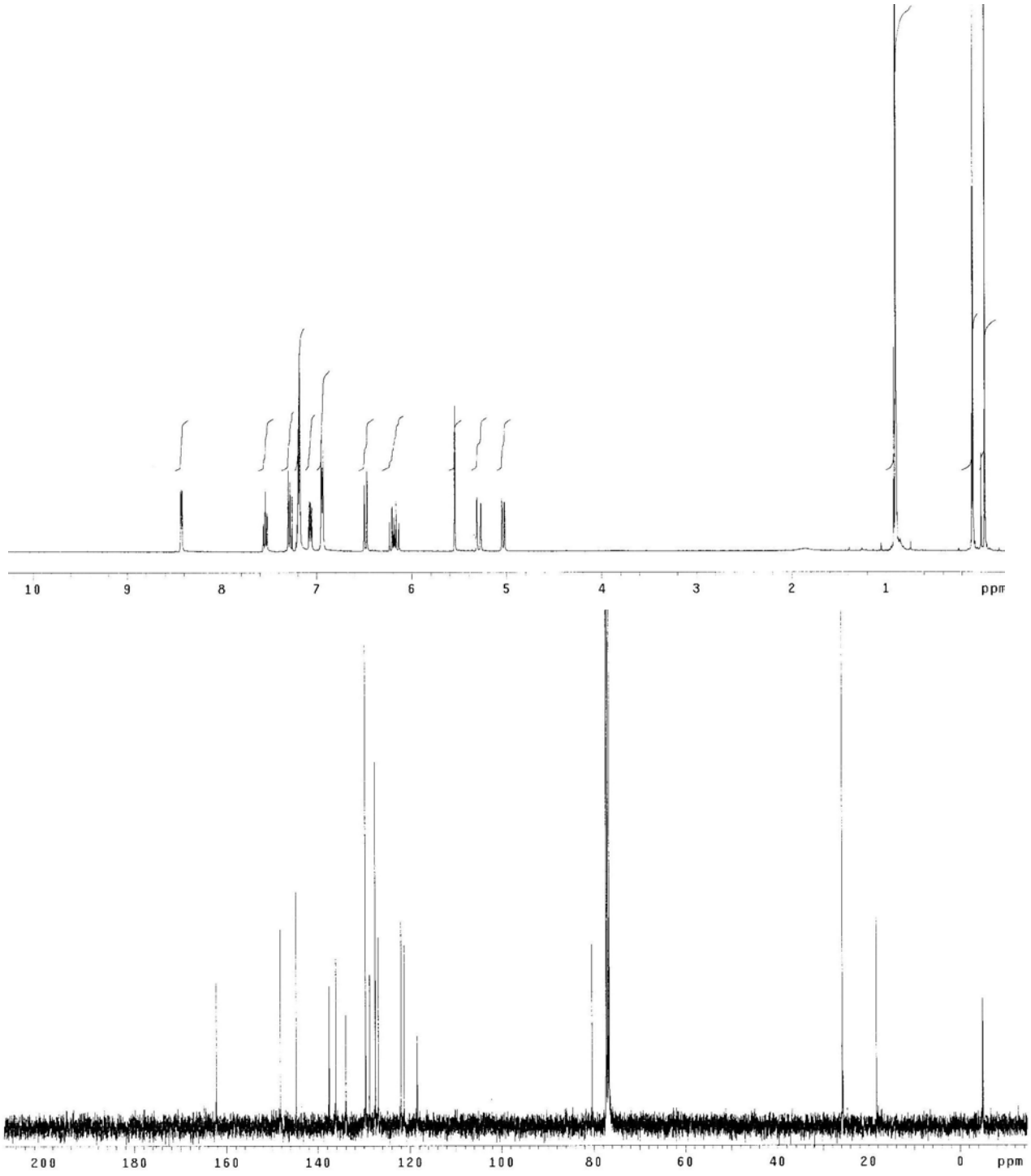
2b

To a solution of 2-phenyl-1-pyridin-2-yl-penta-2,4-dien-1-ol (**2**) (300.0 mg, 1.260 mmol, 100 mol%) and imidazole (170.0 mg, 2.520 mmol, 200 mol%) in dry DMF (4.2 mL) in 25 mL RB flask, *tert*-butyldimethylsilyl chloride (370.0 mg, 2.520 mmol) was added at 0 ^{o}C and and stirred at ambient temperature for 4 hours under argon atmosphere. The reaction mixture was quenched with saturated aqueous ammounium chloride (5.0 mL) and extracted with diethyl ether (2 x 30.0 mL) and washed with brine solution (20.0 mL).The organic layer was dried over anhydrous sodium sulfate and concentrated *in vacuo*. The crude was purified by flash column chromatography (R_f = 0.30, 10% EtOAc/hexanes) to afford (382.0 mg, 1.088 mmol) as a colorless oil (86% yield.).

^{1}H NMR (400 MHz, $CDCl_3$): 8.43 (ddd, *J* = 4.8, 2.0, 0.8 Hz, 1H), 7.52 (dt, *J* = 8.0, 1.6 Hz, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.18 (m, 3H), 7.06 (m, 1H), 6.93 (m, 2H), 6.48 (d, *J* = 10.8 Hz, 1H), 6.18 (dt, *J* = 16.8, 10.4 Hz, 1H), 5.51 (s, 1H), 5.29 (dd, *J* = 16.4, 1.6 Hz, 1H), 5.03 (dd, *J* = 10.4, 2.0 Hz, 1H), 0.91 (s, 9H), 0.086 (s, 3H), -0.040 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 162.2, 148.2, 144.7, 137.5, 136.1, 133.9, 129.6, 128.7, 127.5, 126.8, 121.9, 121.2, 118.4, 80.4, 25.8, 18.2, -4.8, -5.0.
HRMS Calcd. for $C_{22}H_{29}NOSi$ (M): 351.2018, Found: 351.2016.
FTIR (NaCl Film): 2954, 2928, 2856, 1588, 1570, 1470, 1433, 1254, 1102, 1102, 1079, 911, 868, 835, 702 cm^{-1}.


Ph
N
OTBS

2b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4
3
2
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ppm
200
180
160
140
120
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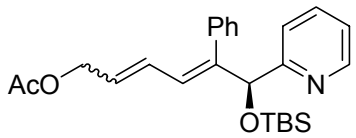
ppm

Acetic acid 6-(tert-butyl-dimethyl-silanyloxy)-5-phenyl-6-pyridin-2-yl-hexa-2,4-dienyl ester



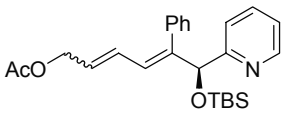
(Mixture of two diastereomers)

25

To a degassed solution of 2-[1-(*tert*-butyl-dimethyl-silanyloxy)-2-phenyl-penta-2,4-dienyl-pyridine (37.0 mg, 0.105 mmol, 100 mol%) and 1,4-diacetoxy-cis-2-butene (36.0 mg, 0.210 mmol, 200 mol%) in dry toluene (1.0 mL, 0.1 M) Grubbs' catalyst (10.0 mg, 0.0105 mmol, 10 mol%) was added in two portions over a period of 12 hours and the reaction mixture was heated at 100 ^{o}C in a sealed tube.[7] Then the reaction mixture was concentrated *in vacuo* and purified by flash column chromatography (R_f = 0.23, 15 % EtOAc/hexanes) to afford (24.0 mg, 0.057 mmol) as an yellow oil (54 % yield, *E*:*Z* = 5:1). The major diastereomer has been characterized.

^{1}H NMR (400 MHz, $CDCl_3$): 8.41 (d, *J* = 2.0 Hz, 1H), 7.54 (dt, *J* = 8.1, 1.8 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.18 (m, 3H), 7.06 (dd, *J* = 7.2, 5.4 Hz, 1H), 6.92 (m, 2H), 6.48 (d, *J* = 10.8 Hz, 1H), 6.11 (dd, *J* = 15.6, 11.2 Hz, 1H), 5.85 (m, 1H) 5.53 (s, 1H), 4.57 (m, 1H), 4.47 (d, *J* = 6.8 Hz, 1H), 2.19 (t, *J* = 4.4 Hz, 1H), 1.89 (s, 3H), 0.88 (s, 9H), 0.07 (s, 3H), -0.06 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 170.6, 162.0, 148.2, 137.2, 136.1, 131.2, 129.5, 128.0, 127.7, 127.5, 127.0, 126.7, 122.0, 121.2, 80.2, 64.8, 63.8, 38.2, 25.7, 18.9, -4.9, -5.0.
HRMS Calcd. for $C_{25}H_{33}NO_3Si$ (M): 422.2230, Found: 422.2232.
FTIR (NaCl Film): 2954, 2929, 2885, 2856, 1742, 1678, 1588, 1471, 1434, 1362, 1227, 1100, 1077, 1024, 836, 703 cm^{-1}.

(7) Kong, J-R.; Ngai, M-Y.; Krische, M. J. *J. Am. Chem. Soc.*, **2006**, *128*, 718.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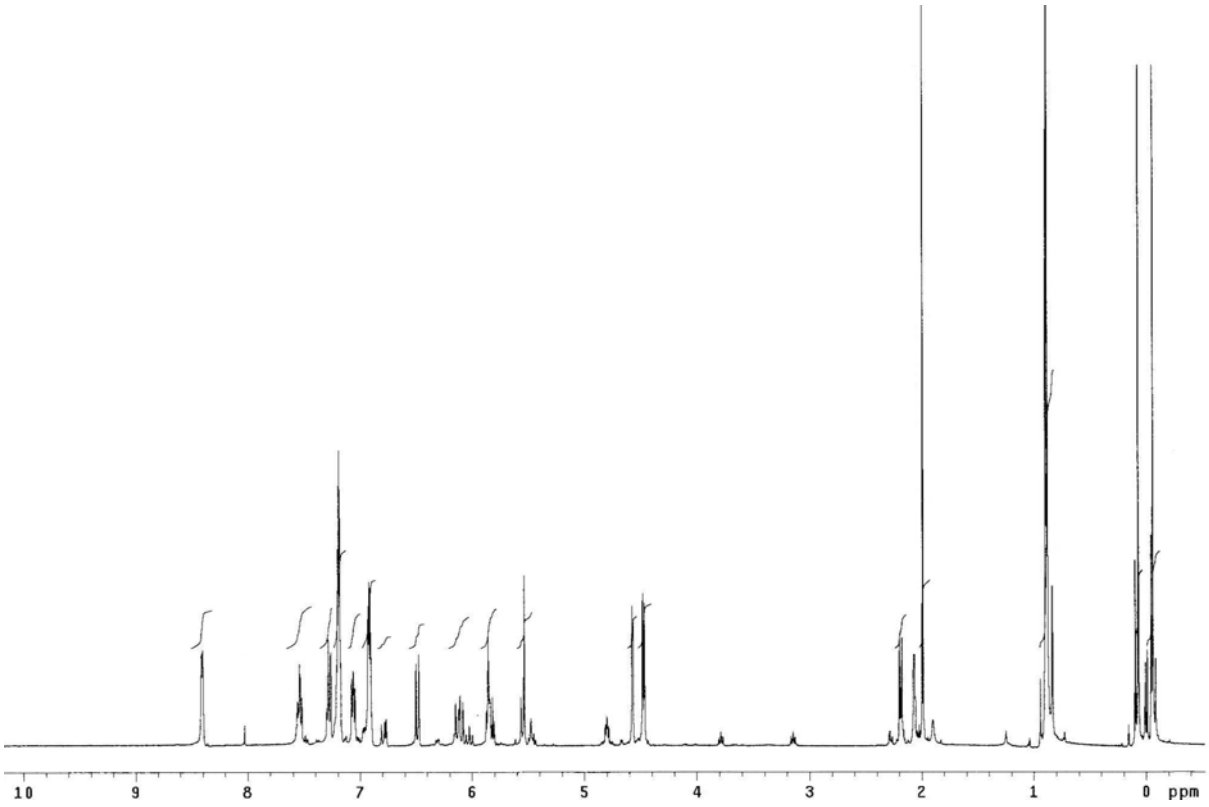
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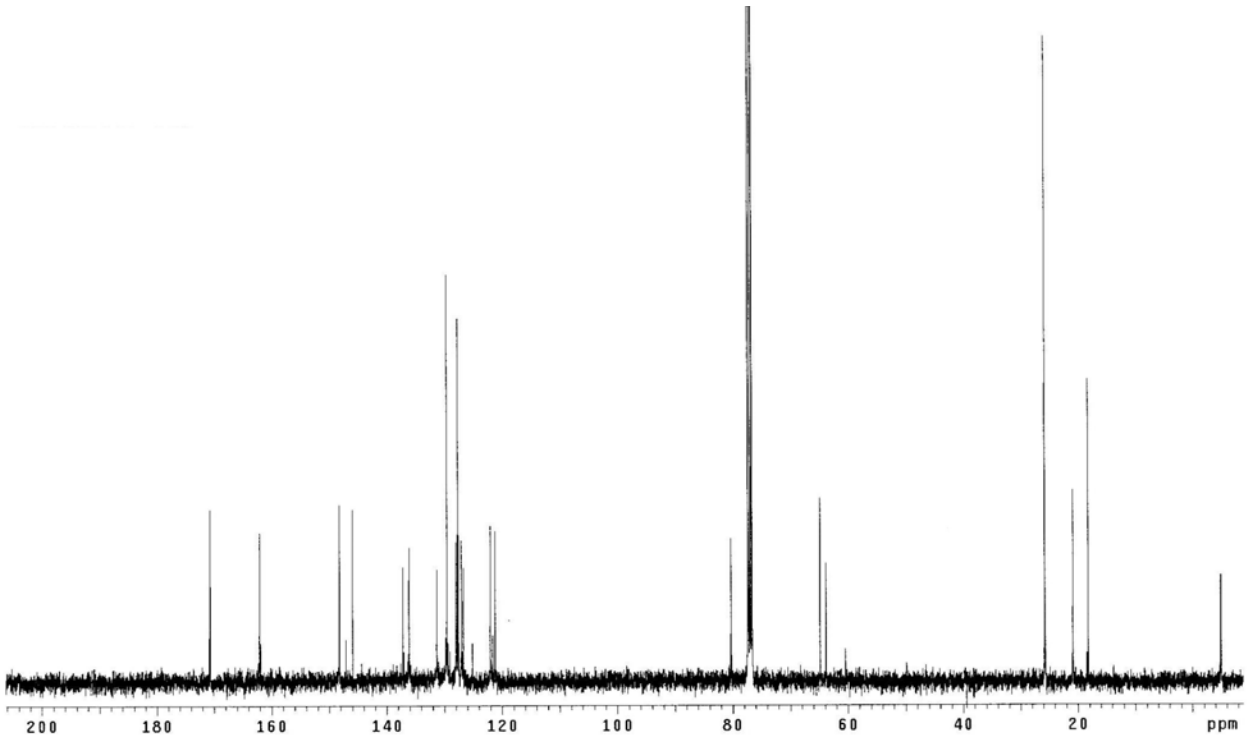
200
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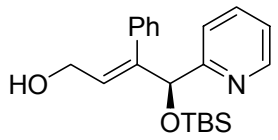
ppm

4-(*tert*-Butyl-dimethyl-silanyloxy)-3-phenyl-4-pyridin-2-yl-but-2-en-1-ol

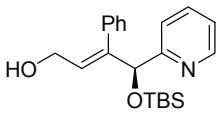


26

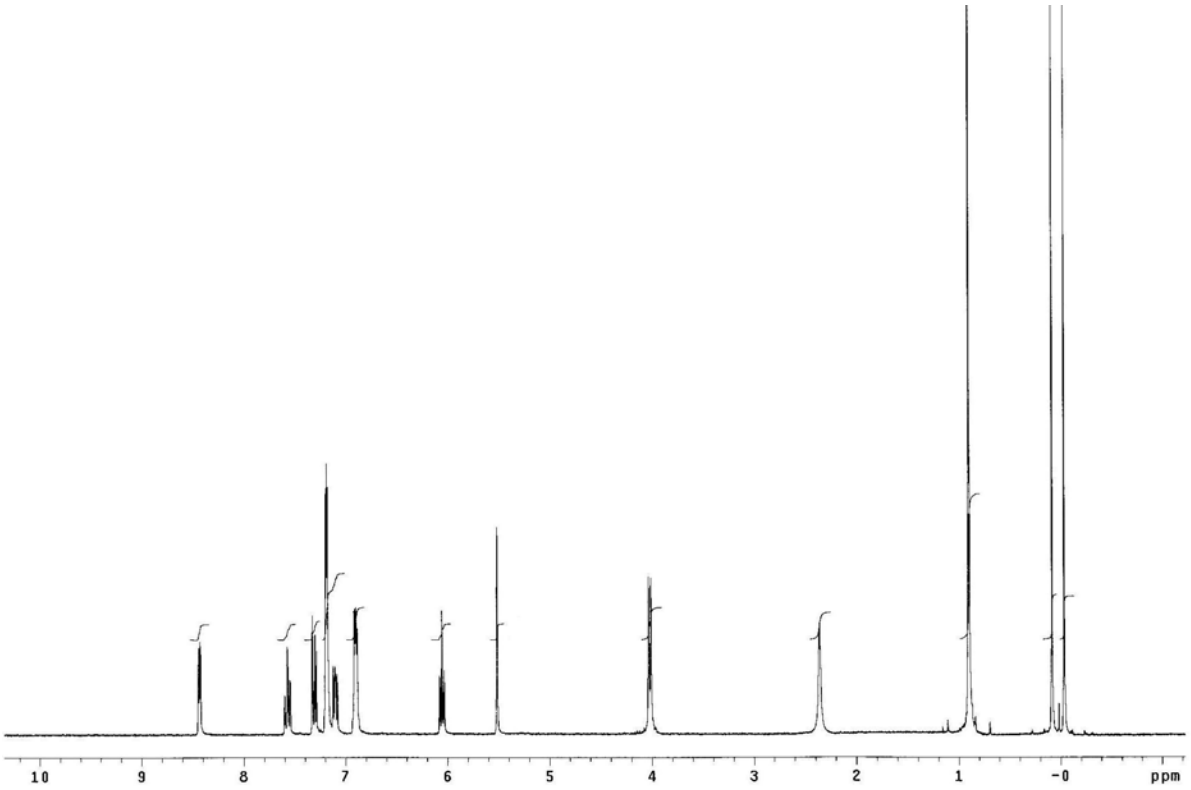
To a suspension of 2-[1-(*tert*-butyl-dimethyl-silanyloxy)-2-phenyl-penta-2,4-dienyl-pyridine (**2b**) (230.0 mg, 0.650 mmol, 100 mol%) in 2.0 mL of water and 4.0 mL of THF in a 25 mL RB flask, OsO_4 (8.0 mg, 0.032 mmol, 5 mol%) was added and then stirred for 5 minutes. While the temperature of the stirred mixture was maintained at 0 °C, sodium periodate (280.0 mg, 1.310 mmol, 200 mol%) was added in portions over a period of 40 minutes. The solution was stirred for an additional 4 hours.[6] The reaction mixture was extracted thoroughly with ether (2 x 30.0 mL) and the combined organic layers were dried (anhydrous Na_2SO_4). The solvent was removed *in vacuo*, and then the corresponding enal was purified by flash silica gel chromatography (R_f = 0.23, 20% EtOAc/hexane) to afford (190.0 mg, 0.788 mmol) as a colorless oil (83% yield).

To a solution of the enal (prepared as mentioned above) (70.0 mg, 0.198 mmol, 100 mol%) in THF (1.0 mL, 0.2 M) in a 10 mL RB flask, sodium borohydride (7.2 mg, 0.198 mmol, 100 mol%) was added at 0 ^oC and stirred for two hours. The reaction mixture was quenched with 0.5 N hydrochloric acid (0.5 mL) and extracted with EtOAc (2 x 20.0 mL). The organic layer was dried (anhydrous Na_2SO_4). The solvent was removed *in vacuo*, and then the corresponding alcohol was purified by flash chromatography (R_f = 0.20, 35% EtOAc/hexanes) to afford (66.0 mg, 0.273 mmol) as a colorless syrup (94% yield).

^{1}H NMR (400 MHz, $CDCl_3$): 8.43 (m, 1H), 7.57 (dt, *J* = 8.1, 1.8 Hz, 1H), 7.31 (d, *J* = 7.8Hz, 1H), 7.18 (m, 2H), 7.10 (m, 2H), 6.90 (m, 2H), 6.05 (t, *J* = 6.9 Hz, 1H), 5.5 (s, 1H), 4.01 (d, *J* = 6.6 Hz, 2H), 2.36 (s, 1H), 0.90 (s, 9H), 0.08 (s, 3H), -0.04 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 161.9, 148.1, 144.7, 136.8, 136.3, 129.1, 128.6, 127.5, 127.0, 122.0, 121.3, 80.1, 59.8, 25.7, 18.2, -4.8, -5.0.
HRMS Calcd. for $C_{15}H_{15}NO_2$ (M): 241.1103, Found: 241.1104.
FTIR (NaCl Film): 3309, 3055, 2954, 2856, 1593, 1572, 1471, 1434, 1254, 1105, 1054, 1004, 867, 779, 702.


Ph
HO
N
OTBS

26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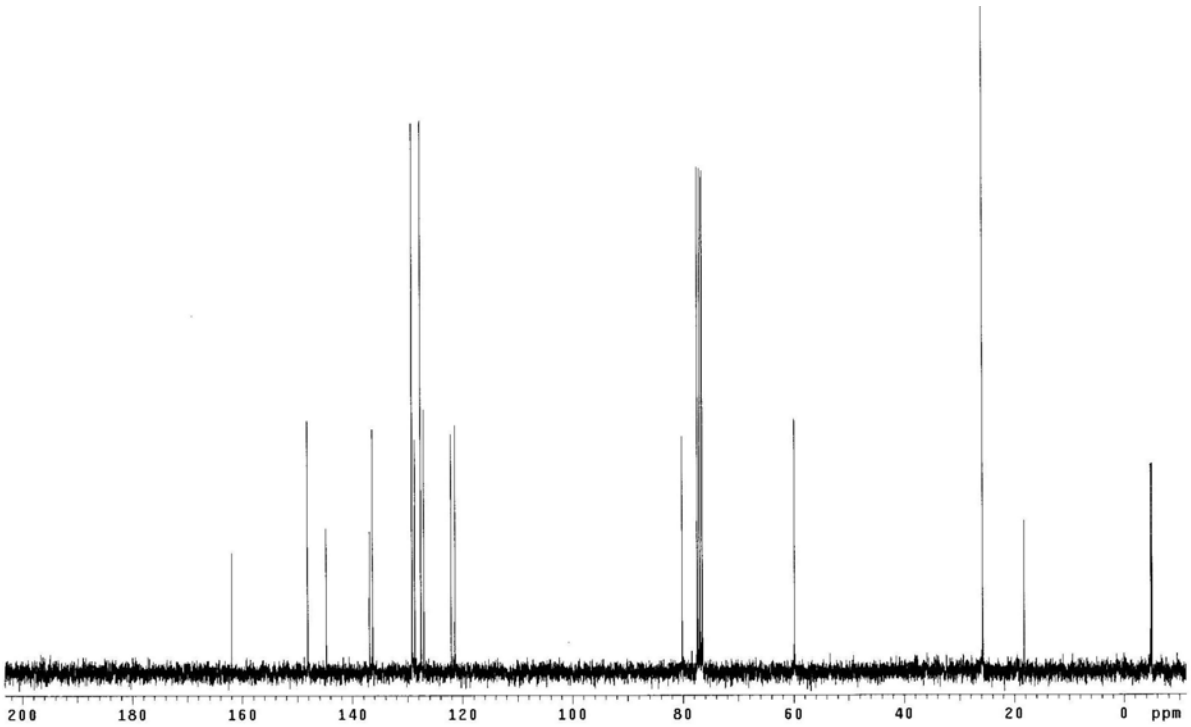
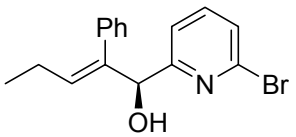
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

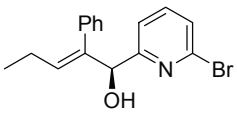
1-(6-Bromo-pyridin-2-yl)-2-phenyl-pent-2-en-1-ol



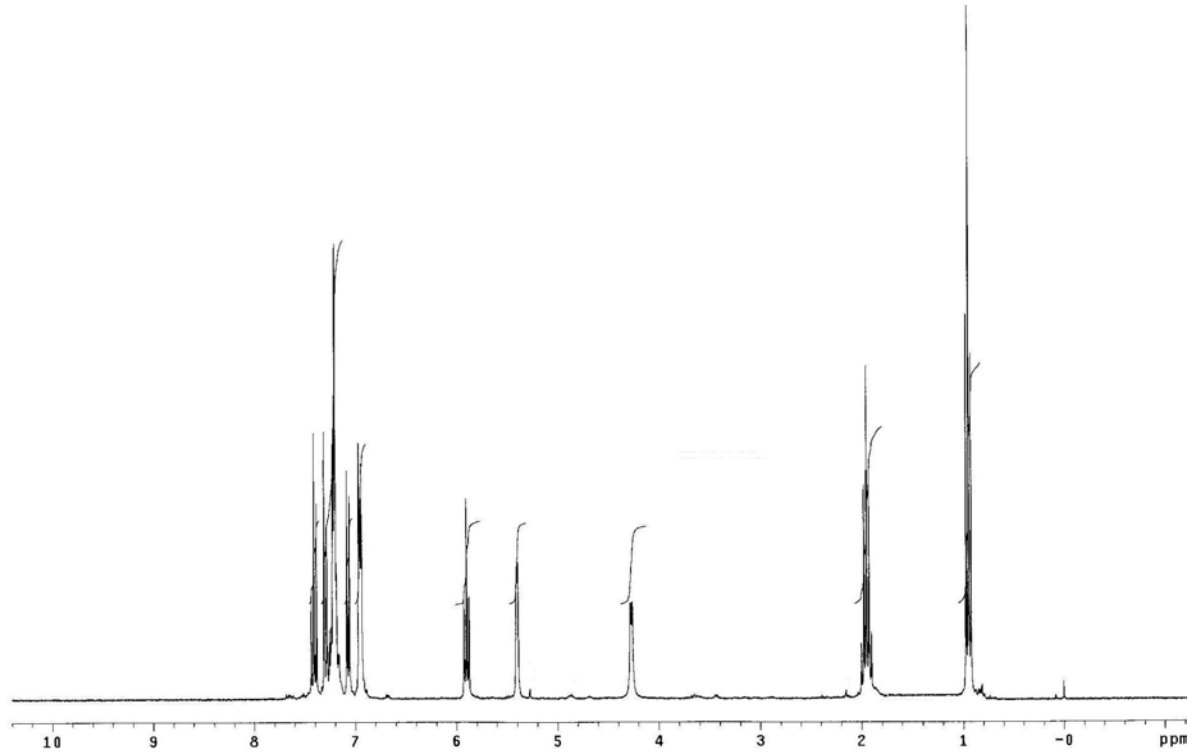
27

To a degassed solution of 1-(6-Bromo-pyridin-2-yl)-2-phenyl-penta-2,4-dien-1-ol (**8**) (180.0 mg, 0.569 mmol, 100 mol%) in toluene (2.8 mL, 0.2 M) in a 13 x 100 mm test tube $RhCl(PPh_3)_3$ (53.0 mg, 0.057 mmol, 10 mol%) was added. The system was purged with argon gas followed by hydrogen gas. The reaction was allowed to stir at 40 ^oC under 1 atm of hydrogen for 24 hours.[7] The solvent was evaporated *in vacuo* and the title compound was purified by flash column chromatography (R_f = 0.3, 8% EtOAc/hexanes) to afford (152.0 mg, 0.479 mmol) as a pale yellow syrup (82% yield).

^{1}H NMR (300 MHz, $CDCl_3$): 7.41 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 10.0Hz, 1H), 7.20 (m, 3H), 5.90 (t, *J* = 14.7Hz, 1H), 5.40 (d, *J* = 3.6 Hz, 1H), 4.27 (d, *J* = 4.8 Hz, 1H), 1.95 (quintet, *J* = 7.5 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$): 161.6, 140.6, 140.4, 138.5, 137.1, 129.3, 127.7, 126.8, 126.4, 120.0, 22.0, 14.1.
HRMS Calcd. for $C_{16}H_{16}BrNO$ (M): 317.0415. Found: 317.0417.
FTIR (NaCl Film): 3020, 3000, 2980, 1747, 1580, 1556, 1493, 1434, 1370, 1227, 1156, 1122, 986, 702 cm^{-1}.


Ph
N
Br
OH

27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6
5
4
3
2
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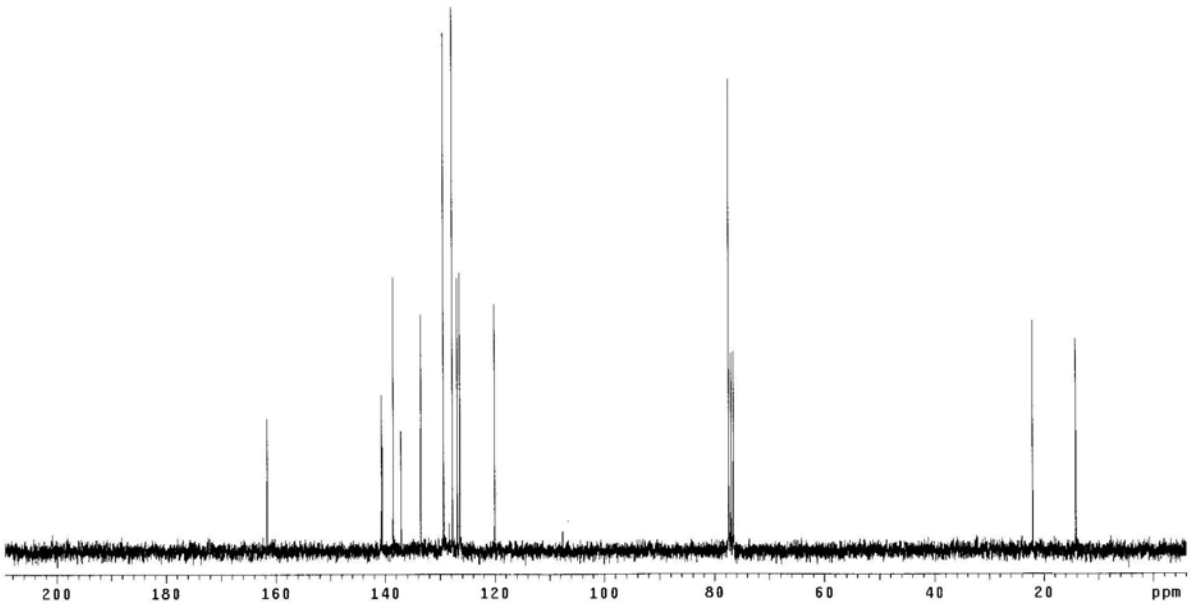
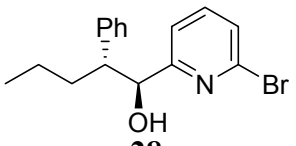
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

1-(6-Bromo-pyridin-2-yl)-2-phenyl-pentane-1-ol

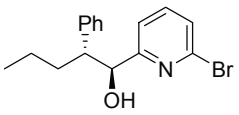


28

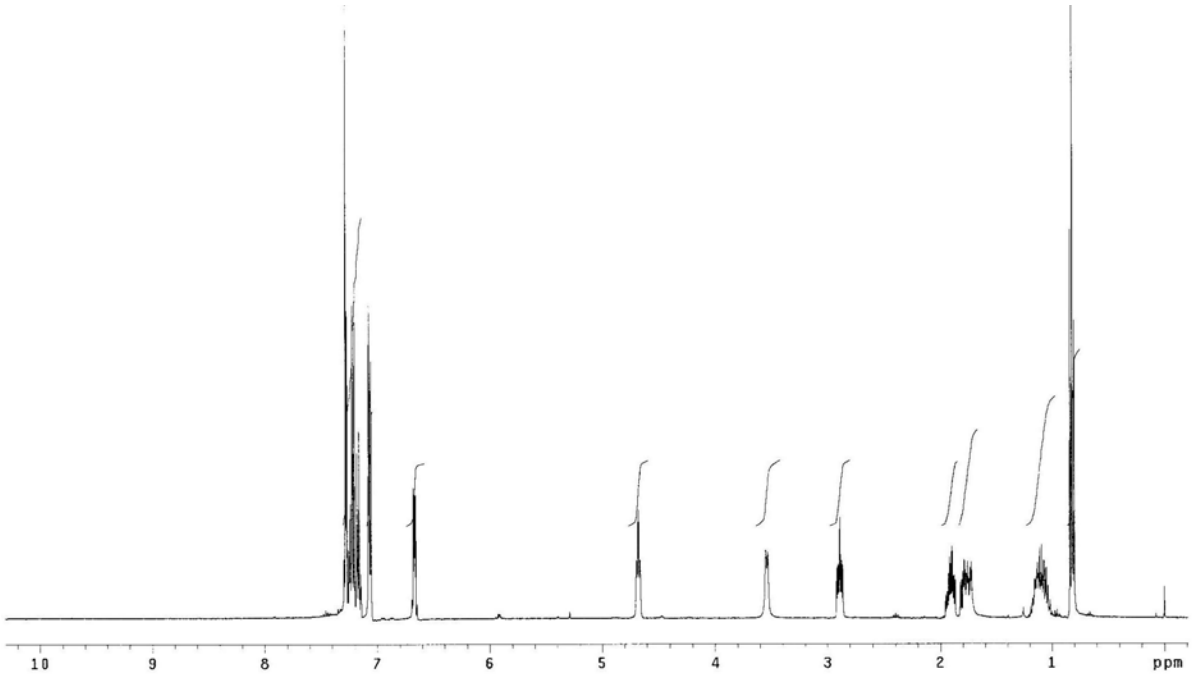
(Mixture of two diastereomers)

To a degassed solution of 1-(6-Bromo-pyridin-2-yl)-2-phenyl-penta-2,4-dien-1-ol **(8)** (100.0 mg, 0.3160 mmol, 100 mol%) in toluene (1.6 mL, 0.2 M) in a 13 x 100 mm test tube at ambient temperature Ir(COD)(Pyr)[P(*c*-Hex)$_3$]PF$_6$ (27.0 mg, 0.0316 mmol, 10 mol%) was added The system was purged with argon gas followed by hydrogen gas. The reaction was allowed to stir at 40 ^{o}C under 1 atm of hydrogen for 24 hours.[7] The title compound was purified by flash column chromatography (R_f = 0.28, 8% EtOAc/hexane) to afford (63.0 mg, 0.196 mmol) as a colorless oil (63% yield, 20:1 diastereomeric ratio).

^{1}H NMR (400 MHz, $CDCl_3$): 7.21 (m, 5H), 7.06 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.66 (dd, *J* = 6.0, 3.2 Hz, 1H), 4.68 (t, *J* = 6.4 Hz, 1H), 3.54 (d, *J* = 7.2 Hz, 1H), 2.89 (m, 1H), 1.91 (m, 1H), 1.77 (m, 1H), 1.10 (m, 2H) 0.81 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 162.6, 141.4, 140.8, 138.1, 128.6, 128.2, 126.5, 126.4, 120.4, 77.4, 53.3, 32.2, 20.4, 14.0.
HRMS Calcd. for $C_{16}H_{18}BrNO$ (M): 320.0650, Found: 320.0645.
FTIR (NaCl Film): 3424, 2955, 2869, 2348, 1581, 1558, 1436, 1408, 1167, 1126, 1049, 701 cm^{-1}.


Ph
N
Br
OH

28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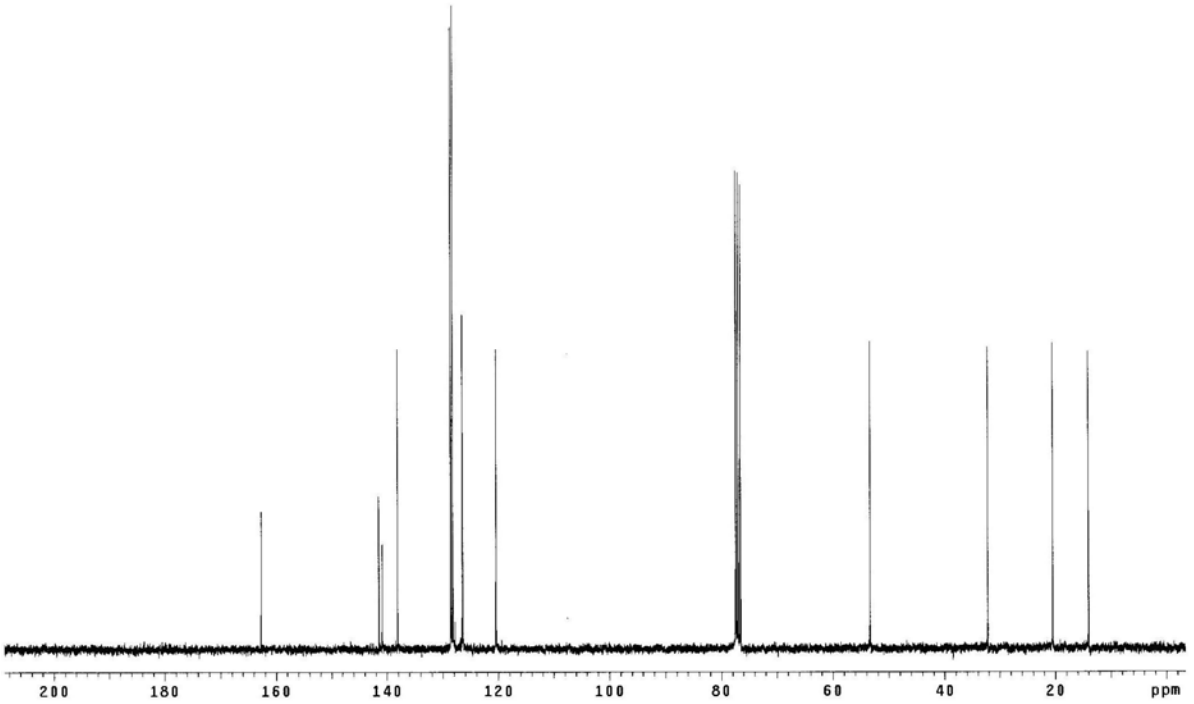
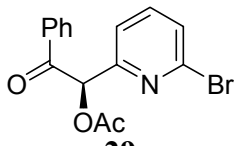
7
6
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

Acetic acid 1-(6-bromo—pyridin-2-yl)-2-oxo-2-phenyl-ethyl ester

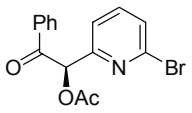


29

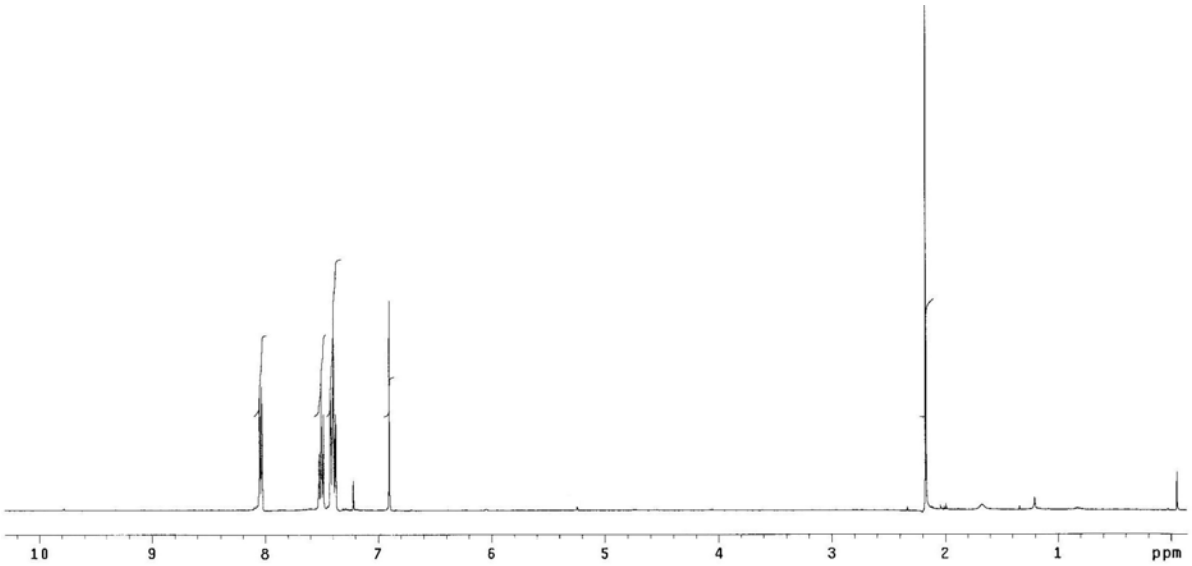
To a solution of 1-(6-bromo-pyridin-2-yl)-2-phenyl-pent-2-en-1-ol (**27**) (100.0 mg, 0.313 mmol) and triethylamine (0.5 mL) in freshly distilled DCM (2.0 mL) in a 10 mL RB flask, acetic anhydride (0.1 mL, 0.626 mmol) was added and catalytic amount of DMAP were added and stirred at ambient temperature for 1 hour. The reaction mixture was quenched with water and extracted with DCM (2 x 10 mL) and washed with brine solution (5.0 mL). The organic layer was dried (anhydrous Na_2SO_4), concentrated and the crude material was purified by flash column chromatography (R_f = 0.32, 4% EtOAc/hexanes) to afford (109.8 mg, 0.329 mmol) as an yellow oil (97% yield).

The acetylated product (90.0 mg, 0.250 mmol, 100 mol%) was dissolved in DCM (3.0 mL, 0.2 M), in a 10 mL RB flsk and the solution was cooled to -78 °C. The solution was sparged with ozone for 2 min, and sparged with argon for 5 min. Then triphenylphosphine (65.0 mg, 0.500 mmol, 200 mol%) was added, and the reaction was allowed to stir for 10 hours while warming gradually to ambient temperature. The solvent was removed *in vacuo*. The title compound was purified by flash column chromatography (R_f = 0.3, 20% EtOA/hexane) to afford (55.0 mg, 0.165 mmol) as a colorless oil (77% yield).

^{1}H NMR (400 MHz, $CDCl_3$): 8.02 (dd, *J* = 7.6, 0.8 Hz, 2H), 7.50 (t, *J* = 8.0, Hz, 2H), 7.39 (m, 4H), 6.90 (s, 1H), 2.17 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): 192.4, 160.7, 154.9, 141.6, 139.3, 134.0, 133.8, 129.2, 128.6, 128.3, 121.8, 78.1, 20.6.
HRMS Calcd. for $C_{15}H_{12}BrNO_3$ (M): 333.0001, Found: 332.9999.
FTIR (NaCl Film): 3065, 2359, 1747, 1697, 1579, 1557, 1434, 1372, 1227, 1123, 1064, 988, 791, 688 cm^{-1}.


Ph
O
N
Br
OAc

29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9
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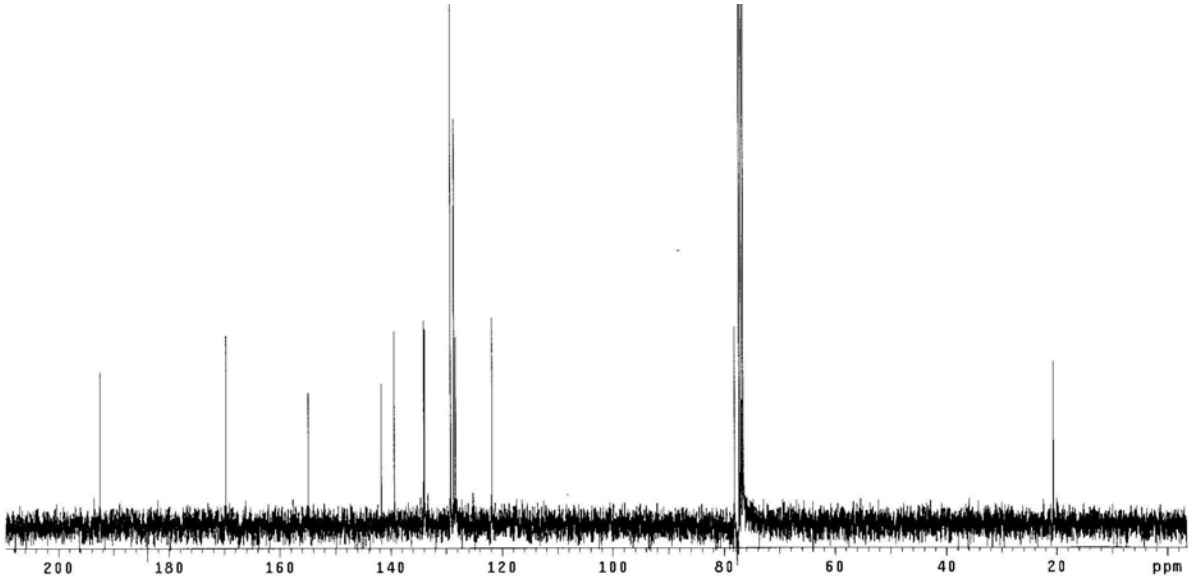
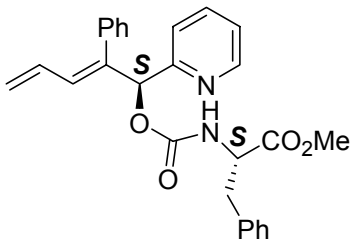
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

III. Absolute Stereochemistry Determination

3-Phenyl-2-(2-phenyl-1-pyridin-2-yl-penta-2,4-dienloxycarbonylamino)-propionic acid methyl ester

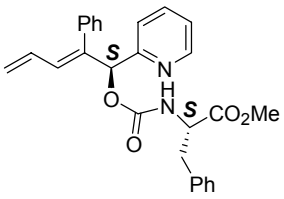


2c

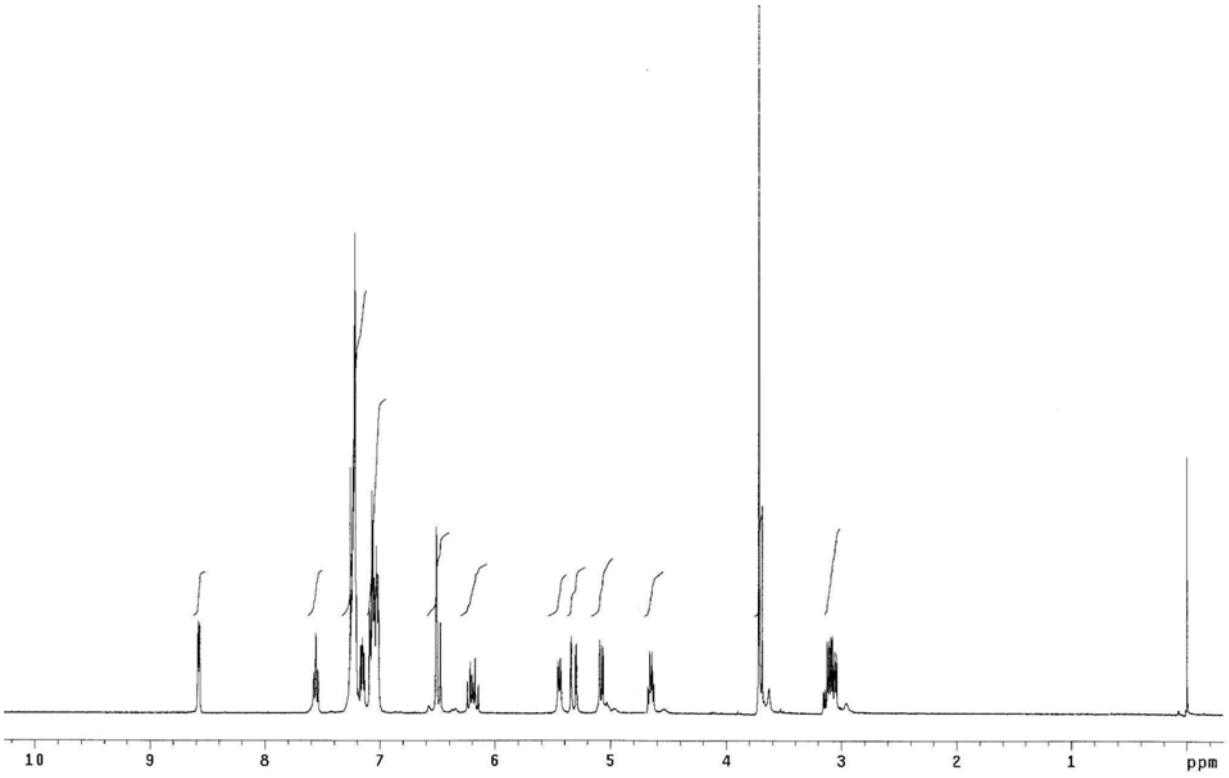
A mixture of 2-phenyl-1-pyridin-2-yl-penta-2,4-dien-1-ol (200.0 mg, 0.843 mmol, 100 mol%) and isocyanate derived from (*L*)- phenylalanine methyl ester (190.0 mg, 0.928 mmol, 110 mol%) was heated in toluene (1.7 mL, 0.5 M) at 90 ^{o}C for 26 hours.[8] The solvent was removed *in vacuo*, and the title compound was purified by flash column chromatography (R_f = 0.23, 35% EtOAc/hexanes) to afford (290.0 mg, 0.654 mmol) as a white solid (78% yield)

^{1}H NMR (400 MHz, $CDCl_3$): 8.57 (dd, *J* = 4.8, 0.8 Hz, 1H), 7.56 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.19 (m, 7H), 7.18 (m, 2H), 7.04 (m, 5H), 6.51 (s, 1H), 6.47 (s, 1H), 6.18 (dt, *J* = 16.8, 10.4 Hz, 1H), 5.44 (d, *J* = 8.0 Hz, 1H), 5.32 (dd, *J* = 17.2, 1.2 Hz, 1H) 5.01 (dd, *J* = 10.0, 1.6 Hz, 1H), 4.65 (m, 2H), 3.71 (s, 3H), 3.09 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 157.7, 154.5, 149.3, 140.2, 137.0, 136.3, 135.6, 133.3, 130.6, 129.5, 129.3, 129.2, 128.5, 128.4, 127.9, 127.3, 127.0, 122.6, 121.6, 80.3, 54.8, 52.3, 38.0.
HRMS Calcd. for $C_{27}H_{26}N_2O_4$ (M+1): 443.1971, Found: 443.1967.
FTIR (NaCl Film): 3345, 3028, 2951, 1726, 1590, 1496, 1435, 1362, 1253, 1212, 1049, 812, 702.
MP 121 ^{o}C.

(8) Paquette, L. A., Wiedeman, P. E, .Bulman, P. C. *J. Org. Chem*., **1988**, *53*, 1441.


Ph
S
N
H
O
N
S
CO2Me
O
Ph

2c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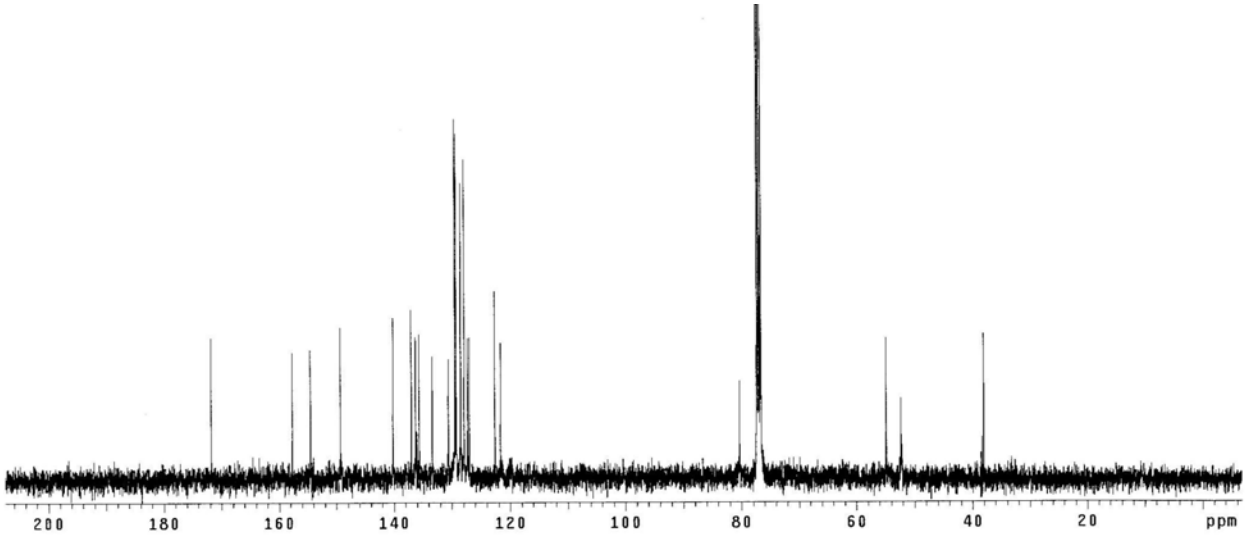
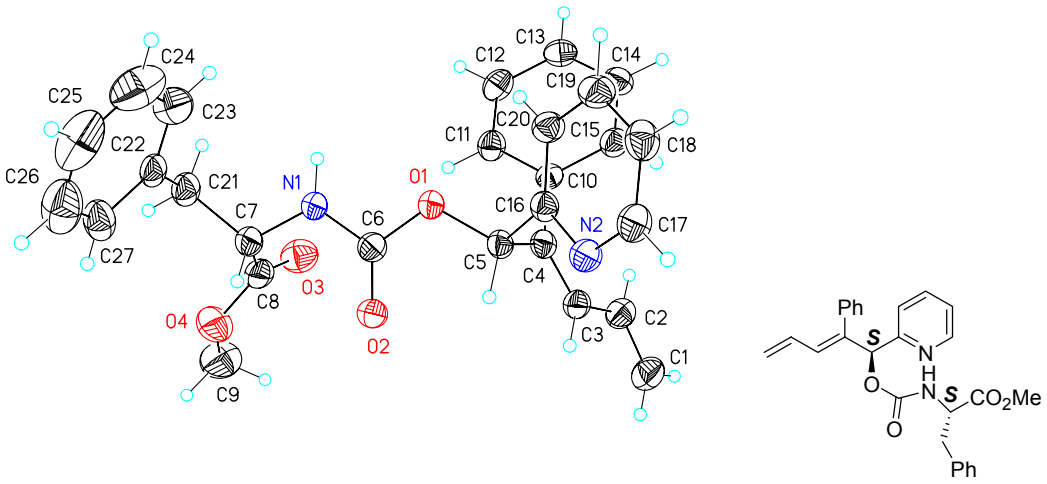
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

X-Ray Crystallographic data

View of the molecule **2c** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



X-ray Experimental.

Table 1. Crystallographic Data

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms.

Table 3. Bond Lengths (Å) and Angles (^{o}) for the non-hydrogen atoms.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms.

Table 6. Torsion Angles (^{o}) for the non-hydrogen atoms.

Table 7. Observed and calculated structure factor amplitudes. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

X-ray Experimental for 2c

Crystals grew as large, colorless prisms by slow evaporation from DCM/hexanes sovent mixture.The data crystal was cut from a larger crystal and had approximate dimensions; 0.28 x 0.28 x 0.25 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073 Å). A total of 173 frames of data were collected using ω-scans with a scan range of 1.5° and a counting time of 64 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The absolute configuration was established by internal comparison to the known configuration at C7. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0434*P)^2 + (1.0685*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0**.**116, with R(F) equal to 0.0455 and a goodness of fit, S, = 1.03. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (2.0(2)x10^{-5})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for **2c**.

Empirical formula	C27 H26 N2 O4	
Formula weight	442.50	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21	
Unit cell dimensions	a = 15.6756(5) Å	α= 90°.
	b = 6.9546(3) Å	β= 90.784(2)°.
	c = 21.4312(9) Å	γ = 90°.
Volume	2336.16(16) $Å^3$	
Z	4	
Density (calculated)	1.258 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	936	
Crystal size	0.28 x 0.28 x 0.25 mm^3	
Theta range for data collection	2.29 to 27.50°.	
Index ranges	-20<=h<=20, -9<=k<=8, -27<=l<=27	
Reflections collected	9634	
Independent reflections	5754 [R(int) = 0.0330]	
Completeness to theta = 27.50°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5754 / 1 / 596	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1086	
R indices (all data)	R1 = 0.0602, wR2 = 0.1162	
Extinction coefficient	2.00(17)x10^{-5}	
Largest diff. peak and hole	0.238 and -0.222 e.$Å^{-3}$	

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

	x	y	z	U(eq)
O1'	4502(1)	2983(3)	7185(1)	35(1)
O2'	5180(1)	2408(3)	6271(1)	35(1)
O3'	6208(1)	7120(4)	6447(1)	47(1)
O4'	6234(1)	6492(4)	5422(1)	46(1)
N1'	4604(2)	5331(4)	6484(1)	29(1)
N2'	3907(2)	-1869(4)	7523(1)	38(1)
C1'	7130(3)	-1505(8)	8601(2)	72(1)
C2'	6499(2)	-221(6)	8573(2)	50(1)
C3'	5916(2)	-75(6)	8043(2)	41(1)
C4'	5268(2)	1168(5)	7984(1)	32(1)
C5'	4696(2)	1051(5)	7406(1)	33(1)
C6'	4799(2)	3489(5)	6614(1)	27(1)
C7'	4910(2)	6159(5)	5911(1)	27(1)
C8'	5856(2)	6641(5)	5967(2)	33(1)
C9'	7147(2)	6858(7)	5419(2)	61(1)
C10'	5011(2)	2551(5)	8482(1)	33(1)
C11'	5096(2)	4527(5)	8405(2)	45(1)
C12'	4839(3)	5795(6)	8860(2)	56(1)
C13'	4477(2)	5106(6)	9408(2)	46(1)
C14'	4395(2)	3150(6)	9495(2)	43(1)
C15'	4660(2)	1885(5)	9038(2)	37(1)
C16'	3871(2)	51(5)	7553(1)	31(1)
C17'	3190(3)	-2842(6)	7669(2)	50(1)
C18'	2429(2)	-1987(6)	7830(2)	46(1)
C19'	2410(2)	-11(6)	7854(2)	44(1)
C20'	3141(2)	1016(6)	7717(2)	41(1)
C21'	4429(2)	8011(5)	5731(1)	31(1)
C22'	3499(2)	7669(5)	5578(1)	31(1)
C23'	3231(2)	7139(5)	4981(1)	37(1)
C24'	2375(2)	6855(5)	4847(2)	43(1)
C25'	1775(2)	7030(5)	5312(2)	42(1)
C26'	2034(2)	7521(6)	5903(2)	44(1)
C27'	2886(2)	7863(5)	6035(1)	38(1)
O1	9215(1)	8313(3)	7741(1)	29(1)
O2	10202(2)	8701(4)	8523(1)	43(1)
O3	11151(2)	4312(4)	8237(1)	50(1)
O4	11328(2)	4469(4)	9275(1)	53(1)
N1	9498(2)	5868(4)	8388(1)	31(1)
N2	8559(2)	13087(4)	7471(1)	33(1)
C1	11856(2)	13034(6)	6461(2)	47(1)
C2	11239(2)	11725(5)	6431(2)	37(1)
C3	10639(2)	11442(5)	6928(1)	30(1)
C4	10010(2)	10131(5)	6955(1)	28(1)
C5	9420(2)	10219(4)	7510(1)	27(1)
C6	9688(2)	7703(5)	8241(1)	31(1)
C7	9943(2)	4976(5)	8909(1)	33(1)
C8	10868(2)	4550(5)	8750(2)	38(1)
C9	12245(2)	4194(8)	9209(2)	64(1)
C10	9799(2)	8717(4)	6453(1)	26(1)
C11	9835(2)	6738(5)	6562(2)	33(1)
C12	9600(2)	5442(5)	6101(2)	37(1)

C13	9324(2)	6095(5)	5520(1)	35(1)
C14	9300(2)	8041(5)	5401(1)	34(1)
C15	9529(2)	9345(5)	5864(1)	32(1)
C16	8587(2)	11199(5)	7335(1)	27(1)
C17	7854(2)	14039(5)	7297(1)	38(1)
C18	7168(2)	13216(6)	6994(2)	39(1)
C19	7201(2)	11278(6)	6857(2)	37(1)
C20	7926(2)	10258(5)	7030(1)	33(1)
C21	9487(2)	3143(5)	9116(1)	37(1)
C22	8687(2)	3541(5)	9475(1)	33(1)
C23	7886(2)	3563(6)	9199(2)	51(1)
C24	7174(3)	3945(7)	9566(2)	70(1)
C25	7292(3)	4290(7)	10200(2)	73(1)
C26	8081(3)	4264(7)	10463(2)	68(1)
C27	8775(3)	3914(6)	10112(2)	46(1)

Table 3. Bond lengths [Å] and angles [°] for **2c**.

O1'-C6'	1.362(3)	C24'-C25'	1.385(5)
O1'-C5'	1.456(4)	C24'-H24B	0.95
O2'-C6'	1.213(4)	C25'-C26'	1.368(5)
O3'-C8'	1.207(4)	C25'-H25B	0.95
O4'-C8'	1.320(4)	C26'-C27'	1.383(4)
O4'-C9'	1.454(4)	C26'-H26B	0.95
N1'-C6'	1.346(4)	C27'-H27B	0.95
N1'-C7'	1.444(4)	O1-C6	1.362(3)
N1'-H1'C	0.88	O1-C5	1.452(4)
N2'-C16'	1.338(4)	O2-C6	1.219(4)
N2'-C17'	1.351(5)	O3-C8	1.202(4)
C1'-C2'	1.334(6)	O4-C8	1.328(4)
C1'-H1'A	0.95	O4-C9	1.460(4)
C1'-H1'B	0.95	N1-C6	1.349(4)
C2'-C3'	1.452(5)	N1-C7	1.449(4)
C2'-H2'A	0.95	N1-H1C	0.88
C3'-C4'	1.338(5)	N2-C17	1.337(4)
C3'-H3'A	0.95	N2-C16	1.346(4)
C4'-C10'	1.496(5)	C1-C2	1.330(5)
C4'-C5'	1.521(4)	C1-H1A	0.95
C5'-C16'	1.505(5)	C1-H1B	0.95
C5'-H5'A	1.00	C2-C3	1.445(4)
C7'-C8'	1.524(4)	C2-H2A	0.95
C7'-C21'	1.538(4)	C3-C4	1.345(4)
C7'-H7'A	1.00	C3-H3A	0.95
C9'-H9'A	0.98	C4-C10	1.491(4)
C9'-H9'B	0.98	C4-C5	1.517(4)
C9'-H9'C	0.98	C5-C16	1.516(4)
C10'-C11'	1.391(5)	C5-H5A	1.00
C10'-C15'	1.397(4)	C7-C8	1.524(5)
C11'-C12'	1.380(5)	C7-C21	1.530(5)
C11'-H11B	0.95	C7-H7A	1.00
C12'-C13'	1.396(6)	C9-H9A	0.98
C12'-H12B	0.95	C9-H9B	0.98
C13'-C14'	1.379(6)	C9-H9C	0.98
C13'-H13B	0.95	C10-C11	1.397(5)
C14'-C15'	1.384(5)	C10-C15	1.396(4)
C14'-H14B	0.95	C11-C12	1.385(5)
C15'-H15B	0.95	C11-H11A	0.95
C16'-C20'	1.376(5)	C12-C13	1.389(5)
C17'-C18'	1.380(6)	C12-H12A	0.95
C17'-H17B	0.95	C13-C14	1.377(5)
C18'-C19'	1.376(6)	C13-H13A	0.95
C18'-H18B	0.95	C14-C15	1.388(4)
C19'-C20'	1.385(5)	C14-H14A	0.95
C19'-H19B	0.95	C15-H15A	0.95
C20'-H20B	0.95	C16-C20	1.382(4)
C21'-C22'	1.509(4)	C17-C18	1.373(5)
C21'-H21C	0.99	C17-H17A	0.95
C21'-H21D	0.99	C18-C19	1.380(5)
C22'-C27'	1.388(4)	C18-H18A	0.95
C22'-C23'	1.390(4)	C19-C20	1.386(4)
C23'-C24'	1.383(4)	C19-H19A	0.95
C23'-H23B	0.95	C20-H20A	0.95

C21-C22	1.504(4)	C24-C25	1.389(7)
C21-H21A	0.99	C24-H24A	0.95
C21-H21B	0.99	C25-C26	1.351(7)
C22-C23	1.381(5)	C25-H25A	0.95
C22-C27	1.395(4)	C26-C27	1.354(6)
C23-C24	1.400(6)	C26-H26A	0.95
C23-H23A	0.95	C27-H27A	0.95

C6'-O1'-C5'	117.3(2)	C11'-C12'-C13'	120.1(4)
C8'-O4'-C9'	116.4(3)	C11'-C12'-H12B	119.9
C6'-N1'-C7'	118.6(3)	C13'-C12'-H12B	119.9
C6'-N1'-H1'C	120.7	C14'-C13'-C12'	119.4(4)
C7'-N1'-H1'C	120.7	C14'-C13'-H13B	120.3
C16'-N2'-C17'	117.0(3)	C12'-C13'-H13B	120.3
C2'-C1'-H1'A	120.0	C13'-C14'-C15'	120.2(4)
C2'-C1'-H1'B	120.0	C13'-C14'-H14B	119.9
H1'A-C1'-H1'B	120.0	C15'-C14'-H14B	119.9
C1'-C2'-C3'	122.8(4)	C14'-C15'-C10'	121.2(3)
C1'-C2'-H2'A	118.6	C14'-C15'-H15B	119.4
C3'-C2'-H2'A	118.6	C10'-C15'-H15B	119.4
C4'-C3'-C2'	126.0(3)	N2'-C16'-C20'	122.3(3)
C4'-C3'-H3'A	117.0	N2'-C16'-C5'	114.5(3)
C2'-C3'-H3'A	117.0	C20'-C16'-C5'	123.2(3)
C3'-C4'-C10'	124.0(3)	N2'-C17'-C18'	124.5(4)
C3'-C4'-C5'	118.6(3)	N2'-C17'-H17B	117.8
C10'-C4'-C5'	117.0(3)	C18'-C17'-H17B	117.8
O1'-C5'-C16'	108.5(3)	C19'-C18'-C17'	117.3(4)
O1'-C5'-C4'	109.5(3)	C19'-C18'-H18B	121.3
C16'-C5'-C4'	110.6(2)	C17'-C18'-H18B	121.3
O1'-C5'-H5'A	109.4	C18'-C19'-C20'	119.2(4)
C16'-C5'-H5'A	109.4	C18'-C19'-H19B	120.4
C4'-C5'-H5'A	109.4	C20'-C19'-H19B	120.4
O2'-C6'-N1'	125.2(3)	C16'-C20'-C19'	119.7(3)
O2'-C6'-O1'	124.1(3)	C16'-C20'-H20B	120.1
N1'-C6'-O1'	110.7(3)	C19'-C20'-H20B	120.1
N1'-C7'-C8'	110.8(2)	C22'-C21'-C7'	113.0(3)
N1'-C7'-C21'	112.3(2)	C22'-C21'-H21C	109.0
C8'-C7'-C21'	108.0(2)	C7'-C21'-H21C	109.0
N1'-C7'-H7'A	108.6	C22'-C21'-H21D	109.0
C8'-C7'-H7'A	108.6	C7'-C21'-H21D	109.0
C21'-C7'-H7'A	108.6	H21C-C21'-H21D	107.8
O3'-C8'-O4'	124.7(3)	C27'-C22'-C23'	118.2(3)
O3'-C8'-C7'	124.1(3)	C27'-C22'-C21'	120.4(3)
O4'-C8'-C7'	111.2(3)	C23'-C22'-C21'	121.4(3)
O4'-C9'-H9'A	109.5	C24'-C23'-C22'	120.7(3)
O4'-C9'-H9'B	109.5	C24'-C23'-H23B	119.7
H9'A-C9'-H9'B	109.5	C22'-C23'-H23B	119.7
O4'-C9'-H9'C	109.5	C25'-C24'-C23'	120.2(3)
H9'A-C9'-H9'C	109.5	C25'-C24'-H24B	119.9
H9'B-C9'-H9'C	109.5	C23'-C24'-H24B	119.9
C11'-C10'-C15'	117.9(3)	C26'-C25'-C24'	119.5(3)
C11'-C10'-C4'	121.5(3)	C26'-C25'-H25B	120.2
C15'-C10'-C4'	120.5(3)	C24'-C25'-H25B	120.2
C12'-C11'-C10'	121.2(4)	C25'-C26'-C27'	120.4(3)
C12'-C11'-H11B	119.4	C25'-C26'-H26B	119.8
C10'-C11'-H11B	119.4	C27'-C26'-H26B	119.8

C26'-C27'-C22'	121.0(3)	C11-C12-C13	120.2(3)
C26'-C27'-H27B	119.5	C11-C12-H12A	119.9
C22'-C27'-H27B	119.5	C13-C12-H12A	119.9
C6-O1-C5	115.6(2)	C14-C13-C12	119.7(3)
C8-O4-C9	116.5(3)	C14-C13-H13A	120.2
C6-N1-C7	118.7(3)	C12-C13-H13A	120.2
C6-N1-H1C	120.7	C13-C14-C15	120.2(3)
C7-N1-H1C	120.7	C13-C14-H14A	119.9
C17-N2-C16	116.9(3)	C15-C14-H14A	119.9
C2-C1-H1A	120.0	C14-C15-C10	120.9(3)
C2-C1-H1B	120.0	C14-C15-H15A	119.5
H1A-C1-H1B	120.0	C10-C15-H15A	119.5
C1-C2-C3	122.6(3)	N2-C16-C20	122.5(3)
C1-C2-H2A	118.7	N2-C16-C5	114.6(3)
C3-C2-H2A	118.7	C20-C16-C5	122.8(3)
C4-C3-C2	127.5(3)	N2-C17-C18	124.3(3)
C4-C3-H3A	116.2	N2-C17-H17A	117.8
C2-C3-H3A	116.2	C18-C17-H17A	117.8
C3-C4-C10	124.9(3)	C17-C18-C19	118.4(3)
C3-C4-C5	117.4(3)	C17-C18-H18A	120.8
C10-C4-C5	117.4(2)	C19-C18-H18A	120.8
O1-C5-C16	107.4(2)	C18-C19-C20	118.4(3)
O1-C5-C4	111.8(2)	C18-C19-H19A	120.8
C16-C5-C4	111.0(2)	C20-C19-H19A	120.8
O1-C5-H5A	108.9	C16-C20-C19	119.4(3)
C16-C5-H5A	108.9	C16-C20-H20A	120.3
C4-C5-H5A	108.9	C19-C20-H20A	120.3
O2-C6-N1	124.7(3)	C22-C21-C7	113.0(3)
O2-C6-O1	124.2(3)	C22-C21-H21A	109.0
N1-C6-O1	111.1(3)	C7-C21-H21A	109.0
N1-C7-C8	111.1(3)	C22-C21-H21B	109.0
N1-C7-C21	111.0(2)	C7-C21-H21B	109.0
C8-C7-C21	110.7(3)	H21A-C21-H21B	107.8
N1-C7-H7A	108.0	C23-C22-C27	119.6(3)
C8-C7-H7A	108.0	C23-C22-C21	122.9(3)
C21-C7-H7A	108.0	C27-C22-C21	117.5(3)
O3-C8-O4	124.5(3)	C22-C23-C24	119.3(4)
O3-C8-C7	126.5(3)	C22-C23-H23A	120.4
O4-C8-C7	109.0(3)	C24-C23-H23A	120.4
O4-C9-H9A	109.5	C25-C24-C23	119.1(4)
O4-C9-H9B	109.5	C25-C24-H24A	120.4
H9A-C9-H9B	109.5	C23-C24-H24A	120.4
O4-C9-H9C	109.5	C26-C25-C24	120.9(4)
H9A-C9-H9C	109.5	C26-C25-H25A	119.5
H9B-C9-H9C	109.5	C24-C25-H25A	119.5
C11-C10-C15	118.1(3)	C25-C26-C27	120.6(4)
C11-C10-C4	121.4(3)	C25-C26-H26A	119.7
C15-C10-C4	120.5(3)	C27-C26-H26A	119.7
C12-C11-C10	120.8(3)	C26-C27-C22	120.5(4)
C12-C11-H11A	119.6	C26-C27-H27A	119.7
C10-C11-H11A	119.6	C22-C27-H27A	119.7

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1'	51(1)	23(1)	31(1)	6(1)	7(1)	5(1)
O2'	43(1)	27(1)	36(1)	1(1)	8(1)	5(1)
O3'	40(1)	44(2)	57(1)	-3(1)	-14(1)	-2(1)
O4'	32(1)	49(2)	56(1)	1(1)	10(1)	-7(1)
N1'	35(1)	22(1)	29(1)	0(1)	6(1)	2(1)
N2'	56(2)	23(1)	36(1)	1(1)	9(1)	1(1)
C1'	68(3)	69(3)	77(3)	-2(3)	-13(2)	26(3)
C2'	42(2)	50(2)	58(2)	2(2)	-3(2)	6(2)
C3'	45(2)	34(2)	44(2)	1(2)	5(1)	0(2)
C4'	38(2)	26(2)	32(2)	5(1)	1(1)	-2(1)
C5'	46(2)	22(2)	32(2)	3(1)	2(1)	3(1)
C6'	27(1)	26(2)	27(1)	0(1)	-1(1)	-3(1)
C7'	29(1)	23(2)	31(1)	0(1)	2(1)	-1(1)
C8'	30(1)	23(2)	46(2)	2(1)	-1(1)	3(1)
C9'	32(2)	52(3)	99(3)	0(3)	18(2)	-9(2)
C10'	34(2)	30(2)	33(2)	-1(1)	-2(1)	-1(1)
C11'	68(2)	28(2)	40(2)	-1(2)	2(2)	-10(2)
C12'	81(3)	27(2)	58(2)	-7(2)	-8(2)	-4(2)
C13'	53(2)	43(2)	42(2)	-13(2)	-7(2)	8(2)
C14'	46(2)	46(2)	36(2)	-3(2)	2(1)	6(2)
C15'	41(2)	30(2)	40(2)	3(2)	2(1)	1(2)
C16'	46(2)	26(2)	21(1)	2(1)	-5(1)	0(1)
C17'	68(2)	29(2)	54(2)	0(2)	13(2)	-7(2)
C18'	52(2)	46(2)	39(2)	5(2)	1(2)	-15(2)
C19'	41(2)	44(2)	46(2)	5(2)	-2(2)	1(2)
C20'	46(2)	30(2)	46(2)	3(2)	-4(2)	5(2)
C21'	33(1)	26(2)	36(2)	3(1)	-1(1)	0(1)
C22'	32(1)	21(2)	39(2)	4(1)	-1(1)	1(1)
C23'	38(2)	39(2)	35(2)	-2(2)	1(1)	1(2)
C24'	44(2)	36(2)	49(2)	-2(2)	-12(2)	1(2)
C25'	31(2)	28(2)	67(2)	3(2)	-9(2)	3(1)
C26'	35(2)	38(2)	58(2)	5(2)	9(2)	4(2)
C27'	37(2)	42(2)	36(2)	-3(2)	1(1)	6(2)
O1	34(1)	25(1)	28(1)	3(1)	-3(1)	-1(1)
O2	55(1)	30(1)	43(1)	5(1)	-19(1)	-7(1)
O3	44(1)	53(2)	54(1)	-5(1)	5(1)	-4(1)
O4	47(1)	56(2)	57(1)	7(1)	-16(1)	6(1)
N1	39(1)	25(1)	31(1)	4(1)	-6(1)	-3(1)
N2	35(1)	29(2)	35(1)	0(1)	-2(1)	2(1)
C1	45(2)	43(2)	53(2)	6(2)	3(2)	-10(2)
C2	37(2)	32(2)	41(2)	1(2)	1(1)	-1(2)
C3	32(1)	25(2)	35(2)	1(1)	-3(1)	2(1)
C4	29(1)	24(2)	31(1)	2(1)	-4(1)	5(1)
C5	33(1)	23(2)	25(1)	1(1)	-2(1)	1(1)
C6	34(1)	26(2)	32(1)	-1(1)	-1(1)	2(1)
C7	41(2)	27(2)	32(2)	3(1)	-4(1)	-1(1)
C8	43(2)	26(2)	46(2)	5(2)	-8(2)	-1(2)
C9	44(2)	60(3)	89(3)	6(3)	-17(2)	5(2)
C10	23(1)	25(2)	29(1)	-1(1)	2(1)	0(1)
C11	36(2)	28(2)	35(2)	1(1)	1(1)	3(1)
C12	43(2)	25(2)	44(2)	-3(1)	6(1)	2(1)

C13	32(2)	35(2)	37(2)	-9(2)	2(1)	-1(1)
C14	36(2)	36(2)	30(1)	-3(1)	-4(1)	-1(2)
C15	32(2)	28(2)	36(2)	1(1)	0(1)	1(1)
C16	32(1)	26(2)	24(1)	0(1)	2(1)	1(1)
C17	42(2)	28(2)	44(2)	0(2)	-1(1)	7(2)
C18	35(2)	40(2)	43(2)	7(2)	1(1)	7(2)
C19	28(1)	40(2)	44(2)	1(2)	-2(1)	-1(1)
C20	34(2)	29(2)	35(2)	-3(1)	-1(1)	-1(1)
C21	48(2)	26(2)	36(2)	3(1)	1(1)	2(2)
C22	49(2)	20(2)	30(1)	3(1)	2(1)	-2(1)
C23	49(2)	50(2)	55(2)	1(2)	-2(2)	-5(2)
C24	48(2)	50(3)	114(4)	-4(3)	5(2)	-2(2)
C25	86(3)	44(3)	89(3)	-6(3)	50(3)	4(3)
C26	96(3)	53(3)	55(2)	-1(2)	24(2)	4(3)
C27	71(2)	36(2)	32(2)	0(2)	4(2)	3(2)

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

	x	y	z	U(eq)
H1'C	4296	6017	6742	34
H1'A	7212	-2375	8266	86
H1'B	7497	-1551	8958	86
H2'A	6428	635	8914	60
H3'A	6002	-941	7707	49
H5'A	4997	324	7072	40
H7'A	4829	5199	5568	33
H9'A	7358	6722	4993	91
H9'B	7439	5933	5693	91
H9'C	7259	8167	5569	91
H11B	5335	5013	8032	54
H12B	4908	7139	8801	67
H13B	4289	5976	9719	55
H14B	4157	2669	9869	51
H15B	4601	541	9103	44
H17B	3212	-4207	7661	60
H18B	1939	-2734	7919	55
H19B	1902	642	7965	52
H20B	3138	2381	7735	49
H21C	4473	8935	6082	38
H21D	4706	8599	5365	38
H23B	3640	6969	4663	44
H24B	2197	6540	4434	52
H25B	1188	6810	5221	50
H26B	1625	7627	6225	52
H27B	3055	8236	6445	46
H1C	9111	5225	8171	38
H1A	11916	13828	6819	57
H1B	12238	13176	6123	57
H2A	11190	10946	6068	44
H3A	10696	12278	7277	37
H5A	9707	10966	7852	33
H7A	9941	5902	9266	40
H9A	12519	4169	9622	96
H9B	12482	5253	8964	96
H9C	12352	2973	8995	96
H11A	10022	6277	6958	40
H12A	9627	4100	6182	45
H13A	9154	5205	5206	41
H14A	9124	8492	5001	41
H15A	9502	10685	5779	38
H17A	7826	15374	7388	45
H18A	6682	13962	6882	47
H19A	6738	10659	6649	45
H20A	7969	8924	6940	39
H21A	9339	2366	8743	44
H21B	9882	2375	9381	44
H23A	7819	3322	8765	61
H24A	6618	3969	9385	85
H25A	6812	4547	10453	87

H26A	8148	4493	10898	81
H27A	9327	3922	10301	56

Table 6 Torsion angles [°] for **2c**.

C1'-C2'-C3'-C4'	179.6(4)	C25'-C26'-C27'-C22'	-1.7(6)
C2'-C3'-C4'-C10'	-3.6(6)	C23'-C22'-C27'-C26'	0.6(5)
C2'-C3'-C4'-C5'	-177.2(3)	C21'-C22'-C27'-C26'	-178.9(3)
C6'-O1'-C5'-C16'	-123.6(3)	C1-C2-C3-C4	-177.8(3)
C6'-O1'-C5'-C4'	115.5(3)	C2-C3-C4-C10	-1.5(5)
C3'-C4'-C5'-O1'	-138.7(3)	C2-C3-C4-C5	-175.5(3)
C10'-C4'-C5'-O1'	47.3(4)	C6-O1-C5-C16	-140.3(2)
C3'-C4'-C5'-C16'	101.7(3)	C6-O1-C5-C4	97.7(3)
C10'-C4'-C5'-C16'	-72.3(4)	C3-C4-C5-O1	-139.7(3)
C7'-N1'-C6'-O2'	-4.2(4)	C10-C4-C5-O1	45.8(3)
C7'-N1'-C6'-O1'	176.5(2)	C3-C4-C5-C16	100.4(3)
C5'-O1'-C6'-O2'	3.3(4)	C10-C4-C5-C16	-74.1(3)
C5'-O1'-C6'-N1'	-177.4(2)	C7-N1-C6-O2	-1.5(5)
C6'-N1'-C7'-C8'	-76.2(3)	C7-N1-C6-O1	179.9(2)
C6'-N1'-C7'-C21'	163.0(2)	C5-O1-C6-O2	6.4(4)
C9'-O4'-C8'-O3'	2.8(5)	C5-O1-C6-N1	-175.0(2)
C9'-O4'-C8'-C7'	-178.1(3)	C6-N1-C7-C8	-71.8(4)
N1'-C7'-C8'-O3'	-31.5(4)	C6-N1-C7-C21	164.6(3)
C21'-C7'-C8'-O3'	91.9(4)	C9-O4-C8-O3	4.1(5)
N1'-C7'-C8'-O4'	149.4(3)	C9-O4-C8-C7	-176.2(3)
C21'-C7'-C8'-O4'	-87.2(3)	N1-C7-C8-O3	-24.7(5)
C3'-C4'-C10'-C11'	113.6(4)	C21-C7-C8-O3	99.1(4)
C5'-C4'-C10'-C11'	-72.7(4)	N1-C7-C8-O4	155.7(3)
C3'-C4'-C10'-C15'	-67.8(4)	C21-C7-C8-O4	-80.5(3)
C5'-C4'-C10'-C15'	105.9(3)	C3-C4-C10-C11	120.0(3)
C15'-C10'-C11'-C12'	-0.3(6)	C5-C4-C10-C11	-66.0(4)
C4'-C10'-C11'-C12'	178.4(3)	C3-C4-C10-C15	-62.4(4)
C10'-C11'-C12'-C13'	-0.7(6)	C5-C4-C10-C15	111.6(3)
C11'-C12'-C13'-C14'	1.3(6)	C15-C10-C11-C12	-0.6(5)
C12'-C13'-C14'-C15'	-0.8(6)	C4-C10-C11-C12	177.0(3)
C13'-C14'-C15'-C10'	-0.1(5)	C10-C11-C12-C13	0.0(5)
C11'-C10'-C15'-C14'	0.7(5)	C11-C12-C13-C14	1.1(5)
C4'-C10'-C15'-C14'	-178.0(3)	C12-C13-C14-C15	-1.5(5)
C17'-N2'-C16'-C20'	-0.7(5)	C13-C14-C15-C10	0.9(5)
C17'-N2'-C16'-C5'	178.1(3)	C11-C10-C15-C14	0.2(4)
O1'-C5'-C16'-N2'	155.1(3)	C4-C10-C15-C14	-177.4(3)
C4'-C5'-C16'-N2'	-84.7(3)	C17-N2-C16-C20	0.1(4)
O1'-C5'-C16'-C20'	-26.1(4)	C17-N2-C16-C5	176.6(3)
C4'-C5'-C16'-C20'	94.1(3)	O1-C5-C16-N2	142.0(2)
C16'-N2'-C17'-C18'	1.6(5)	C4-C5-C16-N2	-95.5(3)
N2'-C17'-C18'-C19'	-1.4(6)	O1-C5-C16-C20	-41.5(3)
C17'-C18'-C19'-C20'	0.3(6)	C4-C5-C16-C20	81.0(4)
N2'-C16'-C20'-C19'	-0.3(5)	C16-N2-C17-C18	0.2(5)
C5'-C16'-C20'-C19'	-179.0(3)	N2-C17-C18-C19	-0.2(5)
C18'-C19'-C20'-C16'	0.5(5)	C17-C18-C19-C20	-0.1(5)
N1'-C7'-C21'-C22'	-65.2(3)	N2-C16-C20-C19	-0.4(5)
C8'-C7'-C21'-C22'	172.4(2)	C5-C16-C20-C19	-176.6(3)
C7'-C21'-C22'-C27'	93.5(4)	C18-C19-C20-C16	0.4(5)
C7'-C21'-C22'-C23'	-86.0(4)	N1-C7-C21-C22	-75.1(3)
C27'-C22'-C23'-C24'	1.4(5)	C8-C7-C21-C22	161.0(2)
C21'-C22'-C23'-C24'	-179.2(3)	C7-C21-C22-C23	96.0(4)
C22'-C23'-C24'-C25'	-2.3(6)	C7-C21-C22-C27	-83.6(4)
C23'-C24'-C25'-C26'	1.2(6)	C27-C22-C23-C24	-0.5(6)
C24'-C25'-C26'-C27'	0.7(6)	C21-C22-C23-C24	180.0(4)

C22-C23-C24-C25	-0.1(7)
C23-C24-C25-C26	0.2(8)
C24-C25-C26-C27	0.5(8)
C25-C26-C27-C22	-1.1(7)
C23-C22-C27-C26	1.1(6)
C21-C22-C27-C26	-179.3(4)

Table 7.Observed and calculated structure factors for **2c** Page 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	0	0	216	232	2	12	4	0	112	116	2	8	0	1	290	291	5	17	2	1	73	74	6	-8	5	1	90	89	8
4	0	0	1034	1025	14	13	4	0	68	67	4	9	0	1	260	258	3	18	2	1	15	24	15	-7	5	1	186	183	2
5	0	0	314	322	3	14	4	0	69	73	4	10	0	1	31	41	2	19	2	1	41	39	7	-6	5	1	125	116	2
6	0	0	138	124	1	15	4	0	16	37	16	11	0	1	98	95	1	-19	3	1	67	66	11	-5	5	1	99	98	1
7	0	0	181	186	2	16	4	0	42	48	7	12	0	1	25	18	2	-18	3	1	46	38	8	-4	5	1	81	88	2
8	0	0	126	127	1	17	4	0	44	41	5	13	0	1	113	111	1	-17	3	1	20	16	19	-3	5	1	176	170	2
9	0	0	134	131	1	18	4	0	38	32	8	14	0	1	117	112	2	-16	3	1	43	42	4	-2	5	1	203	201	2
10	0	0	48	58	1	1	5	0	77	71	2	15	0	1	268	241	4	-15	3	1	28	28	6	-1	5	1	236	236	2
11	0	0	69	72	1	2	5	0	227	227	2	16	0	1	57	48	3	-14	3	1	99	105	2	0	5	1	20	17	6
12	0	0	328	322	3	3	5	0	27	32	4	17	0	1	0	8	1	-13	3	1	132	138	1	1	5	1	182	177	2
13	0	0	84	80	1	4	5	0	90	92	1	18	0	1	60	56	6	-12	3	1	152	152	1	2	5	1	196	191	2
14	0	0	145	152	2	5	5	0	154	150	2	19	0	1	19	8	18	-11	3	1	54	61	1	3	5	1	175	175	2
15	0	0	156	153	2	6	5	0	64	66	2	20	0	1	0	35	1	-10	3	1	140	137	2	4	5	1	42	44	2
16	0	0	46	49	4	7	5	0	275	275	3	-20	1	1	50	42	6	-9	3	1	113	113	1	5	5	1	117	114	1
17	0	0	52	42	6	8	5	0	236	237	11	-19	1	1	14	6	14	-8	3	1	111	110	3	6	5	1	282	284	3
18	0	0	56	45	9	9	5	0	227	227	3	-18	1	1	34	42	8	-7	3	1	255	257	2	7	5	1	252	248	9
19	0	0	58	66	10	10	5	0	184	181	2	-17	1	1	38	37	5	-6	3	1	98	94	2	8	5	1	268	262	3
20	0	0	58	45	10	11	5	0	132	130	2	-16	1	1	42	45	3	-5	3	1	402	409	5	9	5	1	23	22	7
2	1	0	157	130	2	12	5	0	32	24	15	-15	1	1	121	116	1	-4	3	1	221	209	3	10	5	1	147	147	5
3	1	0	1090	1055	9	13	5	0	53	50	7	-14	1	1	119	112	1	-3	3	1	59	60	3	11	5	1	59	61	6
4	1	0	438	435	6	14	5	0	51	37	9	-13	1	1	150	150	3	-2	3	1	723	723	7	12	5	1	199	193	3
5	1	0	365	387	2	15	5	0	86	79	8	-12	1	1	78	76	1	-1	3	1	349	360	3	13	5	1	108	105	8
6	1	0	431	443	3	16	5	0	48	33	9	-11	1	1	187	182	2	0	3	1	290	293	2	14	5	1	81	84	5
7	1	0	173	176	1	0	6	0	190	203	5	-10	1	1	28	34	1	1	3	1	341	354	3	15	5	1	108	104	7
8	1	0	336	326	2	1	6	0	86	89	3	-9	1	1	88	89	1	2	3	1	577	549	6	16	5	1	26	21	26
9	1	0	104	107	1	2	6	0	97	89	3	-8	1	1	244	235	2	3	3	1	23	15	2	-15	6	1	97	94	9
10	1	0	116	122	1	3	6	0	121	133	3	-7	1	1	389	386	3	4	3	1	206	208	2	-14	6	1	115	102	8
11	1	0	86	90	1	4	6	0	122	125	3	-6	1	1	149	119	4	5	3	1	347	344	3	-13	6	1	32	30	10
12	1	0	56	60	2	5	6	0	216	219	6	-5	1	1	704	705	6	6	3	1	113	119	1	-12	6	1	32	40	11
13	1	0	33	32	2	6	6	0	190	186	6	-4	1	1	216	215	2	7	3	1	237	233	3	-11	6	1	34	30	7
14	1	0	125	125	2	7	6	0	152	151	4	-2	1	1	329	343	2	8	3	1	129	130	1	-10	6	1	26	28	11
15	1	0	105	100	1	8	6	0	37	43	5	0	1	1	269	280	3	9	3	1	161	154	1	-9	6	1	104	107	3
16	1	0	34	32	3	9	6	0	106	105	5	1	1	1	300	309	6	10	3	1	118	119	2	-8	6	1	67	82	3
17	1	0	64	63	2	10	6	0	75	83	4	2	1	1	561	615	5	11	3	1	84	91	1	-7	6	1	89	84	4
18	1	0	50	53	6	11	6	0	83	87	4	3	1	1	1304	1219	21	12	3	1	47	48	1	-6	6	1	52	41	3
19	1	0	43	42	7	12	6	0	54	52	6	4	1	1	397	400	3	13	3	1	97	100	1	-5	6	1	62	49	6
20	1	0	65	63	6	13	6	0	121	122	8	5	1	1	551	552	4	14	3	1	45	40	3	-4	6	1	67	79	3
0	2	0	576	566	7	14	6	0	92	92	7	6	1	1	529	546	4	15	3	1	59	69	5	-3	6	1	17	3	17
1	2	0	774	771	12	15	6	0	54	53	11	7	1	1	298	304	2	16	3	1	45	40	4	-2	6	1	71	81	3
2	2	0	503	509	5	1	7	0	65	62	5	8	1	1	273	260	2	17	3	1	28	26	7	-1	6	1	78	77	4
3	2	0	173	184	2	2	7	0	81	85	4	9	1	1	164	171	1	18	3	1	51	54	7	0	6	1	81	79	3
4	2	0	81	64	2	3	7	0	93	96	3	10	1	1	168	172	1	19	3	1	41	50	17	1	6	1	121	116	3
5	2	0	177	172	1	4	7	0	0	14	1	11	1	1	78	75	2	-18	4	1	29	33	10	2	6	1	22	13	9
6	2	0	242	248	2	5	7	0	35	46	6	12	1	1	136	145	1	-17	4	1	20	17	20	3	6	1	56	54	4
7	2	0	176	172	1	6	7	0	79	85	4	13	1	1	65	67	2	-16	4	1	68	61	4	4	6	1	90	95	3
8	2	0	138	137	1	7	7	0	27	25	18	14	1	1	67	71	1	-15	4	1	67	56	7	5	6	1	128	135	5
9	2	0	275	279	2	8	7	0	45	44	6	15	1	1	116	120	1	-14	4	1	115	120	3	6	6	1	157	158	3
10	2	0	56	57	4	9	7	0	15	16	15	16	1	1	38	40	3	-13	4	1	133	134	2	7	6	1	80	75	5
11	2	0	71	68	1	10	7	0	87	85	5	17	1	1	117	108	2	-12	4	1	54	61	2	8	6	1	82	87	2
12	2	0	56	61	1	11	7	0	52	57	8	18	1	1	39	44	6	-11	4	1	178	175	3	9	6	1	156	157	3
13	2	0	78	81	1	12	7	0	60	46	14	19	1	1	83	76	5	-10	4	1	38	45	3	10	6	1	93	87	4
14	2	0	85	87	1	0	8	0	0	21	1	20	1	1	71	45	11	-9	4	1	131	137	1	11	6	1	13	29	13
15	2	0	85	84	2	1	8	0	57	53	7	-19	2	1	71	72	9	-8	4	1	61	60	3	12	6	1	79	83	4
16	2	0	65	67	8	2	8	0	56	55	7	-18	2	1	44	42	6	-7	4	1	109	107	1	13	6	1	36	26	16
17	2	0	88	86	3	3	8	0	59	50	9	-17	2	1	17	10	16	-6	4	1	33	26	2	14	6	1	38	51	27
18	2	0	43	34	12	4	8	0	74	72	9	-16	2	1	68	77	2	-5	4	1	108	95	5	15	6	1	85	82	7
19	2	0	123	123	7	5	8	0	154	136	7	-15	2	1	43	43	4	-4	4	1	331	334	4	-12	7	1	18	13	17
1	3	0	404	408	3	6	8	0	137	134	5	-14	2	1	81	88	2	-3	4	1	285	299	9	-11	7	1	53	55	7
2	3	0	186	180	3	7	8	0	59	53	8	-13	2	1	82	82	2	-2	4	1	634	599	6	-10	7	1	67	77	6
3	3	0	438	442	5	8	8	0	108	102	9	-12	2	1	152	158	3	-1	4	1	257	251	2	-9	7	1	43	52	6
4	3	0	321	335	2	9	8	0	66	55	7	-11	2	1	111	111	1	0	4	1	108	107	1	-8	7	1	43	48	9
5	3	0	137	138	1	1	9	0	28	2	27	-10	2	1	175	176	1	1	4	1	175	163	2	-7	7	1	42	43	6
6	3	0	138	128	1	-20	0	1	34	40	23	-9	2	1	193	192	1	2	4	1	597	570	6	-6	7	1	84	84	5
7	3	0	147	151	7	-19	0	1	31	1	30	-8	2	1	117	113	2	3	4	1	137	134	2	-5	7	1	27	30	12
8	3	0	136	140	1	-18	0	1	67	70	7	-7	2	1	315	310	3	4	4	1	372	375	3	-4	7	1	57	50	3
9	3	0	92	95	1	-17	0	1	57	49	4	-6	2	1	374	380	3	5	4	1	246	247	2	-3	7	1	22	10	21
10	3	0	116	116	1	-16	0	1	12	18	12	-5	2	1	69	57	1	6	4	1	142	140	1	-2	7	1	39	49	7
11	3	0	139	134	1	-15	0	1	289	280	4	-4	2	1	261	262	2	7	4	1	130	129	1	-1	7	1	143	147	4
12	3	0	84	86	1	-14	0	1	87	82	2	-3	2	1	216	220	2	8	4	1	100	100	2	0	7	1	194	196	3
13	3	0	232	235	2	-13	0	1	211	204	3	-2	2	1	614	639	5	9	4	1	106	101	3	1	7	1	153	146	3
14	3	0	73	75	2	-12	0	1	33	38	4	-1	2	1	301	285	3	10	4	1	56	61	2	2	7	1	25	9	10
15	3	0	56	62	4	-11	0	1	97	94	1	1	2	1	428	446	3	11	4	1	59	60	2	3	7	1	5	26	5
16	3	0	74	78	3	-10	0	1	91	91	1	2	2	1	510	519	12	12	4	1	164	166	2	4	7	1	53	45	5
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4	3	3	346	332	5	-13	6	3	35	40	18	-5	0	4	699	704	9	4	2	4	380	381	4	16	4	4	67	67	6
5	3	3	86	72	2	-12	6	3	20	16	20	-4	0	4	660	627	9	5	2	4	268	263	2	17	4	4	0	21	1
6	3	3	243	244	2	-11	6	3	28	33	12	-3	0	4	1075	1052	14	6	2	4	316	324	2	-16	5	4	17	59	17
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8	3	3	100	98	6	-9	6	3	67	70	4	-1	0	4	79	54	1	8	2	4	171	165	2	-14	5	4	71	67	8
9	3	3	220	221	2	-8	6	3	202	195	5	0	0	4	141	156	1	9	2	4	168	165	2	-13	5	4	13	29	12
10	3	3	82	78	3	-7	6	3	165	170	3	1	0	4	155	143	1	10	2	4	176	183	1	-12	5	4	31	35	11
11	3	3	57	57	1	-6	6	3	268	270	4	2	0	4	1342	1263	23	11	2	4	80	85	2	-11	5	4	74	85	4
12	3	3	57	63	1	-5	6	3	183	182	5	3	0	4	1234	1182	14	12	2	4	95	94	1	-10	5	4	119	120	4
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14	3	3	70	71	3	-3	6	3	129	122	6	5	0	4	604	607	6	14	2	4	61	64	2	-8	5	4	154	158	2
15	3	3	144	144	2	-2	6	3	236	237	4	6	0	4	546	558	5	15	2	4	57	58	3	-7	5	4	119	120	2
16	3	3	30	34	6	-1	6	3	167	168	3	7	0	4	271	288	2	16	2	4	18	21	14	-6	5	4	265	259	3
17	3	3	48	48	3	0	6	3	135	144	3	8	0	4	316	327	3	17	2	4	24	33	8	-5	5	4	199	199	8
18	3	3	3	18	3	1	6	3	98	96	3	9	0	4	87	88	1	18	2	4	29	34	8	-4	5	4	229	219	4
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-16	4	3	18	7	17	5	6	3	120	113	2	13	0	4	221	220	2	-16	3	4	57	58	3	0	5	4	329	333	5
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-11	4	3	165	167	3	10	6	3	82	74	4	19	0	4	28	27	27	-11	3	4	170	161	2	5	5	4	243	252	3
-10	4	3	67	77	3	11	6	3	99	92	3	20	0	4	0	2	1	-10	3	4	94	97	1	6	5	4	299	294	3
-9	4	3	184	187	2	12	6	3	69	69	11	-20	1	4	34	28	12	-9	3	4	169	177	2	7	5	4	121	124	5
-8	4	3	120	122	1	13	6	3	51	57	13	-19	1	4	74	62	7	-8	3	4	213	219	2	8	5	4	58	55	3
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-5	4	3	96	93	2	-12	7	3	14	12	14	-16	1	4	67	70	3	-5	3	4	215	215	2	11	5	4	124	119	3
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0	4	3	175	163	7	-7	7	3	85	88	4	-11	1	4	150	156	2	0	3	4	299	301	9	16	5	4	51	55	13
1	4	3	258	257	2	-6	7	3	22	25	16	-10	1	4	360	360	3	1	3	4	264	251	3	-14	6	4	44	32	15
2	4	3	237	249	2	-5	7	3	32	29	9	-9	1	4	296	291	2	2	3	4	382	368	3	-13	6	4	83	78	7
3	4	3	170	157	2	-4	7	3	46	36	5	-8	1	4	537	541	4	3	3	4	288	297	2	-12	6	4	43	43	9
4	4	3	102	109	3	-3	7	3	62	63	4	-7	1	4	391	393	3	4	3	4	286	277	2	-11	6	4	47	37	8
5	4	3	132	128	1	-2	7	3	76	84	3	-6	1	4	346	343	3	5	3	4	232	227	2	-10	6	4	92	94	4
6	4	3	47	33	5	-1	7	3	62	58	4	-5	1	4	410	422	3	6	3	4	116	126	1	-9	6	4	62	58	5
7	4	3	98	95	1	0	7	3	245	245	4	-4	1	4	269	289	2	7	3	4	152	145	4	-8	6	4	136	140	3
8	4	3	51	49	2	1	7	3	81	91	3	-3	1	4	217	238	5	8	3	4	202	196	3	-7	6	4	104	101	2
9	4	3	120	123	2	2	7	3	72	70	3	-2	1	4	254	267	4	9	3	4	228	223	2	-6	6	4	136	128	7
10	4	3	12	12	12	3	7	3	58	57	4	-1	1	4	962	956	9	10	3	4	25	21	2	-5	6	4	72	77	2
11	4	3	55	58	2	4	7	3	45	38	5	1	1	4	792	783	7	11	3	4	210	204	3	-4	6	4	79	72	3
12	4	3	57	59	2	5	7	3	48	54	5	2	1	4	307	321	2	12	3	4	60	62	1	-3	6	4	167	174	6
13	4	3	20	35	8	6	7	3	48	48	7	3	1	4	232	240	1	13	3	4	105	111	1	-2	6	4	217	213	4
14	4	3	75	76	6	7	7	3	97	91	4	4	1	4	56	54	1	14	3	4	48	43	3	-1	6	4	141	139	3
15	4	3	42	46	7	8	7	3	57	52	6	5	1	4	515	522	4	15	3	4	81	93	3	0	6	4	111	116	2
16	4	3	53	58	10	9	7	3	30	13	12	6	1	4	344	352	4	16	3	4	38	41	5	1	6	4	41	12	5
17	4	3	29	30	14	10	7	3	20	45	20	7	1	4	204	197	7	17	3	4	69	68	7	2	6	4	250	244	4
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-15	5	3	55	55	13	12	7	3	70	60	8	9	1	4	268	255	2	-18	4	4	38	41	27	4	6	4	52	57	4
-14	5	3	85	79	4	-9	8	3	21	19	21	10	1	4	301	298	2	-17	4	4	35	56	35	5	6	4	113	118	3
-13	5	3	77	77	5	-8	8	3	45	44	8	11	1	4	103	104	1	-16	4	4	31	28	8	6	6	4	226	224	4
-12	5	3	88	94	9	-6	8	3	89	95	8	12	1	4	185	185	2	-15	4	4	105	105	3	7	6	4	231	226	3
-11	5	3	103	101	3	-5	8	3	84	81	5	13	1	4	115	110	2	-14	4	4	79	84	4	8	6	4	99	97	2
-10	5	3	50	47	8	-4	8	3	44	42	9	14	1	4	128	129	1	-13	4	4	44	43	5	9	6	4	211	210	4
-9	5	3	119	118	2	-3	8	3	87	85	7	15	1	4	12	14	12	-12	4	4	14	26	14	10	6	4	91	90	3
-8	5	3	206	204	3	-2	8	3	27	28	15	16	1	4	63	59	3	-11	4	4	113	122	2	11	6	4	82	80	4
-7	5	3	66	63	7	-1	8	3	57	48	6	17	1	4	23	32	8	-10	4	4	152	153	2	12	6	4	78	79	9
-6	5	3	322	328	6	0	8	3	142	134	7	18	1	4	64	60	3	-9	4	4	69	74	4	13	6	4	97	74	8
-5	5	3	465	473	12	1	8	3	106	109	4	19	1	4	66	73	4	-8	4	4	270	272	7	14	6	4	27	31	27

Table 7. Observed and calculated structure factors for 1 Page 4

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s

-12	7	4	42	39	8	-15	1	5	35	36	3	-5	3	5	80	65	4	12	5	5	42	55	11	-8	0	6	253	253	3
-11	7	4	53	40	7	-14	1	5	109	120	2	-4	3	5	257	261	2	13	5	5	75	72	6	-7	0	6	380	375	5
-10	7	4	65	66	6	-13	1	5	91	94	1	-3	3	5	75	71	4	14	5	5	16	18	16	-6	0	6	308	307	4
-9	7	4	24	20	19	-12	1	5	147	141	1	-2	3	5	234	226	2	15	5	5	101	114	5	-5	0	6	83	65	3
-8	7	4	57	48	7	-11	1	5	173	173	1	-1	3	5	171	174	2	16	5	5	63	56	9	-4	0	6	179	167	2
-7	7	4	13	27	13	-10	1	5	79	79	2	0	3	5	486	483	10	-14	6	5	99	94	5	-3	0	6	1212	1171	16
-6	7	4	68	68	6	-9	1	5	154	147	6	1	3	5	233	228	2	-13	6	5	9	19	9	-2	0	6	102	107	2
-5	7	4	33	19	7	-8	1	5	296	306	2	2	3	5	201	208	3	-12	6	5	28	22	27	-1	0	6	769	761	8
-4	7	4	27	30	13	-7	1	5	505	507	4	3	3	5	42	36	2	-11	6	5	50	58	7	0	0	6	432	435	4
-3	7	4	103	103	3	-6	1	5	418	428	3	4	3	5	269	273	2	-10	6	5	56	59	8	1	0	6	1199	1179	16
-2	7	4	98	101	3	-5	1	5	212	190	3	5	3	5	218	216	2	-9	6	5	70	71	5	2	0	6	167	192	1
-1	7	4	93	87	3	-4	1	5	487	506	4	6	3	5	221	218	2	-8	6	5	89	94	4	3	0	6	532	482	6
0	7	4	92	91	4	-3	1	5	508	533	4	7	3	5	147	141	2	-7	6	5	101	104	4	4	0	6	275	287	2
1	7	4	60	55	4	-2	1	5	532	558	5	8	3	5	130	132	1	-6	6	5	204	198	7	5	0	6	315	344	3
2	7	4	129	133	3	-1	1	5	545	576	13	9	3	5	123	132	1	-5	6	5	91	91	4	6	0	6	177	164	2
3	7	4	72	79	4	0	1	5	254	278	2	10	3	5	137	136	1	-4	6	5	216	212	6	7	0	6	169	160	2
4	7	4	46	51	8	1	1	5	591	590	4	11	3	5	140	141	4	-3	6	5	25	30	11	8	0	6	246	248	2
5	7	4	51	52	6	2	1	5	371	379	6	12	3	5	98	94	2	-2	6	5	99	97	4	9	0	6	166	174	1
6	7	4	37	24	8	3	1	5	351	328	2	13	3	5	47	52	3	-1	6	5	139	125	4	10	0	6	262	261	2
7	7	4	87	82	4	4	1	5	196	184	7	14	3	5	51	63	4	0	6	5	218	209	3	11	0	6	137	136	2
8	7	4	46	41	6	5	1	5	504	529	4	15	3	5	65	64	3	1	6	5	216	212	4	12	0	6	80	79	2
9	7	4	33	40	11	6	1	5	212	205	5	16	3	5	39	42	4	2	6	5	240	237	4	13	0	6	418	410	7
10	7	4	14	3	14	7	1	5	591	587	4	17	3	5	63	66	7	3	6	5	132	131	2	14	0	6	125	127	3
11	7	4	50	43	13	8	1	5	168	170	4	18	3	5	82	78	4	4	6	5	207	208	3	15	0	6	161	157	4
12	7	4	41	40	22	9	1	5	393	384	3	-17	4	5	85	84	9	5	6	5	155	153	3	16	0	6	0	6	1
-9	8	4	42	49	11	10	1	5	322	327	2	-16	4	5	86	74	4	6	6	5	100	94	2	17	0	6	35	29	10
-8	8	4	30	38	13	11	1	5	52	47	4	-15	4	5	56	50	9	7	6	5	73	73	3	18	0	6	25	13	24
-7	8	4	69	78	7	12	1	5	203	196	2	-14	4	5	64	76	6	8	6	5	52	61	4	19	0	6	0	4	1
-6	8	4	47	38	7	13	1	5	118	119	2	-13	4	5	150	145	3	9	6	5	119	122	3	-19	1	6	24	20	18
-5	8	4	31	34	14	14	1	5	184	182	3	-12	4	5	62	63	3	10	6	5	122	117	3	-18	1	6	57	55	5
-4	8	4	69	78	6	15	1	5	35	42	3	-11	4	5	77	78	4	11	6	5	48	56	10	-17	1	6	101	99	3
-3	8	4	59	68	8	16	1	5	74	73	7	-10	4	5	155	147	4	12	6	5	156	149	6	-16	1	6	75	74	3
-2	8	4	42	41	8	17	1	5	36	41	4	-9	4	5	227	230	3	13	6	5	45	37	16	-15	1	6	54	54	2
-1	8	4	75	74	5	18	1	5	26	18	9	-8	4	5	64	62	2	14	6	5	70	81	10	-14	1	6	83	81	2
0	8	4	30	14	13	19	1	5	71	79	4	-7	4	5	64	39	11	-12	7	5	51	39	8	-13	1	6	159	152	2
1	8	4	49	47	9	-19	2	5	44	40	6	-6	4	5	173	176	1	-11	7	5	0	25	1	-12	1	6	59	64	2
2	8	4	33	35	12	-18	2	5	0	24	1	-5	4	5	171	175	2	-10	7	5	95	88	9	-11	1	6	209	209	3
3	8	4	0	21	1	-17	2	5	20	19	20	-4	4	5	118	121	2	-9	7	5	31	19	9	-10	1	6	142	140	1
4	8	4	74	66	6	-16	2	5	0	8	1	-3	4	5	185	192	2	-8	7	5	17	10	17	-9	1	6	71	68	1
5	8	4	36	37	11	-15	2	5	81	86	2	-2	4	5	220	188	2	-7	7	5	21	18	21	-8	1	6	243	236	2
6	8	4	42	41	8	-14	2	5	114	115	3	-1	4	5	359	363	3	-6	7	5	78	79	4	-7	1	6	139	142	1
7	8	4	78	78	6	-13	2	5	122	118	2	0	4	5	86	93	1	-5	7	5	53	59	6	-6	1	6	523	528	4
8	8	4	90	101	6	-12	2	5	44	42	2	1	4	5	213	197	2	-4	7	5	31	20	30	-5	1	6	272	286	4
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-17	0	5	37	28	6	-8	2	5	219	203	2	5	4	5	141	138	1	0	7	5	118	119	3	-1	1	6	319	312	2
-16	0	5	20	18	19	-7	2	5	327	327	3	6	4	5	77	72	1	1	7	5	92	100	4	0	1	6	84	100	1
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-13	0	5	369	368	7	-4	2	5	205	193	2	9	4	5	31	7	4	4	7	5	34	23	7	3	1	6	291	298	1
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-4	0	5	142	76	4	5	2	5	354	370	3	-16	5	5	44	27	13	-8	8	5	5	34	5	12	1	6	167	164	5
-3	0	5	76	89	1	6	2	5	253	252	2	-15	5	5	44	53	34	-7	8	5	91	94	5	13	1	6	154	156	1
-2	0	5	1534	1400	30	7	2	5	170	165	5	-14	5	5	85	82	7	-6	8	5	36	31	9	14	1	6	31	34	5
-1	0	5	368	407	3	8	2	5	88	81	3	-13	5	5	107	105	4	-5	8	5	56	46	9	15	1	6	21	13	4
0	0	5	91	86	1	9	2	5	141	135	1	-12	5	5	102	100	6	-4	8	5	27	32	21	16	1	6	36	40	6
1	0	5	111	73	1	10	2	5	151	148	2	-11	5	5	57	57	4	-3	8	5	81	89	4	17	1	6	33	45	9
2	0	5	1032	976	9	11	2	5	145	140	2	-10	5	5	116	111	3	-2	8	5	48	47	7	18	1	6	37	37	6
3	0	5	36	31	1	12	2	5	124	121	2	-9	5	5	40	37	6	-1	8	5	124	119	5	19	1	6	27	25	27
4	0	5	525	542	4	13	2	5	94	93	4	-8	5	5	67	66	3	0	8	5	47	48	6	-19	2	6	35	25	10
5	0	5	116	120	1	14	2	5	189	191	2	-7	5	5	164	160	5	1	8	5	93	95	5	-18	2	6	73	73	7
6	0	5	138	144	1	15	2	5	35	25	10	-6	5	5	138	126	3	2	8	5	43	30	9	-17	2	6	45	37	4
7	0	5	229	235	2	16	2	5	57	50	5	-5	5	5	231	234	4	3	8	5	82	89	5	-16	2	6	120	114	6
8	0	5	24	32	1	17	2	5	80	72	3	-4	5	5	122	117	5	4	8	5	65	67	6	-15	2	6	69	71	2
9	0	5	63	53	1	18	2	5	76	69	4	-3	5	5	194	193	2	5	8	5	43	60	8	-14	2	6	53	56	3
10	0	5	110	110	1	19	2	5	42	34	8	-2	5	5	45	41	3	6	8	5	0	8	1	-13	2	6	131	131	1
11	0	5	131	134	1	-18	3	5	37	33	9	-1	5	5	160	166	5	7	8	5	56	60	6	-12	2	6	128	129	1
12	0	5	166	169	1	-17	3	5	21	11	14	0	5	5	96	101	2	8	8	5	30	26	20	-11	2	6	98	103	3
13	0	5	53	57	1	-16	3	5	44	44	9	1	5	5	50	48	3	-19	0	6	64	60	8	-10	2	6	193	190	2
14	0	5	82	75	1	-15	3	5	25	29	8	2	5	5	72	71	2	-18	0	6	5	3	5	-9	2	6	68	59	3
15	0	5	205	198	4	-14	3	5	23	13	6	3	5	5	215	205	3	-17	0	6	58	64	7	-8	2	6	242	244	2
16	0	5	25	32	10	-13	3	5	119	112	2	4	5	5	255	261	4	-16	0	6	8	14	7	-7	2	6	71	64	2
17	0	5	0	45	1	-12	3	5	189	188	2	5	5	5	122	118	6	-15	0	6	0	11	1	-6	2	6	308	307	4
18	0	5	99	99	6	-11	3	5	32	36	3	6	5	5	275	271	3	-14	0	6	111	114	3	-5	2	6	403	394	3
19	0	5	0	15	1	-10	3	5	117	119	1	7	5	5	220	227	6	-13	0	6	85	83	4	-4	2	6	419	407	3
-19	1	5	27	28	18	-9	3	5	16	16	15	8	5	5	203	210	3	-12	0	6	93	106	3	-3	2	6	300	308	2
-18	1	5	63	61	4	-8	3	5	131	128	2	9	5	5	155	160	2	-11	0	6	194	194	3	-2	2	6	290	278	3
-17	1	5	103	103	3	-7	3	5	279	283	3	10	5	5	92	87	2	-10	0	6	129	121	3	-1	2	6	367	375	3
-16	1	5	99	98	2	-6	3	5	268	268	5	11	5	5	102	99	3	-9	0	6	129	136	3	0	2	6	99	97	2

Table 7. Observed and calculated structure factors for 1 Page 5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	2	6	302	296	5	14	4	6	39	43	7	9	7	6	11	33	10	8	1	7	99	90	2	18	3	7	0	16	1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	2	6	300	309	2	15	4	6	24	19	24	10	7	6	0	23	1	9	1	7	77	77	1	-17	4	7	42	31	20
3	2	6	250	246	2	16	4	6	76	83	6	11	7	6	47	51	12	10	1	7	237	234	3	-16	4	7	40	16	9
4	2	6	452	443	4	17	4	6	57	41	9	12	7	6	48	20	16	11	1	7	110	113	1	-15	4	7	36	38	9
5	2	6	195	195	3	-16	5	6	25	36	24	-8	8	6	76	75	5	12	1	7	269	265	2	-14	4	7	93	88	5
6	2	6	298	287	4	-15	5	6	30	18	18	-7	8	6	80	80	4	13	1	7	100	105	3	-13	4	7	29	41	10
7	2	6	258	255	1	-14	5	6	51	59	7	-6	8	6	48	47	9	14	1	7	116	121	2	-12	4	7	39	41	5
8	2	6	339	336	3	-13	5	6	21	31	20	-5	8	6	30	41	24	15	1	7	72	74	4	-11	4	7	52	56	7
9	2	6	302	297	3	-12	5	6	173	171	4	-4	8	6	82	80	5	16	1	7	122	113	6	-10	4	7	179	178	3
10	2	6	83	81	1	-11	5	6	53	64	6	-3	8	6	33	37	12	17	1	7	75	68	4	-9	4	7	46	21	15
11	2	6	118	119	2	-10	5	6	44	35	6	-2	8	6	93	95	6	18	1	7	82	88	4	-8	4	7	106	100	2
12	2	6	79	75	5	-9	5	6	194	198	3	-1	8	6	51	35	7	19	1	7	27	35	10	-7	4	7	183	187	3
13	2	6	42	36	3	-8	5	6	21	7	14	0	8	6	48	43	6	-19	2	7	48	54	9	-6	4	7	214	222	2
14	2	6	165	159	2	-7	5	6	158	157	2	1	8	6	90	87	5	-18	2	7	91	82	5	-5	4	7	35	30	3
15	2	6	47	44	3	-6	5	6	140	140	3	2	8	6	99	109	5	-17	2	7	37	41	5	-4	4	7	56	52	1
16	2	6	119	110	3	-5	5	6	88	81	5	3	8	6	50	52	7	-16	2	7	0	13	1	-3	4	7	27	31	8
17	2	6	28	34	7	-4	5	6	90	95	3	4	8	6	78	73	6	-15	2	7	84	89	3	-2	4	7	66	64	9
18	2	6	75	78	5	-3	5	6	94	94	6	5	8	6	42	47	11	-14	2	7	88	91	1	-1	4	7	86	79	2
19	2	6	33	27	8	-2	5	6	99	100	2	6	8	6	27	27	19	-13	2	7	81	79	1	0	4	7	128	139	2
-18	3	6	44	47	11	-1	5	6	110	101	1	7	8	6	32	36	13	-12	2	7	36	39	2	1	4	7	141	144	1
-17	3	6	0	15	1	0	5	6	128	124	2	8	8	6	63	52	6	-11	2	7	149	146	2	2	4	7	109	117	1
-16	3	6	41	32	4	1	5	6	175	172	2	-19	0	7	48	49	12	-10	2	7	96	99	2	3	4	7	12	18	12
-15	3	6	0	26	1	2	5	6	101	102	2	-18	0	7	118	118	4	-9	2	7	106	102	2	4	4	7	72	73	1
-14	3	6	69	67	4	3	5	6	62	63	2	-17	0	7	48	53	8	-8	2	7	211	211	2	5	4	7	66	72	1
-13	3	6	92	92	2	4	5	6	60	66	6	-16	0	7	12	29	12	-7	2	7	279	288	2	6	4	7	67	63	2
-12	3	6	70	78	2	5	5	6	98	95	2	-15	0	7	35	28	7	-6	2	7	210	205	2	7	4	7	169	169	2
-11	3	6	145	146	2	6	5	6	58	58	11	-14	0	7	366	353	6	-5	2	7	280	288	4	8	4	7	50	61	3
-10	3	6	29	25	3	7	5	6	157	159	2	-13	0	7	177	172	3	-4	2	7	232	222	3	9	4	7	276	275	4
-9	3	6	68	75	1	8	5	6	171	171	3	-12	0	7	111	102	3	-3	2	7	324	325	3	10	4	7	37	33	3
-8	3	6	48	43	4	9	5	6	85	81	2	-11	0	7	334	333	5	-2	2	7	48	48	2	11	4	7	76	80	2
-7	3	6	138	138	2	10	5	6	64	62	3	-10	0	7	215	212	3	-1	2	7	527	515	4	12	4	7	81	84	5
-6	3	6	129	134	1	11	5	6	27	24	9	-9	0	7	206	214	3	0	2	7	177	186	1	13	4	7	53	49	7
-5	3	6	222	223	4	12	5	6	48	42	10	-8	0	7	32	51	5	1	2	7	466	456	4	14	4	7	91	95	5
-4	3	6	128	134	1	13	5	6	0	24	1	-7	0	7	152	148	2	2	2	7	34	16	2	15	4	7	39	40	10
-3	3	6	128	128	1	14	5	6	36	36	11	-6	0	7	68	59	2	3	2	7	260	255	2	16	4	7	88	82	6
-2	3	6	98	80	1	15	5	6	48	48	12	-5	0	7	56	19	3	4	2	7	281	276	2	17	4	7	27	10	17
-1	3	6	346	343	3	16	5	6	53	60	10	-4	0	7	352	378	4	5	2	7	192	182	3	-16	5	7	53	43	11
0	3	6	93	83	3	-14	6	6	0	2	1	-3	0	7	107	28	3	6	2	7	201	199	1	-15	5	7	57	46	8
1	3	6	232	225	3	-13	6	6	53	59	9	-2	0	7	498	484	5	7	2	7	361	365	2	-14	5	7	47	39	7
2	3	6	145	139	1	-12	6	6	27	21	16	-1	0	7	369	397	3	8	2	7	220	229	2	-13	5	7	102	95	4
3	3	6	196	197	1	-11	6	6	9	20	9	0	0	7	287	290	2	9	2	7	280	284	2	-12	5	7	73	68	5
4	3	6	109	113	1	-10	6	6	86	90	4	1	0	7	217	216	2	10	2	7	187	190	2	-11	5	7	143	143	3
5	3	6	92	65	3	-9	6	6	95	92	6	2	0	7	986	968	8	11	2	7	230	235	4	-10	5	7	101	100	3
6	3	6	34	29	1	-8	6	6	196	197	5	3	0	7	414	445	3	12	2	7	169	164	2	-9	5	7	124	118	4
7	3	6	132	125	1	-7	6	6	83	82	4	4	0	7	111	94	2	13	2	7	72	75	3	-8	5	7	59	59	7
8	3	6	173	176	2	-6	6	6	180	179	3	5	0	7	214	229	1	14	2	7	124	118	2	-7	5	7	171	166	8
9	3	6	48	48	2	-5	6	6	44	43	6	6	0	7	86	75	1	15	2	7	49	48	3	-6	5	7	116	108	2
10	3	6	37	28	2	-4	6	6	121	125	3	7	0	7	86	88	1	16	2	7	63	66	3	-5	5	7	168	168	3
11	3	6	51	62	2	-3	6	6	45	46	5	8	0	7	112	109	1	17	2	7	29	28	9	-4	5	7	119	114	2
12	3	6	194	192	3	-2	6	6	129	124	5	9	0	7	152	152	2	18	2	7	31	39	9	-3	5	7	154	148	3
13	3	6	27	27	6	-1	6	6	69	74	4	10	0	7	235	236	3	19	2	7	86	83	8	-2	5	7	42	21	8
14	3	6	73	76	3	0	6	6	179	185	3	11	0	7	142	142	3	-18	3	7	36	32	35	-1	5	7	203	201	3
15	3	6	19	20	9	1	6	6	97	103	3	12	0	7	63	64	3	-17	3	7	38	30	7	0	5	7	57	56	3
16	3	6	98	97	3	2	6	6	199	207	3	13	0	7	218	214	4	-16	3	7	48	54	4	1	5	7	234	238	3
17	3	6	25	30	12	3	6	6	64	58	4	14	0	7	167	165	3	-15	3	7	90	92	6	2	5	7	151	146	2
18	3	6	0	14	1	4	6	6	144	131	3	15	0	7	62	67	4	-14	3	7	37	42	5	3	5	7	212	207	3
-17	4	6	64	58	8	5	6	6	75	76	2	16	0	7	106	104	3	-13	3	7	180	180	3	4	5	7	90	89	2
-16	4	6	76	73	5	6	6	6	73	62	3	17	0	7	36	3	17	-12	3	7	96	92	1	5	5	7	120	122	7
-15	4	6	37	34	18	7	6	6	93	92	3	18	0	7	84	78	6	-11	3	7	235	230	3	6	5	7	231	229	3
-14	4	6	47	43	10	8	6	6	90	87	4	19	0	7	27	17	26	-10	3	7	265	263	3	7	5	7	112	108	2
-13	4	6	51	57	6	9	6	6	171	170	4	-19	1	7	64	64	6	-9	3	7	164	157	2	8	5	7	67	62	2
-12	4	6	41	52	8	10	6	6	23	29	15	-18	1	7	34	31	11	-8	3	7	177	182	2	9	5	7	230	227	3
-11	4	6	96	91	3	11	6	6	69	71	7	-17	1	7	49	44	4	-7	3	7	87	89	2	10	5	7	77	74	3
-10	4	6	111	108	3	12	6	6	23	29	23	-16	1	7	47	51	5	-6	3	7	297	295	3	11	5	7	41	36	5
-9	4	6	115	121	2	13	6	6	40	46	14	-15	1	7	97	111	2	-5	3	7	133	137	2	12	5	7	109	103	5
-8	4	6	153	157	5	14	6	6	45	32	19	-14	1	7	81	83	2	-4	3	7	175	175	3	13	5	7	89	97	6
-7	4	6	181	181	2	-12	7	6	44	51	12	-13	1	7	53	53	3	-3	3	7	140	128	2	14	5	7	66	69	7
-6	4	6	72	69	1	-11	7	6	56	50	8	-12	1	7	153	159	3	-2	3	7	167	159	2	15	5	7	36	54	20
-5	4	6	140	142	2	-10	7	6	0	14	1	-11	1	7	163	167	2	-1	3	7	172	170	1	-14	6	7	13	25	13
-4	4	6	110	107	2	-9	7	6	2	8	1	-10	1	7	163	168	3	0	3	7	173	168	1	-13	6	7	72	73	9
-3	4	6	132	130	2	-8	7	6	66	62	6	-9	1	7	176	173	2	1	3	7	80	67	3	-12	6	7	55	51	14
-2	4	6	94	89	2	-7	7	6	48	34	7	-8	1	7	67	69	2	2	3	7	276	277	2	-11	6	7	136	133	5
-1	4	6	177	170	3	-6	7	6	39	45	8	-7	1	7	190	191	4	3	3	7	238	235	2	-10	6	7	171	165	4
0	4	6	336	328	9	-5	7	6	43	36	8	-6	1	7	219	221	3	4	3	7	207	204	1	-9	6	7	29	30	13
1	4	6	230	236	4	-4	7	6	81	74	5	-5	1	7	486	494	4	5	3	7	226	225	2	-8	6	7	28	36	10
2	4	6	92	93	2	-3	7	6	96	98	4	-4	1	7	281	277	2	6	3	7	307	304	2	-7	6	7	73	55	9
3	4	6	236	242	3	-2	7	6	111	108	3	-3	1	7	346	351	3	7	3	7	194	202	1	-6	6	7	105	105	3
4	4	6	125	123	1	-1	7	6	29	22	12	-2	1	7	327	348	2	8	3	7	127	132	1	-5	6	7	106	93	16
5	4	6	154	156	1	0	7	6	144	147	4	-1	1	7	499	500	4	9	3	7	71	75	1	-4	6	7	51	61	5
6	4	6	103	107	1	1	7	6	30	28	8	0	1	7	186	187	1	10	3	7	193	192	3	-3	6	7	67	63	4
7	4	6	52	45	6	2	7	6	117	108	3	1	1	7	381	402	2	11	3	7	99	109	2	-2	6	7	163	178	10
8	4	6	29	23	3	3	7	6	99	106	4	2	1	7	164	154	2	12	3	7	64	69	3	-1	6	7	134	123	3
9	4	6	133	137	2	4	7	6	172	168	4	3	1	7	304	305	3	13	3	7	134	135	2	0	6	7	279	276	5
10	4	6	157	148	2	5	7	6	88	95	4	4	1	7	464	462	2	14	3	7	15	26	14	1	6	7	202	197	10
11	4	6	90	92	1	6	7	6	56	48	6	5	1	7	360	357	2	15	3	7	74	78	4	2	6	7	142	150	3
12	4	6	106	100	2	7	7	6	97	98	4	6	1	7	262	253	3	16	3	7	31	26	7	3	6	7	131	134	3
13	4	6	50	48	8	8	7	6	39	44	9	7	1	7	104	101	1	17	3	7	82	85	4	4	6	7	56	47	5

Table 7. Observed and calculated structure factors for 1 Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	6	7	229	232	4	19	0	8	117	104	7	-9	3	8	135	132	2	8	5	8	211	208	3	-6	0	9	114	123	2
6	6	7	44	43	4	-19	1	8	97	101	5	-8	3	8	38	37	5	9	5	8	96	95	3	-5	0	9	111	117	2
7	6	7	249	244	4	-18	1	8	78	74	7	-7	3	8	189	194	2	10	5	8	181	170	4	-4	0	9	61	50	1

8	6	7	31	30	6	-17	1	8	93	93	3	-6	3	8	129	133	2	11	5	8	48	55	9	-3	0	9	443	444	4
9	6	7	16	17	16	-16	1	8	54	49	4	-5	3	8	165	152	2	12	5	8	24	35	24	-2	0	9	104	86	1
10	6	7	60	62	4	-15	1	8	41	47	9	-4	3	8	84	78	4	13	5	8	37	31	10	-1	0	9	22	13	3
11	6	7	16	31	16	-14	1	8	54	61	4	-3	3	8	294	286	4	14	5	8	75	72	8	0	0	9	88	85	1
12	6	7	39	32	10	-13	1	8	120	119	2	-2	3	8	260	259	2	15	5	8	23	32	23	1	0	9	94	100	1
13	6	7	33	27	17	-12	1	8	266	263	3	-1	3	8	90	79	4	-14	6	8	106	102	6	2	0	9	215	231	1
14	6	7	33	16	32	-11	1	8	364	355	5	0	3	8	221	217	2	-13	6	8	80	78	5	3	0	9	411	406	3
-11	7	7	62	68	7	-10	1	8	148	152	4	1	3	8	230	227	5	-12	6	8	52	49	7	4	0	9	215	215	1
-10	7	7	48	57	10	-9	1	8	150	156	2	2	3	8	160	151	2	-11	6	8	35	32	9	5	0	9	59	53	1
-9	7	7	62	54	7	-8	1	8	111	115	1	3	3	8	108	98	1	-10	6	8	185	175	4	6	0	9	75	85	1
-8	7	7	22	16	21	-7	1	8	68	67	1	4	3	8	45	39	1	-9	6	8	44	46	10	7	0	9	117	103	2
-7	7	7	66	66	7	-6	1	8	136	129	4	5	3	8	176	175	1	-8	6	8	138	144	4	8	0	9	174	179	1
-6	7	7	29	36	14	-5	1	8	168	177	1	6	3	8	172	171	1	-7	6	8	105	109	8	9	0	9	259	275	2
-5	7	7	114	119	6	-4	1	8	418	420	5	7	3	8	107	100	2	-6	6	8	184	190	3	10	0	9	52	55	3
-4	7	7	76	70	4	-3	1	8	204	204	3	8	3	8	48	51	1	-5	6	8	95	80	6	11	0	9	350	361	6
-3	7	7	129	136	4	-2	1	8	103	100	2	9	3	8	251	256	4	-4	6	8	261	256	5	12	0	9	294	288	5
-2	7	7	33	17	12	-1	1	8	331	331	2	10	3	8	156	151	3	-3	6	8	173	165	6	13	0	9	371	358	6
-1	7	7	65	68	4	0	1	8	163	164	1	11	3	8	24	23	8	-2	6	8	103	92	3	14	0	9	107	116	3
0	7	7	53	54	6	1	1	8	90	59	1	12	3	8	77	72	2	-1	6	8	136	136	3	15	0	9	0	10	1
1	7	7	99	95	3	2	1	8	212	203	1	13	3	8	121	120	2	0	6	8	165	156	4	16	0	9	18	21	17
2	7	7	68	61	5	3	1	8	234	240	1	14	3	8	42	49	3	1	6	8	120	112	3	17	0	9	24	22	23
3	7	7	105	106	4	4	1	8	366	351	4	15	3	8	89	95	8	2	6	8	131	138	6	18	0	9	44	61	11
4	7	7	56	59	6	5	1	8	230	219	1	16	3	8	83	82	3	3	6	8	152	151	3	19	0	9	55	46	14
5	7	7	89	89	4	6	1	8	334	342	3	17	3	8	18	21	17	4	6	8	147	141	3	-19	1	9	47	54	6
6	7	7	56	59	6	7	1	8	139	140	1	18	3	8	38	35	13	5	6	8	210	209	4	-18	1	9	69	56	5
7	7	7	54	44	5	8	1	8	149	147	1	-17	4	8	66	54	11	6	6	8	135	133	3	-17	1	9	53	53	4
8	7	7	63	59	5	9	1	8	66	57	3	-16	4	8	40	51	11	7	6	8	118	121	3	-16	1	9	99	94	3
9	7	7	16	24	16	10	1	8	172	174	1	-15	4	8	3	28	3	8	6	8	85	84	4	-15	1	9	121	113	5
10	7	7	131	127	8	11	1	8	139	142	8	-14	4	8	46	55	7	9	6	8	39	30	7	-14	1	9	91	85	4
11	7	7	33	38	32	12	1	8	113	115	6	-13	4	8	138	132	8	10	6	8	65	55	8	-13	1	9	135	135	4
-8	8	7	82	82	7	13	1	8	169	166	6	-12	4	8	29	30	11	11	6	8	41	55	11	-12	1	9	32	33	28
-7	8	7	40	48	11	14	1	8	96	93	1	-11	4	8	63	55	4	12	6	8	25	16	25	-11	1	9	136	137	2
-6	8	7	50	66	13	15	1	8	84	88	3	-10	4	8	3	21	3	13	6	8	40	43	13	-10	1	9	221	221	3
-5	8	7	29	19	17	16	1	8	76	76	3	-9	4	8	94	69	6	-11	7	8	61	64	7	-9	1	9	94	99	2
-4	8	7	74	74	6	17	1	8	42	47	9	-8	4	8	155	165	2	-10	7	8	71	69	7	-8	1	9	137	138	3
-3	8	7	47	58	10	18	1	8	31	35	31	-7	4	8	111	115	10	-9	7	8	13	14	12	-7	1	9	162	157	1
-2	8	7	51	35	8	19	1	8	41	46	7	-6	4	8	138	134	2	-8	7	8	42	44	24	-6	1	9	179	177	1
-1	8	7	124	122	5	-19	2	8	67	54	10	-5	4	8	101	93	4	-7	7	8	21	17	20	-5	1	9	324	318	2
0	8	7	79	88	6	-18	2	8	16	24	15	-4	4	8	81	78	2	-6	7	8	21	25	20	-4	1	9	318	324	2
1	8	7	65	57	7	-17	2	8	34	39	6	-3	4	8	264	272	2	-5	7	8	28	6	15	-3	1	9	596	593	12
2	8	7	47	55	8	-16	2	8	103	95	6	-2	4	8	58	63	3	-4	7	8	83	79	4	-2	1	9	231	233	1
3	8	7	58	76	8	-15	2	8	88	85	5	-1	4	8	92	98	2	-3	7	8	22	28	22	-1	1	9	217	202	1
4	8	7	8	8	7	-14	2	8	91	95	2	0	4	8	117	112	1	-2	7	8	125	122	4	0	1	9	270	286	2
5	8	7	60	58	7	-13	2	8	220	214	2	1	4	8	72	77	2	-1	7	8	4	8	3	1	1	9	341	352	2
6	8	7	16	23	16	-12	2	8	94	96	1	2	4	8	55	69	2	0	7	8	63	64	4	2	1	9	156	152	1
7	8	7	39	38	8	-11	2	8	250	244	2	3	4	8	104	98	5	1	7	8	17	20	17	3	1	9	415	400	3
-19	0	8	87	94	5	-10	2	8	196	198	2	4	4	8	127	137	1	2	7	8	197	195	4	4	1	9	131	119	1
-18	0	8	65	81	10	-9	2	8	54	46	7	5	4	8	199	209	2	3	7	8	18	33	17	5	1	9	134	111	1
-17	0	8	112	118	6	-8	2	8	197	203	2	6	4	8	161	168	2	4	7	8	96	101	4	6	1	9	161	151	1
-16	0	8	146	142	5	-7	2	8	180	175	5	7	4	8	239	237	2	5	7	8	39	39	10	7	1	9	222	224	2
-15	0	8	52	60	6	-6	2	8	87	75	2	8	4	8	47	43	2	6	7	8	46	55	6	8	1	9	155	159	1
-14	0	8	292	284	6	-5	2	8	337	331	3	9	4	8	356	351	4	7	7	8	62	62	4	9	1	9	179	176	5
-13	0	8	177	180	3	-4	2	8	87	92	2	10	4	8	29	33	3	8	7	8	58	62	5	10	1	9	187	182	1
-12	0	8	60	63	4	-3	2	8	461	449	4	11	4	8	145	153	2	9	7	8	94	85	9	11	1	9	284	281	4
-11	0	8	165	161	3	-2	2	8	165	161	3	12	4	8	95	95	4	10	7	8	23	27	23	12	1	9	241	239	2
-10	0	8	189	192	3	-1	2	8	346	347	2	13	4	8	60	68	6	11	7	8	32	34	19	13	1	9	134	131	3
-9	0	8	15	0	15	0	2	8	226	232	1	14	4	8	58	55	7	-7	8	8	43	33	10	14	1	9	59	59	3
-8	0	8	152	148	2	1	2	8	250	232	2	15	4	8	41	50	13	-6	8	8	36	13	36	15	1	9	157	154	3
-7	0	8	74	52	4	2	2	8	322	325	2	16	4	8	21	18	21	-5	8	8	37	52	12	16	1	9	47	52	4
-6	0	8	87	53	5	3	2	8	571	569	7	17	4	8	21	22	21	-4	8	8	81	83	5	17	1	9	129	126	3
-5	0	8	346	344	4	4	2	8	114	104	1	-16	5	8	76	59	13	-3	8	8	32	47	14	18	1	9	62	56	6
-4	0	8	285	290	3	5	2	8	330	322	5	-15	5	8	0	22	1	-2	8	8	37	13	13	19	1	9	77	87	7
-3	0	8	327	335	3	6	2	8	305	297	2	-14	5	8	37	44	12	-1	8	8	45	41	8	-18	2	9	24	31	23
-2	0	8	162	164	2	7	2	8	163	166	2	-13	5	8	70	72	5	0	8	8	55	63	6	-17	2	9	10	19	10
-1	0	8	67	44	2	8	2	8	40	35	5	-12	5	8	96	96	6	1	8	8	40	50	9	-16	2	9	78	75	5
0	0	8	54	49	1	9	2	8	283	288	2	-11	5	8	130	121	4	2	8	8	50	50	7	-15	2	9	69	71	3
1	0	8	303	332	2	10	2	8	231	238	2	-10	5	8	115	121	4	3	8	8	56	59	7	-14	2	9	48	48	3
2	0	8	35	23	2	11	2	8	131	124	1	-9	5	8	42	45	7	4	8	8	0	24	1	-13	2	9	57	56	3
3	0	8	465	482	3	12	2	8	128	131	5	-8	5	8	108	100	4	5	8	8	26	25	26	-12	2	9	208	206	2
4	0	8	85	65	2	13	2	8	123	122	2	-7	5	8	101	100	6	6	8	8	91	94	6	-11	2	9	109	109	1
5	0	8	103	76	2	14	2	8	83	86	3	-6	5	8	379	381	6	7	8	8	98	94	5	-10	2	9	164	164	3
6	0	8	370	373	3	15	2	8	45	43	4	-5	5	8	129	137	2	-19	0	9	54	53	7	-9	2	9	58	62	3
7	0	8	235	236	2	16	2	8	95	93	4	-4	5	8	81	78	2	-18	0	9	24	28	23	-8	2	9	143	143	1
8	0	8	162	159	1	17	2	8	24	25	10	-3	5	8	295	296	3	-17	0	9	171	170	8	-7	2	9	169	173	1
9	0	8	191	196	3	18	2	8	51	47	5	-2	5	8	54	43	3	-16	0	9	48	47	8	-6	2	9	436	433	4
10	0	8	28	26	5	-18	3	8	80	77	10	-1	5	8	284	286	4	-15	0	9	119	125	5	-5	2	9	200	202	4
11	0	8	57	51	2	-17	3	8	0	27	1	0	5	8	22	27	9	-14	0	9	61	69	6	-4	2	9	364	362	3
12	0	8	238	240	5	-16	3	8	41	42	8	1	5	8	219	211	4	-13	0	9	67	62	8	-3	2	9	155	157	1
13	0	8	111	110	2	-15	3	8	122	119	3	2	5	8	148	145	5	-12	0	9	90	88	4	-2	2	9	260	264	2
14	0	8	51	46	3	-14	3	8	57	69	3	3	5	8	210	199	3	-11	0	9	108	102	4	-1	2	9	279	280	2
15	0	8	16	33	16	-13	3	8	141	143	3	4	5	8	168	169	2	-10	0	9	16	27	16	0	2	9	268	266	2
16	0	8	130	125	4	-12	3	8	105	112	2	5	5	8	91	97	2	-9	0	9	116	105	3	1	2	9	157	150	1
17	0	8	25	19	11	-11	3	8	133	141	4	6	5	8	152	129	4	-8	0	9	83	82	3	2	2	9	160	150	2
18	0	8	46	41	9	-10	3	8	0	8	1	7	5	8	91	86	2	-7	0	9	303	295	4	3	2	9	132	116	3

Table 7. Observed and calculated structure factors for 1 Page 7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	2	9	137	121	1	-13	5	9	0	9	1	3	8	9	34	47	16	-10	2	10	205	214	2	7	4	10	131	131	2
5	2	9	155	157	1	-12	5	9	30	37	13	4	8	9	79	87	6	-9	2	10	111	122	3	8	4	10	207	210	2
6	2	9	235	224	2	-11	5	9	19	14	18	5	8	9	50	57	8	-8	2	10	194	192	2	9	4	10	125	130	2
7	2	9	166	170	1	-10	5	9	20	13	19	6	8	9	67	66	7	-7	2	10	105	114	1	10	4	10	225	223	3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
8	2	9	49	56	2	-9	5	9	286	273	6	-19	0	10	91	94	5	-6	2	10	231	234	2	11	4	10	85	89	5
9	2	9	55	63	1	-8	5	9	145	136	9	-18	0	10	121	115	6	-5	2	10	169	169	2	12	4	10	40	44	11
10	2	9	141	141	1	-7	5	9	145	138	8	-17	0	10	0	2	1	-4	2	10	92	68	2	13	4	10	111	114	3
11	2	9	81	88	2	-6	5	9	126	124	5	-16	0	10	60	70	10	-3	2	10	290	287	2	14	4	10	37	31	9
12	2	9	113	111	2	-5	5	9	116	112	3	-15	0	10	28	26	28	-2	2	10	179	161	1	15	4	10	110	110	5
13	2	9	33	37	3	-4	5	9	217	218	7	-14	0	10	0	8	1	-1	2	10	311	298	2	16	4	10	53	58	7
14	2	9	43	52	3	-3	5	9	125	116	6	-13	0	10	118	117	4	0	2	10	296	287	2	-15	5	10	23	24	22
15	2	9	52	55	3	-2	5	9	149	141	4	-12	0	10	247	246	5	1	2	10	109	79	2	-14	5	10	51	48	10
16	2	9	86	77	6	-1	5	9	99	89	15	-11	0	10	131	133	3	2	2	10	226	215	1	-13	5	10	65	69	7
17	2	9	21	26	20	0	5	9	208	200	6	-10	0	10	67	72	4	3	2	10	65	10	4	-12	5	10	51	37	8
18	2	9	95	92	4	1	5	9	187	183	4	-9	0	10	62	55	6	4	2	10	337	330	2	-11	5	10	64	63	6
-18	3	9	40	44	23	2	5	9	253	259	3	-8	0	10	91	80	3	5	2	10	213	215	1	-10	5	10	230	221	4
-17	3	9	56	51	6	3	5	9	284	284	5	-7	0	10	28	18	5	6	2	10	185	175	1	-9	5	10	124	120	7
-16	3	9	77	70	4	4	5	9	283	273	4	-6	0	10	473	480	6	7	2	10	32	20	1	-8	5	10	133	132	9
-15	3	9	58	54	4	5	5	9	274	268	3	-5	0	10	172	174	2	8	2	10	251	249	2	-7	5	10	253	251	7
-14	3	9	77	79	3	6	5	9	200	199	3	-4	0	10	388	366	4	9	2	10	162	165	4	-6	5	10	126	123	3
-13	3	9	59	61	3	7	5	9	228	218	3	-3	0	10	63	52	2	10	2	10	93	100	6	-5	5	10	334	319	7
-12	3	9	97	97	2	8	5	9	44	42	3	-2	0	10	144	127	2	11	2	10	60	64	2	-4	5	10	31	26	7
-11	3	9	145	147	2	9	5	9	270	256	4	-1	0	10	212	199	2	12	2	10	116	106	3	-3	5	10	156	155	3
-10	3	9	147	148	2	10	5	9	133	126	3	0	0	10	496	506	4	13	2	10	80	84	2	-2	5	10	122	129	3
-9	3	9	242	242	6	11	5	9	89	92	5	1	0	10	345	352	3	14	2	10	101	105	2	-1	5	10	186	187	3
-8	3	9	106	106	2	12	5	9	81	85	7	2	0	10	410	419	3	15	2	10	24	33	9	0	5	10	28	37	10
-7	3	9	91	94	3	13	5	9	29	35	28	3	0	10	118	131	1	16	2	10	75	84	3	1	5	10	200	204	3
-6	3	9	73	79	2	14	5	9	38	38	12	4	0	10	481	480	3	17	2	10	37	29	6	2	5	10	71	71	3
-5	3	9	89	96	5	15	5	9	0	36	1	5	0	10	135	143	1	18	2	10	43	57	6	3	5	10	120	115	3
-4	3	9	237	241	3	-13	6	9	35	42	25	6	0	10	104	79	4	-17	3	10	26	31	25	4	5	10	104	107	3
-3	3	9	132	130	3	-12	6	9	25	18	24	7	0	10	112	112	1	-16	3	10	52	50	7	5	5	10	258	251	6
-2	3	9	70	62	2	-11	6	9	104	96	9	8	0	10	183	181	1	-15	3	10	65	65	6	6	5	10	61	60	3
-1	3	9	73	72	1	-10	6	9	47	41	8	9	0	10	239	236	2	-14	3	10	40	22	7	7	5	10	205	197	3
0	3	9	279	281	2	-9	6	9	28	2	22	10	0	10	141	154	3	-13	3	10	64	67	4	8	5	10	62	63	3
1	3	9	163	169	1	-8	6	9	103	102	6	11	0	10	32	28	6	-12	3	10	83	78	2	9	5	10	63	69	3
2	3	9	267	271	2	-7	6	9	73	70	7	12	0	10	63	48	5	-11	3	10	110	105	5	10	5	10	58	64	7
3	3	9	177	179	3	-6	6	9	108	115	4	13	0	10	0	12	1	-10	3	10	22	22	21	11	5	10	111	121	5
4	3	9	249	242	2	-5	6	9	83	78	10	14	0	10	0	7	1	-9	3	10	274	264	9	12	5	10	48	39	11
5	3	9	34	26	3	-4	6	9	240	236	4	15	0	10	27	36	8	-8	3	10	110	119	5	13	5	10	42	46	10
6	3	9	178	184	1	-3	6	9	132	133	3	16	0	10	85	89	4	-7	3	10	38	42	4	14	5	10	41	48	11
7	3	9	65	69	3	-2	6	9	121	120	4	17	0	10	140	133	5	-6	3	10	128	128	3	-13	6	10	0	24	1
8	3	9	98	97	1	-1	6	9	124	129	3	18	0	10	101	93	6	-5	3	10	124	127	3	-12	6	10	113	115	5
9	3	9	69	71	1	0	6	9	144	143	5	-18	1	10	109	111	4	-4	3	10	175	165	2	-11	6	10	90	92	10
10	3	9	116	117	2	1	6	9	161	161	3	-17	1	10	30	26	14	-3	3	10	108	99	2	-10	6	10	47	50	12
11	3	9	92	96	3	2	6	9	160	165	6	-16	1	10	13	24	13	-2	3	10	163	164	2	-9	6	10	0	26	1
12	3	9	34	42	5	3	6	9	83	90	3	-15	1	10	60	57	5	-1	3	10	105	92	1	-8	6	10	60	50	8
13	3	9	62	61	5	4	6	9	71	51	5	-14	1	10	63	60	4	0	3	10	81	77	1	-7	6	10	95	96	4
14	3	9	131	126	3	5	6	9	132	127	3	-13	1	10	54	54	4	1	3	10	254	254	2	-6	6	10	66	55	19
15	3	9	107	110	3	6	6	9	51	53	4	-12	1	10	67	66	4	2	3	10	75	70	1	-5	6	10	47	51	6
16	3	9	42	51	6	7	6	9	159	158	3	-11	1	10	199	194	5	3	3	10	289	279	5	-4	6	10	168	166	5
17	3	9	39	44	8	8	6	9	57	62	5	-10	1	10	171	167	6	4	3	10	54	53	1	-3	6	10	67	68	4
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-12	4	9	145	143	4	-11	7	9	11	11	10	-4	1	10	277	283	2	10	3	10	120	118	5	3	6	10	100	100	3
-11	4	9	210	207	4	-10	7	9	100	101	6	-3	1	10	489	487	6	11	3	10	154	154	2	4	6	10	143	143	3
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-5	4	9	179	186	2	-4	7	9	27	15	27	3	1	10	254	230	2	17	3	10	0	12	1	10	6	10	40	44	14
-4	4	9	90	102	2	-3	7	9	39	45	8	4	1	10	145	138	1	-16	4	10	54	48	9	11	6	10	48	43	8
-3	4	9	85	87	2	-2	7	9	36	44	9	5	1	10	255	252	3	-15	4	10	35	34	11	12	6	10	35	66	19
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-1	4	9	158	153	2	0	7	9	94	98	6	7	1	10	139	137	1	-13	4	10	25	42	20	-10	7	10	60	44	19
0	4	9	80	84	4	1	7	9	79	77	5	8	1	10	79	86	1	-12	4	10	53	54	5	-9	7	10	0	23	1
1	4	9	84	81	2	2	7	9	42	45	6	9	1	10	239	245	3	-11	4	10	40	39	8	-8	7	10	37	34	12
2	4	9	238	241	2	3	7	9	63	57	5	10	1	10	141	137	2	-10	4	10	105	100	4	-7	7	10	34	22	33
3	4	9	150	153	2	4	7	9	112	112	4	11	1	10	220	218	2	-9	4	10	152	142	3	-6	7	10	25	10	20
4	4	9	90	94	2	5	7	9	46	53	6	12	1	10	213	212	3	-8	4	10	43	47	6	-5	7	10	72	65	9
5	4	9	104	99	1	6	7	9	68	71	5	13	1	10	56	56	2	-7	4	10	189	190	4	-4	7	10	49	44	7
6	4	9	76	79	2	7	7	9	69	72	5	14	1	10	49	54	4	-6	4	10	31	34	7	-3	7	10	102	94	5
7	4	9	174	175	2	8	7	9	43	41	7	15	1	10	52	47	4	-5	4	10	92	92	3	-2	7	10	23	29	16
8	4	9	169	160	2	9	7	9	0	19	1	16	1	10	58	57	4	-4	4	10	116	109	3	-1	7	10	35	46	10
9	4	9	98	102	1	10	7	9	31	28	30	17	1	10	48	50	9	-3	4	10	144	145	2	0	7	10	48	47	7
10	4	9	34	28	2	-6	8	9	53	57	16	18	1	10	0	7	1	-2	4	10	246	247	2	1	7	10	33	13	11
11	4	9	90	83	6	-5	8	9	48	44	8	-18	2	10	31	32	13	-1	4	10	256	254	2	2	7	10	24	19	13
12	4	9	75	91	5	-4	8	9	12	32	12	-17	2	10	43	31	10	0	4	10	105	112	4	3	7	10	188	183	5
13	4	9	43	21	10	-3	8	9	60	54	5	-16	2	10	24	29	10	1	4	10	300	300	3	4	7	10	55	45	6
14	4	9	75	70	5	-2	8	9	0	22	1	-15	2	10	75	71	6	2	4	10	99	84	2	5	7	10	109	107	4
15	4	9	39	32	8	-1	8	9	0	15	1	-14	2	10	31	21	5	3	4	10	187	190	2	6	7	10	77	83	5
16	4	9	36	46	8	0	8	9	33	39	13	-13	2	10	43	45	3	4	4	10	198	193	2	7	7	10	124	126	4
-15	5	9	28	9	25	1	8	9	0	20	1	-12	2	10	185	187	2	5	4	10	237	238	2	8	7	10	51	53	9
-14	5	9	36	46	20	2	8	9	65	60	7	-11	2	10	29	25	2	6	4	10	118	125	2	9	7	10	60	62	11

Table 7. Observed and calculated structure factors for 1 Page 8

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
10	7	10	81	83	12	-18	2	11	46	51	10	-1	4	11	40	37	1	3	7	11	58	46	5	16	1	12	113	95	3
-6	8	10	68	62	8	-17	2	11	48	49	8	0	4	11	59	59	1	4	7	11	88	94	4	17	1	12	56	54	6
-5	8	10	75	66	14	-16	2	11	67	68	13	1	4	11	125	123	1	5	7	11	100	102	5	18	1	12	79	71	6
-4	8	10	0	5	1	-15	2	11	46	44	4	2	4	11	222	220	2	6	7	11	42	53	8	-17	2	12	100	99	5
-3	8	10	76	79	8	-14	2	11	90	84	5	3	4	11	63	61	2	7	7	11	66	58	4	-16	2	12	57	49	27
-2	8	10	58	61	5	-13	2	11	78	80	3	4	4	11	114	121	2	8	7	11	55	58	12	-15	2	12	28	19	27

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	8	10	45	37	7	-12	2	11	101	98	3	5	4	11	45	39	3	9	7	11	76	70	12	-14	2	12	11	22	10
0	8	10	56	50	6	-11	2	11	171	170	2	6	4	11	51	53	2	-5	8	11	95	81	7	-13	2	12	35	37	4
1	8	10	53	56	8	-10	2	11	171	171	2	7	4	11	161	163	2	-4	8	11	68	77	7	-12	2	12	79	77	2
2	8	10	38	46	9	-9	2	11	151	150	1	8	4	11	124	120	2	-3	8	11	49	50	13	-11	2	12	49	56	2
3	8	10	30	8	16	-8	2	11	54	54	4	9	4	11	86	83	2	-2	8	11	33	30	27	-10	2	12	149	145	2
4	8	10	55	46	8	-7	2	11	122	121	4	10	4	11	58	54	6	-1	8	11	22	29	21	-9	2	12	182	182	2
5	8	10	31	13	21	-6	2	11	211	213	1	11	4	11	78	88	3	0	8	11	57	68	7	-8	2	12	167	176	2
-18	0	11	21	32	21	-5	2	11	138	146	4	12	4	11	25	41	12	1	8	11	38	20	11	-7	2	12	130	127	1
-17	0	11	0	19	1	-4	2	11	261	265	4	13	4	11	70	75	4	2	8	11	32	40	12	-6	2	12	199	201	2
-16	0	11	40	45	14	-3	2	11	139	127	2	14	4	11	57	56	7	3	8	11	0	13	1	-5	2	12	284	281	3
-15	0	11	53	53	8	-2	2	11	124	112	2	15	4	11	29	23	16	4	8	11	0	5	1	-4	2	12	312	304	2
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-12	0	11	226	213	6	1	2	11	76	70	1	-14	5	11	49	38	8	-15	0	12	0	28	1	-1	2	12	106	97	2
-11	0	11	217	225	5	2	2	11	250	250	1	-13	5	11	42	35	12	-14	0	12	33	48	14	0	2	12	70	80	2
-10	0	11	123	130	3	3	2	11	187	191	1	-12	5	11	76	73	5	-13	0	12	0	7	1	1	2	12	150	149	1
-9	0	11	28	1	9	4	2	11	210	204	1	-11	5	11	23	30	22	-12	0	12	163	159	5	2	2	12	115	114	1
-8	0	11	67	74	4	5	2	11	49	46	1	-10	5	11	100	93	4	-11	0	12	241	230	7	3	2	12	119	116	1
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-6	0	11	37	42	5	7	2	11	103	104	1	-8	5	11	65	67	5	-9	0	12	28	35	9	5	2	12	189	192	1
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-3	0	11	219	217	2	10	2	11	105	102	7	-5	5	11	122	119	9	-6	0	12	397	391	5	8	2	12	63	57	1
-2	0	11	178	107	4	11	2	11	240	227	3	-4	5	11	240	235	4	-5	0	12	73	73	2	9	2	12	137	142	2
-1	0	11	69	68	1	12	2	11	55	57	2	-3	5	11	93	98	3	-4	0	12	51	63	2	10	2	12	166	168	3
0	0	11	35	19	3	13	2	11	62	66	2	-2	5	11	62	57	3	-3	0	12	114	112	1	11	2	12	164	159	2
1	0	11	33	1	2	14	2	11	9	23	9	-1	5	11	22	18	13	-2	0	12	165	168	2	12	2	12	143	144	3
2	0	11	670	659	6	15	2	11	21	27	20	0	5	11	17	16	16	-1	0	12	89	103	1	13	2	12	47	40	3
3	0	11	426	456	4	16	2	11	78	83	4	1	5	11	101	95	2	0	0	12	72	67	1	14	2	12	17	28	17
4	0	11	110	72	3	17	2	11	15	22	14	2	5	11	84	87	2	1	0	12	132	130	1	15	2	12	46	45	5
5	0	11	158	154	1	18	2	11	0	18	1	3	5	11	97	96	2	2	0	12	161	161	2	16	2	12	19	28	19
6	0	11	205	196	1	-17	3	11	50	41	8	4	5	11	74	71	3	3	0	12	33	35	2	17	2	12	65	58	5
7	0	11	60	67	1	-16	3	11	34	46	11	5	5	11	130	130	4	4	0	12	111	109	1	-17	3	12	64	57	8
8	0	11	287	293	2	-15	3	11	48	49	7	6	5	11	109	108	2	5	0	12	98	104	1	-16	3	12	32	13	20
9	0	11	0	5	1	-14	3	11	22	20	21	7	5	11	18	13	8	6	0	12	171	159	3	-15	3	12	121	116	4
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13	0	11	0	2	1	-10	3	11	117	124	5	11	5	11	83	81	6	10	0	12	183	187	3	-11	3	12	74	73	5
14	0	11	57	52	4	-9	3	11	74	74	4	12	5	11	44	52	8	11	0	12	366	354	6	-10	3	12	57	56	4
15	0	11	22	22	11	-8	3	11	128	126	6	13	5	11	57	60	8	12	0	12	48	42	4	-9	3	12	186	180	4
16	0	11	44	42	4	-7	3	11	230	225	5	14	5	11	20	25	19	13	0	12	118	120	3	-8	3	12	146	150	3
17	0	11	68	58	6	-6	3	11	33	35	7	-13	6	11	31	31	17	14	0	12	221	211	4	-7	3	12	214	216	3
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0	1	11	271	280	2	14	3	11	46	47	5	7	6	11	68	66	3	-3	1	12	346	353	2	13	3	12	28	32	6
1	1	11	341	358	2	15	3	11	64	69	5	8	6	11	87	86	4	-2	1	12	136	132	2	14	3	12	52	38	5
2	1	11	303	304	2	16	3	11	61	57	4	9	6	11	29	37	17	-1	1	12	191	184	1	15	3	12	70	69	5
3	1	11	590	585	3	17	3	11	41	37	8	10	6	11	57	66	8	0	1	12	180	180	1	16	3	12	49	38	7
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5	1	11	172	173	1	-15	4	11	47	45	9	12	6	11	27	34	27	2	1	12	169	172	1	-15	4	12	17	10	16
6	1	11	129	129	1	-14	4	11	0	24	1	-10	7	11	106	101	6	3	1	12	348	331	4	-14	4	12	48	48	16
7	1	11	55	54	1	-13	4	11	97	97	7	-9	7	11	95	103	6	4	1	12	86	62	4	-13	4	12	23	30	23
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13	1	11	106	97	2	-7	4	11	56	46	6	-3	7	11	127	125	5	10	1	12	69	63	1	-7	4	12	209	200	5
14	1	11	115	117	2	-6	4	11	83	86	4	-2	7	11	64	67	6	11	1	12	196	192	3	-6	4	12	143	134	3
15	1	11	44	47	9	-5	4	11	174	171	7	-1	7	11	67	76	5	12	1	12	76	79	1	-5	4	12	51	52	10
16	1	11	84	90	5	-4	4	11	55	39	6	0	7	11	12	6	12	13	1	12	184	180	3	-4	4	12	145	137	3
17	1	11	57	65	11	-3	4	11	155	159	3	1	7	11	101	109	4	14	1	12	71	66	6	-3	4	12	93	94	2
18	1	11	47	39	6	-2	4	11	163	153	2	2	7	11	23	22	11	15	1	12	55	65	4	-2	4	12	84	85	3

Table 7. Observed and calculated structure factors for 1 Page 9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	4	12	71	82	2	8	7	12	70	54	12	-10	2	13	216	208	2	11	4	13	32	14	7	-4	0	14	77	64	2
0	4	12	71	68	2	9	7	12	44	30	22	-9	2	13	125	133	1	12	4	13	53	52	5	-3	0	14	49	30	2
1	4	12	56	56	2	-3	8	12	54	43	9	-8	2	13	38	28	10	13	4	13	66	55	11	-2	0	14	27	17	2
2	4	12	43	43	2	-2	8	12	39	61	20	-7	2	13	213	210	2	14	4	13	28	13	13	-1	0	14	141	140	1
3	4	12	151	150	2	-1	8	12	22	29	21	-6	2	13	123	127	2	15	4	13	68	73	6	0	0	14	92	89	1
4	4	12	143	137	2	0	8	12	39	49	9	-5	2	13	247	247	7	-14	5	13	71	65	7	1	0	14	41	26	2
5	4	12	73	83	2	1	8	12	81	70	6	-4	2	13	124	127	1	-13	5	13	15	13	14	2	0	14	109	115	1
6	4	12	92	94	2	2	8	12	54	59	7	-3	2	13	97	92	2	-12	5	13	96	97	6	3	0	14	168	173	2

7	4	12	163	155	2	3	8	12	87	86	6	-2	2	13	33	30	2	-11	5	13	73	79	5	4	0	14	163	174	2
8	4	12	131	133	1	-18	0	13	70	79	8	-1	2	13	95	92	1	-10	5	13	63	60	6	5	0	14	256	256	2
9	4	12	167	158	3	-17	0	13	0	3	1	0	2	13	40	46	2	-9	5	13	128	126	4	6	0	14	85	83	1
10	4	12	84	87	12	-16	0	13	29	24	23	1	2	13	112	110	1	-8	5	13	61	66	5	7	0	14	197	193	2
11	4	12	55	49	4	-15	0	13	136	125	5	2	2	13	122	116	1	-7	5	13	129	130	5	8	0	14	190	188	2
12	4	12	48	42	16	-14	0	13	175	179	6	3	2	13	179	178	1	-6	5	13	18	33	17	9	0	14	397	386	4
13	4	12	27	38	9	-13	0	13	42	50	8	4	2	13	184	192	1	-5	5	13	76	79	4	10	0	14	235	220	2
14	4	12	0	12	1	-12	0	13	79	81	6	5	2	13	147	147	1	-4	5	13	212	205	5	11	0	14	39	25	6
15	4	12	37	41	10	-11	0	13	344	332	7	6	2	13	86	89	1	-3	5	13	144	146	13	12	0	14	35	39	7
-14	5	12	20	10	19	-10	0	13	301	290	7	7	2	13	175	171	2	-2	5	13	39	30	5	13	0	14	63	56	4
-13	5	12	139	124	5	-9	0	13	196	199	5	8	2	13	262	267	2	-1	5	13	156	153	2	14	0	14	30	23	7
-12	5	12	53	52	10	-8	0	13	55	61	7	9	2	13	181	170	5	0	5	13	75	72	8	15	0	14	55	53	6
-11	5	12	60	60	6	-7	0	13	39	21	7	10	2	13	122	117	1	1	5	13	178	173	2	16	0	14	31	46	11
-10	5	12	8	30	7	-6	0	13	47	40	3	11	2	13	89	88	2	2	5	13	184	190	2	17	0	14	45	47	8
-9	5	12	73	62	9	-5	0	13	79	27	5	12	2	13	49	47	7	3	5	13	145	144	2	-17	1	14	0	14	1
-8	5	12	92	93	4	-4	0	13	14	27	6	13	2	13	0	19	1	4	5	13	165	164	2	-16	1	14	41	46	8
-7	5	12	0	14	1	-3	0	13	328	330	3	14	2	13	31	29	10	5	5	13	32	24	5	-15	1	14	0	12	1
-6	5	12	43	42	7	-2	0	13	59	18	3	15	2	13	42	47	6	6	5	13	27	25	5	-14	1	14	40	27	11
-5	5	12	51	57	6	-1	0	13	197	192	2	16	2	13	77	67	5	7	5	13	81	79	3	-13	1	14	114	111	4
-4	5	12	153	157	3	0	0	13	157	160	1	17	2	13	56	48	7	8	5	13	37	30	4	-12	1	14	48	42	5
-3	5	12	177	179	3	1	0	13	281	293	2	-16	3	13	30	27	22	9	5	13	46	45	6	-11	1	14	49	46	14
-2	5	12	69	67	5	2	0	13	271	280	2	-15	3	13	18	12	18	10	5	13	119	112	4	-10	1	14	171	165	4
-1	5	12	176	169	2	3	0	13	271	264	2	-14	3	13	46	37	8	11	5	13	72	74	6	-9	1	14	139	139	3
0	5	12	118	127	6	4	0	13	16	11	5	-13	3	13	40	28	8	12	5	13	93	92	5	-8	1	14	112	108	5
1	5	12	146	140	2	5	0	13	302	308	2	-12	3	13	113	111	4	13	5	13	57	53	6	-7	1	14	91	88	1
2	5	12	145	143	3	6	0	13	138	157	1	-11	3	13	131	129	3	-12	6	13	45	55	14	-6	1	14	48	46	3
3	5	12	165	165	3	7	0	13	274	275	3	-10	3	13	47	46	3	-11	6	13	26	22	26	-5	1	14	118	117	1
4	5	12	63	65	3	8	0	13	126	127	1	-9	3	13	126	121	2	-10	6	13	38	54	15	-4	1	14	196	188	2
5	5	12	47	50	4	9	0	13	257	258	3	-8	3	13	59	59	2	-9	6	13	33	43	11	-3	1	14	162	168	2
6	5	12	130	132	2	10	0	13	186	190	2	-7	3	13	119	123	2	-8	6	13	82	84	4	-2	1	14	168	171	2
7	5	12	56	48	5	11	0	13	210	206	4	-6	3	13	45	48	3	-7	6	13	83	86	7	-1	1	14	114	113	1
8	5	12	173	169	4	12	0	13	38	41	5	-5	3	13	25	42	11	-6	6	13	143	145	4	0	1	14	164	161	1
9	5	12	32	64	19	13	0	13	36	30	7	-4	3	13	40	30	3	-5	6	13	132	137	5	1	1	14	179	185	1
10	5	12	58	52	8	14	0	13	72	62	4	-3	3	13	76	78	1	-4	6	13	75	84	6	2	1	14	74	71	1
11	5	12	31	27	30	15	0	13	53	65	5	-2	3	13	156	155	2	-3	6	13	100	100	10	3	1	14	96	85	1
12	5	12	29	27	29	16	0	13	47	62	8	-1	3	13	132	126	1	-2	6	13	28	12	12	4	1	14	244	245	1
13	5	12	40	45	8	17	0	13	67	66	5	0	3	13	60	61	3	-1	6	13	83	83	10	5	1	14	172	180	1
14	5	12	42	29	11	-17	1	13	44	43	10	1	3	13	216	216	2	0	6	13	12	20	12	6	1	14	144	144	1
-12	6	12	137	140	6	-16	1	13	43	47	10	2	3	13	131	127	1	1	6	13	83	84	5	7	1	14	127	133	1
-11	6	12	54	58	9	-15	1	13	26	1	25	3	3	13	123	119	1	2	6	13	137	129	4	8	1	14	123	120	1
-10	6	12	38	36	18	-14	1	13	23	34	17	4	3	13	112	123	1	3	6	13	60	61	6	9	1	14	179	171	2
-9	6	12	44	35	9	-13	1	13	126	114	3	5	3	13	67	73	1	4	6	13	51	64	7	10	1	14	237	228	5
-8	6	12	86	81	5	-12	1	13	190	188	4	6	3	13	47	47	4	5	6	13	73	69	4	11	1	14	166	172	2
-7	6	12	47	40	6	-11	1	13	156	147	6	7	3	13	67	69	1	6	6	13	36	18	8	12	1	14	40	37	3
-6	6	12	71	71	13	-10	1	13	187	193	3	8	3	13	71	69	1	7	6	13	90	93	4	13	1	14	26	40	10
-5	6	12	37	44	6	-9	1	13	83	76	3	9	3	13	42	41	7	8	6	13	33	14	32	14	1	14	62	60	3
-4	6	12	16	18	16	-8	1	13	43	33	6	10	3	13	112	101	2	9	6	13	86	93	7	15	1	14	55	56	5
-3	6	12	46	36	5	-7	1	13	231	236	2	11	3	13	47	36	6	10	6	13	49	41	6	16	1	14	76	74	5
-2	6	12	85	89	4	-6	1	13	127	131	1	12	3	13	56	62	3	11	6	13	78	73	5	17	1	14	45	52	8
-1	6	12	162	151	4	-5	1	13	110	101	2	13	3	13	60	58	3	-8	7	13	0	17	1	-17	2	14	53	42	8
0	6	12	52	44	5	-4	1	13	70	63	2	14	3	13	0	23	1	-7	7	13	59	65	7	-16	2	14	53	60	11
1	6	12	34	24	8	-3	1	13	319	320	2	15	3	13	39	39	9	-6	7	13	0	44	1	-15	2	14	12	14	11
2	6	12	108	117	5	-2	1	13	69	63	2	16	3	13	22	19	22	-5	7	13	57	64	6	-14	2	14	81	90	4
3	6	12	82	87	7	-1	1	13	142	141	1	-15	4	13	58	49	13	-4	7	13	166	165	6	-13	2	14	71	71	5
4	6	12	27	26	9	0	1	13	69	71	1	-14	4	13	47	44	8	-3	7	13	32	24	22	-12	2	14	43	51	6
5	6	12	12	4	12	1	1	13	143	139	1	-13	4	13	39	44	9	-2	7	13	38	37	10	-11	2	14	56	55	3
6	6	12	138	139	3	2	1	13	197	202	1	-12	4	13	63	64	6	-1	7	13	75	80	11	-10	2	14	32	38	3
7	6	12	87	85	3	3	1	13	241	239	1	-11	4	13	126	129	4	0	7	13	46	46	8	-9	2	14	102	98	1
8	6	12	84	84	8	4	1	13	249	249	1	-10	4	13	51	58	6	1	7	13	50	26	7	-8	2	14	121	112	1
9	6	12	123	125	6	5	1	13	223	231	1	-9	4	13	113	110	5	2	7	13	58	54	6	-7	2	14	86	93	3
10	6	12	0	12	1	6	1	13	157	157	1	-8	4	13	98	96	3	3	7	13	108	109	4	-6	2	14	58	59	8
11	6	12	34	41	18	7	1	13	89	82	3	-7	4	13	65	58	4	4	7	13	48	45	8	-5	2	14	109	112	2
-9	7	12	65	72	9	8	1	13	209	219	1	-6	4	13	155	147	4	5	7	13	74	72	6	-4	2	14	96	95	2
-8	7	12	45	42	14	9	1	13	186	191	2	-5	4	13	77	79	12	6	7	13	51	55	6	-3	2	14	91	97	6
-7	7	12	57	63	8	10	1	13	118	116	7	-4	4	13	145	154	4	7	7	13	0	42	1	-2	2	14	125	123	1
-6	7	12	0	18	1	11	1	13	199	188	2	-3	4	13	273	272	5	8	7	13	30	15	29	-1	2	14	20	26	5
-5	7	12	131	122	8	12	1	13	175	169	2	-2	4	13	101	108	3	-17	0	14	24	28	23	0	2	14	225	214	2
-4	7	12	90	104	7	13	1	13	206	196	3	-1	4	13	286	293	4	-16	0	14	0	1	1	1	2	14	26	30	3
-3	7	12	161	158	8	14	1	13	32	26	8	0	4	13	58	55	1	-15	0	14	0	4	1	2	2	14	172	177	3
-2	7	12	57	67	6	15	1	13	83	81	6	1	4	13	269	266	3	-14	0	14	38	46	18	3	2	14	66	65	1
-1	7	12	24	42	23	16	1	13	89	73	14	2	4	13	54	51	4	-13	0	14	54	49	7	4	2	14	143	149	4
0	7	12	48	44	7	17	1	13	0	25	1	3	4	13	314	310	4	-12	0	14	73	67	8	5	2	14	46	40	4
1	7	12	90	84	7	-17	2	13	30	42	30	4	4	13	72	72	2	-11	0	14	39	52	8	6	2	14	63	61	3
2	7	12	13	13	12	-16	2	13	40	44	10	5	4	13	179	174	2	-10	0	14	378	349	9	7	2	14	68	63	3
3	7	12	170	160	4	-15	2	13	8	19	8	6	4	13	251	249	4	-9	0	14	186	189	7	8	2	14	53	56	1
4	7	12	80	81	4	-14	2	13	40	52	8	7	4	13	175	182	3	-8	0	14	179	167	4	9	2	14	86	86	2
5	7	12	47	50	7	-13	2	13	62	55	3	8	4	13	188	184	6	-7	0	14	137	135	4	10	2	14	107	106	3
6	7	12	86	86	5	-12	2	13	131	129	2	9	4	13	180	172	4	-6	0	14	79	84	3	11	2	14	93	92	2
7	7	12	35	46	20	-11	2	13	95	99	2	10	4	13	53	51	5	-5	0	14	272	279	4	12	2	14	39	49	5

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
13	2	14	76	78	3	7	5	14	0	8	1	-9	1	15	59	72	4	13	3	15	59	64	6	2	7	15	23	29	23
14	2	14	0	9	1	8	5	14	80	83	4	-8	1	15	78	78	6	14	3	15	44	43	9	3	7	15	48	40	9
15	2	14	52	48	5	9	5	14	22	17	15	-7	1	15	122	120	3	15	3	15	24	20	23	4	7	15	9	15	9
16	2	14	113	107	5	10	5	14	74	71	5	-6	1	15	56	58	2	-14	4	15	50	57	19	5	7	15	55	40	6
-16	3	14	31	27	13	11	5	14	137	131	5	-5	1	15	111	111	3	-13	4	15	57	59	7	6	7	15	0	23	1
-15	3	14	9	17	9	12	5	14	45	19	9	-4	1	15	42	50	1	-12	4	15	26	15	25	-16	0	16	5	7	5
-14	3	14	41	31	9	13	5	14	68	78	9	-3	1	15	38	38	2	-11	4	15	13	29	13	-15	0	16	24	13	23
-13	3	14	74	73	6	-11	6	14	31	15	31	-2	1	15	259	267	2	-10	4	15	76	82	6	-14	0	16	22	6	21
-12	3	14	136	138	6	-10	6	14	65	68	9	-1	1	15	198	197	1	-9	4	15	32	47	14	-13	0	16	22	35	21
-11	3	14	86	89	4	-9	6	14	52	41	13	0	1	15	100	102	2	-8	4	15	124	124	4	-12	0	16	33	53	33

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-10	3	14	80	85	5	-8	6	14	85	79	9	1	1	15	270	263	2	-7	4	15	117	115	5	-11	0	16	40	46	10
-9	3	14	49	50	3	-7	6	14	1	33	1	2	1	15	200	192	1	-6	4	15	200	212	3	-10	0	16	24	36	24
-8	3	14	27	33	9	-6	6	14	62	56	6	3	1	15	213	212	1	-5	4	15	255	250	4	-9	0	16	101	80	5
-7	3	14	36	35	10	-5	6	14	51	55	9	4	1	15	37	30	1	-4	4	15	58	63	5	-8	0	16	38	44	11
-6	3	14	61	59	2	-4	6	14	106	111	4	5	1	15	57	58	1	-3	4	15	126	135	3	-7	0	16	171	170	4
-5	3	14	90	93	2	-3	6	14	96	92	6	6	1	15	123	116	1	-2	4	15	168	172	3	-6	0	16	69	68	5
-4	3	14	98	105	5	-2	6	14	39	49	8	7	1	15	191	190	2	-1	4	15	201	200	5	-5	0	16	99	102	4
-3	3	14	94	90	2	-1	6	14	65	69	13	8	1	15	107	98	1	0	4	15	166	160	3	-4	0	16	402	405	5
-2	3	14	187	188	2	0	6	14	75	67	5	9	1	15	158	153	2	1	4	15	97	94	2	-3	0	16	185	194	2
-1	3	14	61	62	2	1	6	14	71	69	6	10	1	15	104	99	2	2	4	15	73	76	2	-2	0	16	151	149	2
0	3	14	92	103	4	2	6	14	40	38	8	11	1	15	34	27	4	3	4	15	76	73	2	-1	0	16	98	94	1
1	3	14	62	65	1	3	6	14	81	88	5	12	1	15	30	28	6	4	4	15	122	124	2	0	0	16	118	118	1
2	3	14	139	130	2	4	6	14	53	52	4	13	1	15	54	47	4	5	4	15	165	155	2	1	0	16	56	53	2
3	3	14	190	196	1	5	6	14	51	58	8	14	1	15	46	35	5	6	4	15	133	128	2	2	0	16	34	26	3
4	3	14	124	114	1	6	6	14	29	28	7	15	1	15	68	71	6	7	4	15	120	122	3	3	0	16	84	74	2
5	3	14	27	29	4	7	6	14	0	9	1	16	1	15	0	22	1	8	4	15	148	144	5	4	0	16	168	155	3
6	3	14	51	52	2	8	6	14	56	53	6	-16	2	15	28	28	27	9	4	15	62	72	4	5	0	16	20	5	6
7	3	14	30	31	2	9	6	14	91	86	5	-15	2	15	26	34	19	10	4	15	40	30	9	6	0	16	47	37	2
8	3	14	45	40	2	10	6	14	52	56	7	-14	2	15	69	74	5	11	4	15	61	53	7	7	0	16	56	56	2
9	3	14	125	122	3	11	6	14	41	46	10	-13	2	15	20	23	20	12	4	15	11	19	10	8	0	16	97	109	1
10	3	14	72	81	3	-7	7	14	42	36	12	-12	2	15	33	34	10	13	4	15	36	39	9	9	0	16	159	151	2
11	3	14	99	105	4	-6	7	14	33	35	18	-11	2	15	21	30	20	14	4	15	30	16	14	10	0	16	25	29	5
12	3	14	50	56	8	-5	7	14	32	22	20	-10	2	15	132	133	5	-13	5	15	33	31	15	11	0	16	74	77	4
13	3	14	43	36	6	-4	7	14	32	33	32	-9	2	15	57	48	1	-12	5	15	27	21	23	12	0	16	17	20	17
14	3	14	32	20	11	-3	7	14	90	81	5	-8	2	15	116	118	2	-11	5	15	71	65	7	13	0	16	86	86	4
15	3	14	76	70	5	-2	7	14	107	107	6	-7	2	15	55	58	2	-10	5	15	31	28	25	14	0	16	83	85	4
16	3	14	25	31	24	-1	7	14	87	79	6	-6	2	15	116	115	3	-9	5	15	65	64	9	15	0	16	122	128	5
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-7	4	14	107	114	4	-17	0	15	0	7	1	3	2	15	36	41	2	0	5	15	75	90	4	-9	1	16	55	65	5
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-5	4	14	253	259	4	-15	0	15	34	2	15	5	2	15	90	95	2	2	5	15	167	168	3	-7	1	16	219	218	6
-4	4	14	158	159	9	-14	0	15	74	77	8	6	2	15	73	80	1	3	5	15	59	53	6	-6	1	16	175	178	2
-3	4	14	142	135	6	-13	0	15	54	49	8	7	2	15	111	108	1	4	5	15	54	46	3	-5	1	16	257	255	3
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0	4	14	9	14	8	-10	0	15	0	12	1	10	2	15	117	114	2	7	5	15	45	44	5	-2	1	16	256	258	2
1	4	14	372	368	4	-9	0	15	148	147	4	11	2	15	120	114	2	8	5	15	100	115	4	-1	1	16	248	248	2
2	4	14	192	195	3	-8	0	15	34	10	13	12	2	15	95	91	3	9	5	15	117	112	8	0	1	16	20	34	3
3	4	14	214	219	3	-7	0	15	0	18	1	13	2	15	66	67	3	10	5	15	70	66	7	1	1	16	109	100	1
4	4	14	57	54	2	-6	0	15	198	192	5	14	2	15	44	36	5	11	5	15	0	12	1	2	1	16	111	95	1
5	4	14	238	236	4	-5	0	15	24	1	10	15	2	15	38	38	27	12	5	15	118	119	5	3	1	16	147	135	1
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8	4	14	85	89	2	-2	0	15	181	179	2	-14	3	15	63	64	5	-8	6	15	0	18	1	6	1	16	49	56	2
9	4	14	54	53	5	-1	0	15	162	165	1	-13	3	15	126	115	4	-7	6	15	38	35	12	7	1	16	122	120	2
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11	4	14	136	133	4	1	0	15	59	41	2	-11	3	15	21	22	21	-5	6	15	26	38	25	9	1	16	36	48	1
12	4	14	62	66	4	2	0	15	98	98	1	-10	3	15	41	44	7	-4	6	15	40	24	19	10	1	16	56	58	2
13	4	14	46	49	7	3	0	15	320	305	3	-9	3	15	0	19	1	-3	6	15	70	71	5	11	1	16	78	77	2
14	4	14	0	8	1	4	0	15	155	150	2	-8	3	15	100	105	5	-2	6	15	23	41	22	12	1	16	66	69	3
-13	5	14	78	71	7	5	0	15	101	101	1	-7	3	15	121	110	2	-1	6	15	103	98	5	13	1	16	49	41	5
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-8	5	14	37	61	9	10	0	15	0	18	1	-2	3	15	128	120	2	4	6	15	60	72	6	-15	2	16	87	87	5
-7	5	14	72	79	4	11	0	15	33	32	7	-1	3	15	107	110	2	5	6	15	63	65	6	-14	2	16	26	30	26
-6	5	14	145	138	4	12	0	15	42	49	6	0	3	15	152	154	2	6	6	15	54	51	4	-13	2	16	81	76	5
-5	5	14	151	153	3	13	0	15	28	42	11	1	3	15	63	54	2	7	6	15	42	47	9	-12	2	16	32	28	13
-4	5	14	41	35	20	14	0	15	0	1	1	2	3	15	149	149	2	8	6	15	69	60	5	-11	2	16	131	133	4
-3	5	14	212	216	7	15	0	15	0	15	1	3	3	15	83	80	1	9	6	15	9	23	8	-10	2	16	62	63	5
-2	5	14	236	235	4	16	0	15	54	55	7	4	3	15	118	119	2	10	6	15	45	41	8	-9	2	16	92	96	2
-1	5	14	55	64	5	-17	1	15	34	30	16	5	3	15	78	82	2	-6	7	15	99	96	6	-8	2	16	52	45	3
0	5	14	161	157	2	-16	1	15	16	29	16	6	3	15	81	85	4	-5	7	15	70	70	9	-7	2	16	84	82	3
1	5	14	111	112	3	-15	1	15	48	44	10	7	3	15	169	169	2	-4	7	15	24	38	24	-6	2	16	169	170	2
2	5	14	153	145	2	-14	1	15	57	61	6	8	3	15	57	47	2	-3	7	15	0	24	1	-5	2	16	66	70	4
3	5	14	162	155	3	-13	1	15	35	48	8	9	3	15	82	82	3	-2	7	15	52	40	8	-4	2	16	336	337	5
4	5	14	81	86	2	-12	1	15	73	72	4	10	3	15	152	147	4	-1	7	15	68	56	6	-3	2	16	135	138	2
5	5	14	37	16	5	-11	1	15	62	60	8	11	3	15	70	67	9	0	7	15	45	35	10	-2	2	16	87	81	2
6	5	14	61	66	3	-10	1	15	0	21	1	12	3	15	55	59	4	1	7	15	77	82	6	-1	2	16	153	155	2

Table 7. Observed and calculated structure factors for 1 Page 11

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	2	16	135	141	2	0	5	16	35	41	11	-4	1	17	153	158	2	-6	4	17	98	96	4	5	0	18	269	271	3
1	2	16	83	77	4	1	5	16	57	60	5	-3	1	17	211	207	2	-5	4	17	129	131	3	6	0	18	242	244	3
2	2	16	174	180	2	2	5	16	75	71	2	-2	1	17	132	118	4	-4	4	17	92	91	8	7	0	18	24	17	6
3	2	16	85	91	1	3	5	16	76	82	3	-1	1	17	316	311	2	-3	4	17	102	110	4	8	0	18	121	116	2
4	2	16	102	76	2	4	5	16	38	40	13	0	1	17	316	315	3	-2	4	17	46	49	5	9	0	18	171	173	3
5	2	16	69	75	1	5	5	16	112	114	9	1	1	17	103	83	4	-1	4	17	154	145	3	10	0	18	70	75	3
6	2	16	131	129	1	6	5	16	50	40	4	2	1	17	343	346	4	0	4	17	74	74	5	11	0	18	50	41	4
7	2	16	130	138	1	7	5	16	97	99	3	3	1	17	184	179	1	1	4	17	171	170	3	12	0	18	0	28	1
8	2	16	147	154	1	8	5	16	97	90	4	4	1	17	74	79	1	2	4	17	50	48	3	13	0	18	24	22	16
9	2	16	155	160	3	9	5	16	34	35	21	5	1	17	275	277	2	3	4	17	82	87	3	14	0	18	115	104	6
10	2	16	119	117	2	10	5	16	70	66	12	6	1	17	160	167	1	4	4	17	107	105	2	15	0	18	58	58	8
11	2	16	34	44	5	11	5	16	80	83	5	7	1	17	163	170	1	5	4	17	71	65	5	-15	1	18	19	5	18

12	2	16	53	53	5	12	5	16	52	48	7	8	1	17	85	84	1	6	4	17	136	136	2	-14	1	18	27	26	23
13	2	16	16	17	16	-9	6	16	27	27	26	9	1	17	168	169	4	7	4	17	60	54	3	-13	1	18	42	54	17
14	2	16	36	40	8	-8	6	16	38	35	15	10	1	17	67	76	2	8	4	17	61	69	5	-12	1	18	0	15	1
15	2	16	26	30	12	-7	6	16	25	34	25	11	1	17	50	47	4	9	4	17	40	35	10	-11	1	18	50	72	6
-15	3	16	72	62	8	-6	6	16	7	13	6	12	1	17	0	14	1	10	4	17	25	3	25	-10	1	18	121	127	4
-14	3	16	19	14	19	-5	6	16	43	50	9	13	1	17	50	22	10	11	4	17	134	123	5	-9	1	18	79	87	4
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-11	3	16	86	84	5	-2	6	16	78	86	5	-15	2	17	29	31	28	-11	5	17	71	75	7	-6	1	18	99	101	5
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-9	3	16	68	71	4	0	6	16	18	21	17	-13	2	17	0	22	1	-9	5	17	82	79	5	-4	1	18	144	142	2
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1	3	16	89	92	2	-5	7	16	52	55	18	-3	2	17	23	10	6	1	5	17	47	53	6	6	1	18	103	106	1
2	3	16	198	201	2	-4	7	16	78	57	8	-2	2	17	108	111	2	2	5	17	114	113	4	7	1	18	96	92	1
3	3	16	269	260	3	-3	7	16	47	26	10	-1	2	17	138	137	2	3	5	17	44	49	10	8	1	18	104	107	1
4	3	16	138	146	2	-2	7	16	22	33	21	0	2	17	28	41	4	4	5	17	70	72	3	9	1	18	131	130	2
5	3	16	28	28	4	-1	7	16	25	29	25	1	2	17	67	70	4	5	5	17	158	150	3	10	1	18	0	22	1
6	3	16	150	155	2	0	7	16	88	81	5	2	2	17	117	121	2	6	5	17	72	79	3	11	1	18	48	51	6
7	3	16	78	80	2	1	7	16	41	39	12	3	2	17	118	117	1	7	5	17	124	124	4	12	1	18	0	8	1
8	3	16	106	112	2	2	7	16	31	19	19	4	2	17	58	54	2	8	5	17	13	21	13	13	1	18	32	37	7
9	3	16	52	37	13	3	7	16	64	68	8	5	2	17	167	170	1	9	5	17	60	64	6	14	1	18	81	74	7
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7	4	16	38	38	5	9	0	17	23	27	7	3	3	17	71	75	3	-14	0	18	84	84	10	11	2	18	100	98	4
8	4	16	59	54	5	10	0	17	131	129	3	4	3	17	36	37	3	-13	0	18	0	10	1	12	2	18	9	4	9
9	4	16	64	57	5	11	0	17	49	61	5	5	3	17	63	72	2	-12	0	18	145	141	6	13	2	18	13	22	13
10	4	16	0	3	1	12	0	17	38	42	8	6	3	17	90	97	2	-11	0	18	69	72	9	14	2	18	48	38	7
11	4	16	53	51	10	13	0	17	41	38	7	7	3	17	106	104	2	-10	0	18	59	51	10	-14	3	18	43	35	12
12	4	16	26	27	13	14	0	17	35	29	11	8	3	17	113	112	5	-9	0	18	115	91	6	-13	3	18	27	35	27
13	4	16	53	31	6	15	0	17	30	27	13	9	3	17	43	43	5	-8	0	18	41	9	14	-12	3	18	56	56	8
-12	5	16	74	68	15	-16	1	17	22	18	21	10	3	17	115	116	3	-7	0	18	5	9	5	-11	3	18	61	67	7
-11	5	16	44	51	13	-15	1	17	80	75	8	11	3	17	46	47	8	-6	0	18	256	251	6	-10	3	18	66	60	8
-10	5	16	33	30	33	-14	1	17	69	76	6	12	3	17	50	50	7	-5	0	18	67	35	6	-9	3	18	34	48	22
-9	5	16	13	28	13	-13	1	17	23	40	22	13	3	17	0	29	1	-4	0	18	56	58	2	-8	3	18	35	52	34
-8	5	16	61	72	6	-12	1	17	90	81	13	14	3	17	28	24	12	-3	0	18	0	16	1	-7	3	18	74	71	8
-7	5	16	53	55	10	-11	1	17	40	32	10	-13	4	17	17	29	16	-2	0	18	48	55	2	-6	3	18	89	88	3
-6	5	16	71	73	5	-10	1	17	78	88	5	-12	4	17	125	120	5	-1	0	18	120	126	2	-5	3	18	138	152	2
-5	5	16	36	22	10	-9	1	17	114	122	8	-11	4	17	92	85	6	0	0	18	69	62	2	-4	3	18	148	153	3
-4	5	16	86	87	6	-8	1	17	144	142	3	-10	4	17	45	43	8	1	0	18	90	91	2	-3	3	18	133	141	3
-3	5	16	98	102	4	-7	1	17	126	122	2	-9	4	17	63	63	7	2	0	18	82	84	2	-2	3	18	51	59	3
-2	5	16	92	84	4	-6	1	17	54	51	2	-8	4	17	70	74	5	3	0	18	15	21	15	-1	3	18	102	88	3
-1	5	16	71	68	8	-5	1	17	175	167	2	-7	4	17	0	23	1	4	0	18	0	1	1	0	3	18	131	121	3

Table 7. Observed and calculated structure factors for 1 Page 12

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	3	18	214	206	4	-2	0	19	160	153	2	0	3	19	191	182	5	4	0	20	11	9	10	10	3	20	29	36	12
2	3	18	46	36	4	-1	0	19	138	135	2	1	3	19	163	158	7	5	0	20	133	132	2	11	3	20	51	62	6
3	3	18	154	153	6	0	0	19	23	24	6	2	3	19	8	22	8	6	0	20	87	95	2	12	3	20	0	13	1
4	3	18	132	135	2	1	0	19	85	84	2	3	3	19	25	15	13	7	0	20	18	14	17	-11	4	20	34	31	19
5	3	18	12	14	12	2	0	19	33	21	4	4	3	19	89	97	2	8	0	20	0	11	1	-10	4	20	19	19	18
6	3	18	17	25	16	3	0	19	147	131	2	5	3	19	105	109	4	9	0	20	104	105	5	-9	4	20	32	34	32
7	3	18	61	68	3	4	0	19	178	181	2	6	3	19	18	16	9	10	0	20	83	85	6	-8	4	20	60	63	7
8	3	18	68	63	3	5	0	19	15	20	15	7	3	19	43	47	3	11	0	20	25	17	24	-7	4	20	25	35	25
9	3	18	35	39	5	6	0	19	47	39	4	8	3	19	40	46	6	12	0	20	24	14	18	-6	4	20	56	59	8
10	3	18	89	87	3	7	0	19	0	2	1	9	3	19	77	71	3	13	0	20	35	30	14	-5	4	20	55	63	6
11	3	18	39	48	8	8	0	19	87	99	3	10	3	19	17	30	17	-14	1	20	43	30	13	-4	4	20	19	13	19
12	3	18	54	54	6	9	0	19	0	10	1	11	3	19	29	23	14	-13	1	20	0	12	1	-3	4	20	46	52	9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
13	3	18	40	46	11	10	0	19	59	59	4	12	3	19	58	66	5	-12	1	20	34	37	13	-2	4	20	100	100	5
-12	4	18	18	14	18	11	0	19	39	46	7	13	3	19	38	50	8	-11	1	20	12	17	12	-1	4	20	85	88	5
-11	4	18	55	39	11	12	0	19	21	16	21	-12	4	19	122	115	6	-10	1	20	65	73	6	0	4	20	65	64	6
-10	4	18	41	29	9	13	0	19	88	92	5	-11	4	19	112	114	5	-9	1	20	33	32	10	1	4	20	48	42	8
-9	4	18	66	54	23	14	0	19	21	9	21	-10	4	19	52	58	8	-8	1	20	55	59	6	2	4	20	74	74	5
-8	4	18	71	76	6	-14	1	19	7	16	6	-9	4	19	70	57	8	-7	1	20	83	88	5	3	4	20	58	60	9
-7	4	18	82	83	6	-13	1	19	0	31	1	-8	4	19	106	107	4	-6	1	20	101	110	3	4	4	20	52	59	6
-6	4	18	76	75	5	-12	1	19	0	5	1	-7	4	19	37	17	11	-5	1	20	119	124	3	5	4	20	57	56	6
-5	4	18	71	65	5	-11	1	19	43	52	8	-6	4	19	46	41	7	-4	1	20	168	173	5	6	4	20	49	47	9
-4	4	18	143	131	4	-10	1	19	86	91	5	-5	4	19	56	44	6	-3	1	20	103	108	1	7	4	20	45	37	8
-3	4	18	18	20	17	-9	1	19	73	78	6	-4	4	19	65	64	6	-2	1	20	108	101	2	8	4	20	25	16	10
-2	4	18	152	154	3	-8	1	19	78	88	4	-3	4	19	92	90	4	-1	1	20	166	164	2	9	4	20	30	39	7
-1	4	18	47	58	6	-7	1	19	36	43	8	-2	4	19	21	33	21	0	1	20	50	54	2	10	4	20	78	73	5
0	4	18	45	58	5	-6	1	19	66	62	2	-1	4	19	29	38	12	1	1	20	88	84	2	-8	5	20	44	43	12
1	4	18	39	43	6	-5	1	19	99	105	2	0	4	19	59	52	5	2	1	20	102	100	2	-7	5	20	92	97	6
2	4	18	79	68	3	-4	1	19	104	107	2	1	4	19	0	26	1	3	1	20	103	93	2	-6	5	20	20	19	20
3	4	18	100	100	2	-3	1	19	46	49	2	2	4	19	67	78	4	4	1	20	68	67	2	-5	5	20	45	48	12
4	4	18	111	109	10	-2	1	19	126	122	1	3	4	19	53	55	4	5	1	20	88	93	2	-4	5	20	81	74	6
5	4	18	45	44	4	-1	1	19	140	133	1	4	4	19	132	133	2	6	1	20	29	22	4	-3	5	20	14	29	13
6	4	18	71	72	7	0	1	19	185	183	2	5	4	19	61	64	3	7	1	20	143	143	3	-2	5	20	30	20	30
7	4	18	80	79	4	1	1	19	133	137	1	6	4	19	77	78	2	8	1	20	86	87	2	-1	5	20	116	109	5
8	4	18	56	52	8	2	1	19	237	235	2	7	4	19	129	128	4	9	1	20	22	32	11	0	5	20	51	48	10
9	4	18	16	22	15	3	1	19	120	121	1	8	4	19	5	11	5	10	1	20	49	52	5	1	5	20	0	13	1
10	4	18	125	115	4	4	1	19	74	77	2	9	4	19	81	83	3	11	1	20	68	56	5	2	5	20	72	77	6
11	4	18	58	55	4	5	1	19	167	169	2	10	4	19	60	55	5	12	1	20	13	10	13	3	5	20	41	33	11
12	4	18	48	44	6	6	1	19	33	35	4	11	4	19	75	83	5	13	1	20	46	18	10	4	5	20	51	53	8
-10	5	18	30	46	24	7	1	19	31	28	4	-9	5	19	41	42	14	-13	2	20	53	47	17	5	5	20	0	26	1
-9	5	18	59	66	8	8	1	19	114	104	2	-8	5	19	47	42	17	-12	2	20	28	10	27	6	5	20	39	56	17
-8	5	18	29	49	29	9	1	19	89	89	4	-7	5	19	0	18	1	-11	2	20	58	44	9	7	5	20	38	32	17
-7	5	18	62	64	7	10	1	19	86	92	3	-6	5	19	59	63	9	-10	2	20	0	16	1	8	5	20	57	53	9
-6	5	18	70	70	7	11	1	19	38	45	5	-5	5	19	89	95	20	-9	2	20	0	6	1	-4	6	20	40	46	18
-5	5	18	51	65	7	12	1	19	48	55	7	-4	5	19	86	86	7	-8	2	20	21	40	21	-3	6	20	18	33	18
-4	5	18	99	101	5	13	1	19	81	73	5	-3	5	19	90	87	5	-7	2	20	195	195	3	-2	6	20	26	22	26
-3	5	18	128	124	4	14	1	19	37	3	8	-2	5	19	49	47	7	-6	2	20	131	129	6	-1	6	20	36	27	36
-2	5	18	82	91	5	-14	2	19	63	64	8	-1	5	19	54	74	13	-5	2	20	127	123	7	0	6	20	136	131	6
-1	5	18	51	49	12	-13	2	19	24	28	23	0	5	19	9	13	8	-4	2	20	119	127	3	1	6	20	90	97	6
0	5	18	49	45	20	-12	2	19	47	33	13	1	5	19	0	21	1	-3	2	20	111	108	2	2	6	20	64	82	9
1	5	18	141	142	4	-11	2	19	33	21	11	2	5	19	25	35	25	-2	2	20	220	214	3	3	6	20	39	46	15
2	5	18	108	111	6	-10	2	19	27	31	21	3	5	19	58	60	5	-1	2	20	53	44	4	-13	0	21	42	15	26
3	5	18	72	79	7	-9	2	19	65	72	6	4	5	19	100	98	4	0	2	20	79	81	6	-12	0	21	34	2	33
4	5	18	113	108	4	-8	2	19	46	31	8	5	5	19	52	50	7	1	2	20	39	43	6	-11	0	21	0	3	1
5	5	18	20	22	20	-7	2	19	38	36	4	6	5	19	64	50	10	2	2	20	118	112	4	-10	0	21	79	80	11
6	5	18	67	72	9	-6	2	19	122	121	2	7	5	19	35	38	21	3	2	20	49	55	3	-9	0	21	9	24	9
7	5	18	44	32	8	-5	2	19	37	25	11	8	5	19	75	67	8	4	2	20	81	79	2	-8	0	21	59	54	12
8	5	18	44	45	7	-4	2	19	77	79	3	9	5	19	8	19	7	5	2	20	93	95	3	-7	0	21	39	57	14
9	5	18	59	68	6	-3	2	19	145	134	7	-6	6	19	84	88	7	6	2	20	125	119	3	-6	0	21	47	1	12
10	5	18	51	59	8	-2	2	19	153	152	2	-5	6	19	48	67	13	7	2	20	60	61	4	-5	0	21	22	16	14
-7	6	18	0	15	1	-1	2	19	29	23	4	-4	6	19	48	51	12	8	2	20	149	140	5	-4	0	21	42	38	4
-6	6	18	47	18	46	0	2	19	61	59	3	-3	6	19	74	74	18	9	2	20	89	79	3	-3	0	21	87	92	2
-5	6	18	59	65	9	1	2	19	80	85	9	-2	6	19	40	50	25	10	2	20	58	59	5	-2	0	21	92	96	2
-4	6	18	78	64	6	2	2	19	146	143	2	-1	6	19	70	78	8	11	2	20	31	30	14	-1	0	21	145	148	2
-3	6	18	64	65	6	3	2	19	171	171	2	0	6	19	47	49	13	12	2	20	48	32	8	0	0	21	167	161	3
-2	6	18	34	39	12	4	2	19	61	69	2	1	6	19	74	54	8	13	2	20	88	87	6	1	0	21	140	134	3
-1	6	18	45	32	8	5	2	19	126	120	2	2	6	19	37	54	12	-12	3	20	64	51	24	2	0	21	28	29	5
0	6	18	73	77	9	6	2	19	114	115	7	3	6	19	18	19	18	-11	3	20	18	9	18	3	0	21	51	53	4
1	6	18	74	78	5	7	2	19	47	52	10	4	6	19	75	74	7	-10	3	20	48	46	14	4	0	21	0	4	1
2	6	18	0	28	1	8	2	19	63	64	3	5	6	19	43	50	10	-9	3	20	64	51	9	5	0	21	53	58	4
3	6	18	58	69	8	9	2	19	151	147	3	-14	0	20	79	57	11	-8	3	20	53	56	6	6	0	21	35	25	6
4	6	18	69	58	6	10	2	19	54	45	5	-13	0	20	0	11	1	-7	3	20	11	8	11	7	0	21	30	31	8
5	6	18	48	64	19	11	2	19	42	51	6	-12	0	20	65	64	9	-6	3	20	38	42	9	8	0	21	63	64	8
6	6	18	28	14	28	12	2	19	20	24	20	-11	0	20	46	40	13	-5	3	20	46	36	4	9	0	21	52	48	8
7	6	18	36	9	24	13	2	19	48	54	8	-10	0	20	0	4	1	-4	3	20	76	84	6	10	0	21	96	89	7
-15	0	19	0	19	1	-13	3	19	25	23	24	-9	0	20	73	65	8	-3	3	20	88	99	5	11	0	21	49	59	9
-14	0	19	39	33	28	-12	3	19	0	31	1	-8	0	20	40	74	8	-2	3	20	118	118	5	12	0	21	0	12	1
-13	0	19	55	56	11	-11	3	19	56	55	10	-7	0	20	45	55	10	-1	3	20	113	113	3	13	0	21	52	51	7
-12	0	19	0	14	1	-10	3	19	54	45	7	-6	0	20	72	78	8	0	3	20	87	95	3	-13	1	21	0	8	1
-11	0	19	33	31	13	-9	3	19	57	58	12	-5	0	20	42	34	4	1	3	20	85	85	4	-12	1	21	56	39	8
-10	0	19	81	86	8	-8	3	19	26	36	16	-4	0	20	41	51	5	2	3	20	59	60	5	-11	1	21	56	49	9
-9	0	19	27	30	21	-7	3	19	44	43	4	-3	0	20	153	148	3	3	3	20	118	117	8	-10	1	21	82	81	5
-8	0	19	42	26	10	-6	3	19	108	119	4	-2	0	20	57	40	3	4	3	20	58	58	4	-9	1	21	39	44	11
-7	0	19	68	79	6	-5	3	19	113	112	4	-1	0	20	63	66	3	5	3	20	81	80	2	-8	1	21	95	94	5
-6	0	19	134	134	4	-4	3	19	80	74	3	0	0	20	277	279	3	6	3	20	91	93	5	-7	1	21	40	23	10
-5	0	19	20	2	20	-3	3	19	97	97	3	1	0	20	82	78	2	7	3	20	18	12	18	-6	1	21	119	121	3
-4	0	19	48	30	10	-2	3	19	43	35	5	2	0	20	228	229	3	8	3	20	74	82	3	-5	1	21	39	37	10
-3	0	19	270	267	3	-1	3	19	58	51	5	3	0	20	23	9	6	9	3	20	25	24	10	-4	1	21	68	64	3

Table 7. Observed and calculated structure factors for 1 Page 13

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-3	1	21	174	179	2	-4	5	21	47	42	11	-7	3	22	32	27	24	7	1	23	18	20	18	-4	1	24	26	22	10
-2	1	21	59	66	2	-3	5	21	134	128	5	-6	3	22	43	46	13	8	1	23	40	53	12	-3	1	24	48	40	17
-1	1	21	23	18	22	-2	5	21	49	52	32	-5	3	22	49	46	8	9	1	23	0	13	1	-2	1	24	35	33	7
0	1	21	17	25	9	-1	5	21	101	92	5	-4	3	22	45	39	13	10	1	23	58	53	7	-1	1	24	50	52	4
1	1	21	16	17	16	0	5	21	26	27	19	-3	3	22	14	14	13	-10	2	23	57	48	8	0	1	24	58	61	4
2	1	21	145	146	2	1	5	21	59	48	7	-2	3	22	53	60	4	-9	2	23	60	61	9	1	1	24	2	11	2
3	1	21	73	62	3	2	5	21	62	53	13	-1	3	22	23	15	10	-8	2	23	47	50	8	2	1	24	64	71	4
4	1	21	88	88	2	3	5	21	37	27	10	0	3	22	140	122	3	-7	2	23	59	63	8	3	1	24	41	51	6
5	1	21	120	117	11	4	5	21	62	68	6	1	3	22	69	77	3	-6	2	23	0	25	1	4	1	24	119	125	3
6	1	21	95	99	2	5	5	21	52	73	17	2	3	22	36	46	8	-5	2	23	101	105	7	5	1	24	40	40	8
7	1	21	98	96	3	6	5	21	53	56	12	3	3	22	46	55	5	-4	2	23	41	39	10	6	1	24	67	58	12
8	1	21	41	34	7	-12	0	22	49	52	16	4	3	22	94	90	7	-3	2	23	114	104	3	7	1	24	0	2	1
9	1	21	42	46	6	-11	0	22	0	18	1	5	3	22	77	86	4	-2	2	23	53	45	5	8	1	24	0	23	1
10	1	21	48	39	6	-10	0	22	50	71	11	6	3	22	22	15	22	-1	2	23	41	38	5	9	1	24	30	54	30

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	1	21	70	60	5	-9	0	22	63	54	11	7	3	22	36	45	9	0	2	23	36	32	8	-9	2	24	37	47	14
12	1	21	58	61	6	-8	0	22	189	176	7	8	3	22	27	32	27	1	2	23	50	60	5	-8	2	24	37	31	24
-12	2	21	25	21	24	-7	0	22	69	72	6	9	3	22	33	31	10	2	2	23	54	48	5	-7	2	24	78	78	6
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-7	2	21	60	49	8	-2	0	22	54	54	3	-5	4	22	27	44	27	7	2	23	66	68	6	-2	2	24	71	67	4
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2	2	21	214	210	3	7	0	22	37	27	7	4	4	22	30	35	14	-4	3	23	45	52	5	7	2	24	26	28	25
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6	2	21	146	142	3	11	0	22	42	39	16	8	4	22	20	32	20	0	3	23	100	97	4	-6	3	24	0	15	1
7	2	21	96	98	11	12	0	22	54	48	9	-5	5	22	18	30	17	1	3	23	46	42	6	-5	3	24	29	21	28
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11	2	21	8	23	7	-9	1	22	73	82	8	-1	5	22	99	96	6	5	3	23	51	68	8	-1	3	24	39	44	9
12	2	21	48	56	8	-8	1	22	115	112	5	0	5	22	36	55	14	6	3	23	67	65	5	0	3	24	60	64	4
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-5	3	21	29	18	20	-1	1	22	76	67	3	-10	0	23	47	58	15	-3	4	23	74	76	6	7	3	24	0	23	1
-4	3	21	86	84	7	0	1	22	45	46	3	-9	0	23	56	52	15	-2	4	23	30	40	21	-5	4	24	38	38	23
-3	3	21	28	44	9	1	1	22	167	163	3	-8	0	23	46	31	19	-1	4	23	0	39	1	-4	4	24	37	9	14
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5	3	21	61	58	4	9	1	22	38	20	13	0	0	23	39	47	6	-2	5	23	40	32	40	4	4	24	17	38	16
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9	3	21	32	38	8	-11	2	22	0	33	1	4	0	23	22	38	22	-10	0	24	20	38	19	-6	0	25	42	48	14
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2	4	21	25	25	24	4	2	22	33	26	11	-4	1	23	23	22	12	5	0	24	88	93	5	-7	1	25	24	40	24
3	4	21	52	48	6	5	2	22	114	119	3	-3	1	23	13	29	13	6	0	24	77	81	4	-6	1	25	59	52	8
4	4	21	60	67	6	6	2	22	64	65	5	-2	1	23	41	32	6	7	0	24	96	95	7	-5	1	25	30	55	29
5	4	21	19	18	19	7	2	22	0	23	1	-1	1	23	84	91	5	8	0	24	103	98	8	-4	1	25	54	50	16
6	4	21	75	66	9	8	2	22	80	88	7	0	1	23	53	42	3	9	0	24	83	93	8	-3	1	25	32	14	9
7	4	21	23	15	22	9	2	22	54	60	6	1	1	23	72	65	4	-10	1	24	0	9	1	-2	1	25	64	64	6
8	4	21	45	46	5	10	2	22	47	43	10	2	1	23	0	16	1	-9	1	24	47	51	11	-1	1	25	11	10	11
9	4	21	28	17	15	11	2	22	77	70	6	3	1	23	61	62	5	-8	1	24	24	22	23	0	1	25	33	35	8
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-5	5	21	91	98	5	-8	3	22	107	105	5	6	1	23	83	81	3	-5	1	24	24	43	24	3	1	25	45	43	7

Table 7. Observed and calculated structure factors for 1 Page 14

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	1	25	56	62	9	7	2	25	34	31	33	0	0	26	43	34	14	6	1	26	90	87	8	-2	0	27	42	33	16
5	1	25	78	80	5	-6	3	25	64	58	15	1	0	26	103	107	6	-5	2	26	79	77	12	-1	0	27	54	81	12
6	1	25	46	47	8	-5	3	25	0	27	1	2	0	26	32	34	16	-4	2	26	55	47	9	0	0	27	39	27	14
7	1	25	71	73	10	-4	3	25	74	80	7	3	0	26	54	61	6	-3	2	26	47	56	9	1	0	27	38	46	14
8	1	25	47	57	11	-3	3	25	15	30	15	4	0	26	45	36	8	-2	2	26	46	50	7	3	0	27	30	39	12
-8	2	25	68	62	8	-2	3	25	73	69	4	5	0	26	35	41	9	-1	2	26	29	36	10	4	0	27	81	78	5
-7	2	25	34	26	17	-1	3	25	63	63	5	6	0	26	0	36	1	0	2	26	45	29	8	-4	1	27	63	74	10
-6	2	25	16	20	15	0	3	25	112	127	4	-7	1	26	91	99	7	1	2	26	11	18	11	-3	1	27	36	24	14
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-4	2	25	16	6	16	2	3	25	99	97	4	-5	1	26	0	34	1	3	2	26	32	22	10	-1	1	27	60	58	6
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-2	2	25	28	30	12	4	3	25	48	54	9	-3	1	26	19	22	19	5	2	26	58	52	7	1	1	27	50	51	6
-1	2	25	59	50	10	5	3	25	56	56	6	-2	1	26	54	53	5	-2	3	26	43	42	8	2	1	27	27	25	15
0	2	25	36	33	36	-7	0	26	0	5	1	-1	1	26	76	76	4	-1	3	26	72	72	5	3	1	27	9	6	8
1	2	25	41	38	6	-6	0	26	70	80	11	0	1	26	37	29	13	0	3	26	0	2	1	4	1	27	33	36	32
2	2	25	59	57	5	-5	0	26	0	12	1	1	1	26	27	26	27	1	3	26	37	32	7	-2	2	27	0	45	1

```
3  2 25   39   30   9    -4  0 26   57   62  11     2  1 26   31   23  11     2  3 26   41   43   8    -1  2 27    0   28   1
4  2 25    8   14   7    -3  0 26    0    3   1     3  1 26   22   19  21    -5  0 27   24   11  23     0  2 27   12   10  12
5  2 25   96  100   6    -2  0 26   51   25  16     4  1 26   75   73   7    -4  0 27   43   30  17     1  2 27   45   48   9
6  2 25   64   67   7    -1  0 26    0   18   1     5  1 26   56   52   7    -3  0 27    0   15   1
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