Application of a New Chiral Phosphepine to the Catalytic Asymmetric Synthesis of Highly Functionalized Cyclopentenes that Bear an Array of Heteroatom-Substituted Quaternary Stereocenters

Yuji Fujiwara and Gregory C. Fu*

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

SUPPORTING INFORMATION

Table of Contents

I. General Information

The following solvents were purchased and used as received: *i*-Pr_2O (anhydrous; Sigma-Aldrich), hexanes (anhydrous; Sigma-Aldrich), and $CHCl_3$ (anhydrous; Sigma-Aldrich).

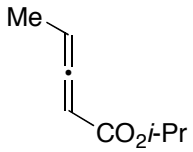
HPLC analyses were carried out on an Agilent 1100 Series system, and supercritical fluid chromatography (SFC) analyses were carried out on a Berger SFC MiniGram system. Daicel CHIRALCEL® columns or Daicel CHIRALPAK® columns (internal diameter 4.6 mm, column length 250 mm, particle size 5 μm or 3 μm) were used for both HPLC and SFC analysis (UV detector at a wavelength of 230 nm).

II. Preparation of Allenes

General Procedure. The alkyl (triphenylphosphoranylidene)acetate (30.0 mmol) and a stir bar were added to a 250-mL flask, which was then evacuated and back-filled with nitrogen (three cycles). CH_2Cl_2 (91 mL) and NEt_3 (4.05 mL, 29.1 mmol) were added via syringe, and the resulting solution was stirred at r.t. for 1 min. Next, the acid chloride (30.0 mmol) was added dropwise via syringe over 2 min to the stirred

solution. The reaction mixture was stirred at r.t. for 1 h, and then it was concentrated under reduced pressure to one-third of the original volume. Hexane (100 mL) and silica gel (5 g) were added, and the mixture was stirred at r.t. for 1 h. Next, the mixture was passed through a pad of silica gel and washed with hexane/Et_2O (150 mL). The filtrate was concentrated under reduced pressure, and the residue was purified by column chromatography, which furnished the allenoate as a colorless oil.

The yields have not been optimized. For the cycloadditions, care should be taken that no carboxylic acid (derived from the acid chloride) is present.



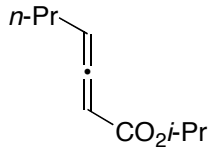
(±)-Isopropyl penta-2,3-dienoate. The title compound was prepared from propionyl chloride according to the General Procedure (purification by distillation under reduced pressure; 51% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.50-5.62 (m, 2H), 5.05 (qq, *J* = 6.0, 6.0 Hz, 1H), 1.75-1.81 (m, 3H), 1.26 (d, *J* = 6.0 Hz, 6H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.7, 165.6, 90.0, 88.0, 67.9, 21.70, 21.68, 12.7;

IR (film) 2982, 2935, 1964, 1713, 1468, 1456, 1411, 1387, 1374, 1335, 1287, 1264, 1171, 1108, 1069, 979, 909, 871, 835, 797, 745, 651, 574 cm^{-1};

LRMS (APCI) calcd for $C_8H_{12}O_2$ (M+) 140.1, found 141.1.



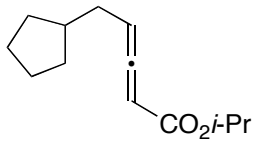
(±)-Isopropyl hepta-2,3-dienoate. The title compound was prepared from valeroyl chloride according to the General Procedure (purification by column chromatography: 20:1 hexane/Et_2O; 56% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.52-5.63 (m, 2H), 5.05 (qq, *J* = 6.2, 6.2 Hz, 1H), 2.08-2.14 (m, 2H), 1.45-1.55 (m, 2H), 1.26 (d, *J* = 6.2 Hz, 3H), 1.25 (d, *J* = 6.2 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.2, 165.8, 95.0, 88.5, 67.9, 29.5, 21.9, 21.77, 21.75, 13.4;

IR (film) 2980, 2936, 2875, 1961, 1713, 1467, 1418, 1386, 1374, 1336, 1324, 1291, 1262, 1170, 1109, 981, 878, 836, 798, 746, 663, 571 cm^{-1};

LRMS (APCI) calcd for $C_{10}H_{17}O_2$ (M+H) 169.1, found 169.2.



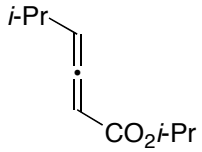
(±)-Isopropyl 5-cyclopentylpenta-2,3-dienoate. The title compound was prepared from 3-cyclopentanoyl chloride according to the General Procedure (purification by column chromatography: 25:1 hexane/Et_2O; 55% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.50-5.61 (m, 2H), 5.05 (qq, *J* = 6.0, 6.0 Hz, 1H), 2.10-2.18 (m, 2H), 1.90-2.02 (m, 1H), 1.75-1.85 (m, 2H), 1.48-1.67 (m, 4H), 1.26 (d, *J* = 6.0 Hz, 3H), 1.25 (d, *J* = 6.0 Hz, 3H), 1.15-1.26 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.5, 165.8, 94.4, 88.1, 67.9, 39.4, 33.9, 32.18, 32.14, 25.19, 25.15, 21.79, 21.78;

IR (film) 2979, 2950, 2869, 1962, 1713, 1468, 1453, 1418, 1386, 1374, 1261, 1168, 1109, 978, 871, 836, 798, 746, 664 cm^{-1};

LRMS (APCI) calcd for $C_{13}H_{21}O_2$ (M+H) 209.2, found 209.2.



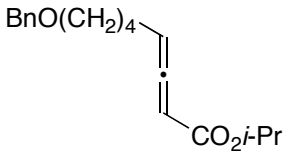
(±)-Isopropyl 5-methylhexa-2,3-dienoate. The title compound was prepared from isovaleroyl chloride according to the General Procedure (purification by column chromatography using gradient elution: 10:0 to 10:1 hexane/Et_2O; 26% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.57-5.64 (m, 2H), 5.04 (qq, *J* = 6.4, 6.4 Hz, 1H), 2.41-2.52 (m, 1H), 1.26 (d, *J* = 6.4 Hz, 3H), 1.25 (d, *J* = 6.4 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 6H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 211.1, 165.7, 102.3, 89.6, 67.8, 27.6, 22.19, 22.12, 21.73, 21.70;

IR (film) 2966, 2874, 1959, 1713, 1468, 1414, 1374, 1318, 1260, 1167, 1110, 980, 873, 838, 807, 748, 668 cm^{-1};

LRMS (APCI) calcd for $C_{10}H_{17}O_2$ (M+H) 169.1, found 169.2.



(±)-Isopropyl 8-(benzyloxy)octa-2,3-dienoate. The title compound was prepared from 6-(benzyloxy)hexanoyl chloride[1] according to the General Procedure (purification by column chromatography: 5:1 hexane/Et_2O; 47% yield).

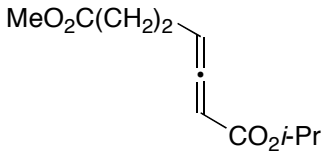
(1) Koch, G.; Loiseleur, O.; Altmann, K.-H. *Synlett* **2004**, 693–697.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.24-7.36 (m, 5H), 5.52-5.61 (m, 2H), 5.03 (qq, *J* = 6.4, 6.4 Hz, 1H), 4.48 (s, 2H), 3.47 (t, *J* = 6.4 Hz, 1H), 2.14 (ddd, *J* = 14.4, 7.2, 3.2 Hz, 1H), 1.65-1.73 (m, 2H), 1.51-1.60 (m, 2H), 1.24 (d, *J* = 6.4 Hz, 3H), 1.23 (d, *J* = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.1, 165.6, 138.5, 128.2, 127.44, 127.36, 94.9, 88.6, 72.7, 69.8, 67.9, 28.8, 27.2, 25.3, 21.71, 21.70;

IR (film) 2980, 2938, 2860, 1961, 1710, 1496, 1454, 1418, 1373, 1262, 1169, 1108, 978, 872, 800, 736 cm^{-1};

LRMS (APCI) calcd for $C_{18}H_{25}O_3$ (M+H) 289.4, found 289.2.



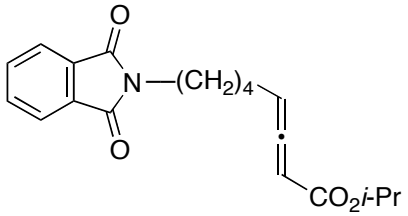
(±)-1-Isopropyl-7-methyl hepta-2,3-dienedioate. The title compound was prepared from methyl 5-chloro-5-oxopentanoate according to the General Procedure (purification by column chromatography using gradient elution: 3:1 to 2:1 hexane/Et_2O; 56% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.66-5.72 (m, 1H), 5.58-5.62 (m, 1H), 5.04 (qq, *J* = 6.4, 6.4 Hz, 1H), 3.69 (s, 3H), 2.40-2.52 (m, 4H), 1.27 (d, *J* = 6.4 Hz, 3H), 1.25 (d, *J* = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 211.8, 172.8, 165.3, 94.1, 89.8, 68.2, 51.6, 32.8, 22.5, 21.74, 21.72;

IR (film) 2982, 2953, 1963, 1740, 1712, 1438, 1420, 1374, 1264, 1171, 1108, 1055, 984, 876, 837, 804, 747, 666 cm^{-1};

LRMS (APCI) calcd for $C_{11}H_{16}NaO_4$ (M+Na) 235.1, found 235.1.



(±)-Isopropyl 8-(1,3-dioxoisoindolin-2-yl)octa-2,3-dienoate. The title compound was prepared from 6-(1, 3-dioxoisoindolin-2-yl)pentanoyl chloride[2] according to the General Procedure (purification by column chromatography using gradient elution: 4:0 to 4:1 hexane/EtOAc; 48% yield).

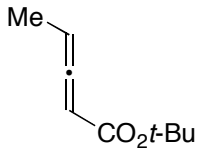
(2) Guénin, E.; Monteil, M.; Bouchemal, N.; Prangé, T.; Lecouvey, M. *Eur. J. Org. Chem.* **2007**, 3380–3391.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82-7.86 (m, 2H), 7.70-7.75 (m, 2H), 5.54-5.62 (m, 2H), 5.02 (qq, *J* = 6.4, 6.4 Hz, 1H), 3.70 (t, *J* = 7.2 Hz, 2H), 2.15-2.24 (m, 2H), 1.72-1.82 (m, 2H), 1.49-1.57 (m, 2H), 1.24 (d, *J* = 6.4 Hz, 3H), 1.22 (d, *J* = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.1, 168.3, 165.6, 133.8, 132.0, 123.1, 94.6, 88.8, 68.0, 37.5, 27.7, 26.9, 25.8, 21.72, 21.70;

IR (film) 2980, 2939, 2864, 1961, 1773, 1710, 1616, 1467, 1437, 1397, 1373, 1337, 1264, 1172, 1108, 1041, 979, 875, 798, 720, 668 cm^{-1};

LRMS (APCI) calcd for $C_{19}H_{21}NNaO_4$ (M+Na) 350.1, found 350.1.



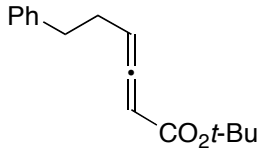
(±)-*tert*-Butyl penta-2,3-dienoate. The title compound was prepared from propionyl chloride according to the General Procedure (purification by distillation under reduced pressure; 23% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.43-5.51 (m, 1H), 5.36-5.41 (m, 1H), 1.69 (dd, *J* = 5.2, 3.2 Hz, 3H), 1.40 (s, 9H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.4, 165.4, 89.8, 89.1, 80.5, 27.9, 12.7;

IR (film) 2979, 2932, 1965, 1707, 1480, 1457, 1407, 1368, 1291, 1257, 1147 cm^{-1};

LRMS (EI) calcd for $C_9H_{14}NaO_2$ (M+Na) 177.09, found 177.09.



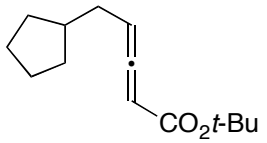
(±)-*tert*-Butyl 6-phenylhexa-2,3-dienoate. The title compound was prepared from 4-phenyl butanoyl chloride according to the General Procedure (purification by column chromatography: 20:1 hexane/Et_2O; 32% yield).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.26-7.31 (m, 2H), 7.17-7.22 (m, 3H), 5.58-5.64 (m, 1H), 5.50-5.54 (m, 1H), 2.71-2.84 (m, 2H), 2.40-2.47 (m, 2H), 1.49 (s, 9H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 211.7, 165.3, 140.9, 128.29, 128.26, 126.0, 94.4, 90.1, 80.6, 35.0, 29.1, 28.0;

IR (film) 3413, 3064, 3028, 2978, 2932, 2860, 1961, 1706, 1604, 1497, 1479, 1455, 1415, 1392, 1368, 1334, 1285, 1256, 1144, 1078, 1031 cm^{-1};

LRMS (EI) calcd for $C_{16}H_{20}NaO_2$ (M+Na) 267.14, found 267.14.



(±)-*tert*-Butyl 5-cyclopentylpenta-2,3-dienoate. The title compound was prepared from 3-cyclopentylpropanoyl chloride according to the General Procedure (purification by column chromatography: 30:1 hexane/Et_2O; 31% yield).

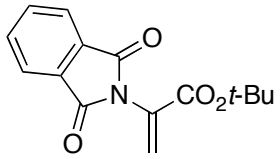
^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.46-5.51 (m, 1H), 5.38-5.42 (m, 1H), 2.04-2.09 (m, 2H), 1.85-1.96 (m, 1H), 1.69-1.78 (m, 2H), 1.44-1.60 (m, 4H), 1.42 (s, 9H), 1.09-1.18 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 212.0, 165.5, 94.2, 89.2, 80.5, 39.4, 33.9, 32.1 (2C), 28.0, 25.2, 25.1;

IR (film) 2951, 2869, 1961, 1706, 1479, 1455, 1416, 1392, 1367, 1281, 1143 cm^{-1};

LRMS (EI) calcd for $C_{14}H_{22}NaO_2$ (M+Na) 245.15, found 245.15.

III. Preparation of Olefins



***tert*-Butyl 2-(1,3-dioxoisoindolin-2-yl)acrylate.** *tert*-Butyl 2-(1,3-dioxoisoindolin-2-yl)-3-hydroxypropanoate[3] (11.7 g, 40.3 mmol) and a stir bar were added to a 500-mL flask, which was then evacuated and back-filled with nitrogen (three cycles). CH_2Cl_2 (250 mL) and NEt_3 (20.2 mL, 145 mmol) were added via syringe, and the resulting solution was stirred in an ice bath for 15 min. Methanesulfonyl chloride (3.89 mL, 50.3 mmol) was then added dropwise via syringe over 3 min to the stirred solution. Next, the ice bath was removed, and the mixture was stirred at r.t. for 1 h. Water (250 mL) was added, the layers were separated, and the aqueous phase was extracted with CH_2Cl_2 (125 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography using gradient elution: 4:1 to 1:1 hexane/Et_2O. The white solid thus obtained was recrystallized from EtOAc (10 mL) and hexane (30 mL) to give the product as a white solid (8.17 g, 74% yield).

Mp 100 °C.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.88-7.94 (m, 2H), 7.76-7.81 (m, 2H), 6.59 (s, 1H), 5.92 (s, 1H), 1.49 (s, 9H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.5, 161.1, 134.3, 131.8, 130.5, 126.6, 123.7, 82.7, 27.8;

(3) Synthesized from (±)-*N*-phthaloyl-*O*-benzyl serine by reaction with *tert*-butyl trichloroacetimidate, followed by hydrogenolysis of benzyl group.

IR (KBr) 2999, 2983, 2967, 1791, 1721, 1646, 1468, 1373, 1288, 1258, 1213, 1141, 1103, 971, 935, 885, 846, 796, 763, 717, 678, 668, 650 cm^{-1};

LRMS (APCI) calcd for $C_{15}H_{15}NNaO_4$ (M+Na) 296.09, found 296.10.

IV. Catalytic Asymmetric [3+2] Cycloadditions

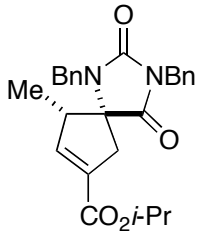
General Procedure A (Table 2). In a glovebox, an oven-dried 20-mL vial was charged with catalyst (*S*)-**1** (13.5 mg, 0.025 mmol), the olefin (0.50 mmol), anhydrous *i*-Pr_2O (4.7 mL), a stir bar, and then the allene (0.75 mmol). The vial was capped and taken out of the glovebox, and the reaction mixture was stirred at r.t. for 24 h. Next, *tert*-butyl hydroperoxide (10 μL; 5-6 M solution in isooctane) was added, the mixture was stirred for 1 min, and then an aqueous solution of $Na_2S_2O_3$ (5 mL; 10%) was added. The aqueous layer was extracted with Et_2O or EtOAc (4 mL x3), and the combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography.

When the [3+2] cycloaddition illustrated in entry 3 of Table 2 was conducted *without* the use of a glovebox, a higher catalyst loading (10%) was necessary to obtain a good yield of product (92%).

General Procedure B (Tables 3–6). In a glovebox, an oven-dried 20-mL vial was charged with catalyst (*S*)-**1** (27.0 mg, 0.050 mmol), the olefin (0.50 mmol), anhydrous *i*-Pr_2O (4.7 mL), a stir bar, and then the allene (1.00 mmol). The vial was capped and taken out of the glovebox, and the reaction mixture was stirred at r.t. for 24 h. Next, *tert*-butyl hydroperoxide (10 μL; 5-6 M solution in isooctane) was added, the mixture was stirred for 1 min, and then an aqueous solution of $Na_2S_2O_3$ (5 mL; 10%) was added. The aqueous layer was extracted with Et_2O or EtOAc (4 mL x3), and the combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography.

For the oxygen-substituted olefin (Table 5), hexane was employed as the solvent (0.4 M), and the reaction time was 48 h.

For the sulfur-substituted olefin (Table 6), chloroform was used as solvent.



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-9-methyl-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 1). The title compound was prepared according to General

Procedure A from (±)-isopropyl penta-2,3-dienoate (105 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (4:1 → 3:1 hexane/EtOAc), the title compound was isolated as a colorless oil (213 mg, 99% yield, rr: 9:1) with 98% ee.

$[\alpha]^{24}_{D}$ = +93 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IC column; 30% 2-PrOH in hexane; 0.7 mL/min; retention times: 11.0 min (major), 17.5 min (minor).

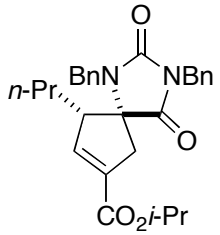
The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 8:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (210 mg, 97% yield, rr: 9:1) with 98% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.21-7.43 (m, 10H), 6.61-6.65 (m, 1H), 5.04 (d, *J* = 15.4 Hz, 1H), 4.98 (qq, *J* = 6.4, 6.4 Hz, 1H), 4.77 (d, *J* = 14.6 Hz, 1H), 4.72 (d, *J* = 14.6 Hz, 1H), 3.84 (d, *J* = 15.4 Hz, 1H), 3.38-3.47 (m, 1H), 3.01 (ddd, *J* = 17.0, 2.8, 2.8 Hz, 1H), 2.34 (d, *J* = 17.0 Hz, 1H), 1.23 (d, *J* = 6.4 Hz, 3H), 1.16 (d, *J* = 6.4 Hz, 3H), 0.91 (d, *J* = 7.6 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.2, 163.0, 155.8, 143.6, 137.1, 136.2, 133.0, 128.64, 128.58, 128.2, 128.0, 127.82, 127.76, 74.2, 67.9, 48.6, 45.2, 42.8, 39.9, 21.75, 21.71, 10.9;

IR (film) 3854, 3745, 2979, 1772, 1710, 1653, 1636, 1559, 1540, 1506, 1497, 1442, 1419, 1362, 1242, 1008, 1075 cm^{-1};

LRMS (APCI) calcd for $C_{26}H_{28}N_2NaO_4$ (M+Na) 455.2, found 455.2.



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-2,4-dioxo-9-propyl-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 2). The title compound was prepared according to General Procedure A from (±)-isopropyl hepta-2,3-dienoate (126 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (5:1 → 4:1 hexane/EtOAc), the title compound was isolated as a colorless oil (228 mg, 99% yield, rr: 14:1) with 97% ee.

$[\alpha]^{24}_{D}$ = +80 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% 2-PrOH in hexane; 1.0 mL/min; retention times: 20.5 min (minor), 27.5 min (major).

The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 15:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (216 mg, 94% yield, rr: >20:1) with 96% ee.

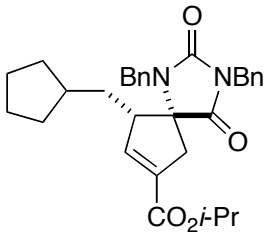
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.17-7.42 (m, 10H), 6.65-6.69 (m, 1H), 4.98 (d, *J* = 15.4 Hz, 1H), 4.95 (qq, *J* = 6.4, 6.4 Hz, 1H), 4.74 (d, *J* = 14.2 Hz, 1H), 4.69 (d, *J* = 14.2 Hz, 1H), 3.83 (d, *J* = 15.4 Hz, 1H), 3.22-3.29 (m, 1H), 2.97 (ddd, *J* = 17.2, 3.0, 3.0 Hz, 1H), 2.30 (d, *J* =

17.2 Hz, 1H), 1.20 (d, J = 6.4 Hz, 3H), 1.14 (d, J = 6.4 Hz, 3H), 0.98-1.30 (m, 4H), 0.70 (d, J = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.4, 163.0, 155.8, 142.4, 137.1, 135.9, 132.8, 128.51 (2C), 128.45, 128.0, 127.8, 127.7, 73.9, 67.8, 53.8, 45.2, 42.8, 40.3, 28.6, 21.70, 21.66, 21.1, 13.8;

IR (film) 3854, 3745, 3629, 1772, 1710, 1653, 1636, 1559, 1540, 1507, 1497, 1442, 1419, 1266, 1109, 754, 700, 668 cm^{-1};

LRMS (APCI) calcd for $C_{28}H_{32}N_2NaO_4$ (M+Na) 483.2, found 483.2.



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-9-(cyclopentylmethyl)-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 3). The title compound was prepared according to General Procedure A from (±)-isopropyl 5-cyclopentylpenta-2,3-dienoate (156 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (3:1 hexane/Et_2O), the title compound was isolated as white semi-solid (235 mg, 94% yield, rr: 14:1) with 92% ee.

$[\alpha]^{24}_D$ = +74 (c = 1.0, $CHCl_3$).

SFC analysis of the product: Daicel CHIRALPAK IC-3 column; 20% MeOH in CO_2; 3.0 mL/min; retention times: 4.4 min (major), 6.0 min (minor).

The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 17:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as white semi-solid (248 mg, 99% yield, rr: 14:1) with 92% ee.

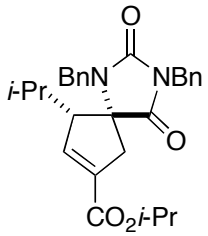
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.20-7.45 (m, 10H), 6.69-6.74 (m, 1H), 4.99 (d, J = 14.8 Hz, 1H), 4.97 (qq, J = 6.4, 6.4 Hz, 1H), 4.75 (d, J = 14.4 Hz, 1H), 4.71 (d, J = 14.4 Hz, 1H), 3.85 (d, J = 14.8 Hz, 1H), 3.26-3.34 (m, 1H), 3.00 (ddd, J = 17.2, 2.8, 2.8 Hz, 1H), 2.33 (d, J = 17.2 Hz, 1H), 1.25-1.64 (m, 8H), 1.23 (d, J = 6.4 Hz, 3H), 1.16 (d, J = 6.4 Hz, 3H), 0.73-1.06 (m, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.2, 163.0, 155.8, 142.6, 137.1, 136.0, 132.8, 128.53, 128.50, 128.47, 128.0, 127.8, 127.7, 74.1, 67.8, 53.1, 45.3, 42.7, 40.1, 38.0, 32.7, 32.6, 32.3, 24.9, 24.8, 21.71, 21.68;

IR (film) 2945, 1768, 1711, 1496, 1442, 1418, 1360, 1265, 1136, 1108, 751, 700, 624 cm^{-1};

LRMS (APCI) calcd for $C_{31}H_{36}N_2NaO_4$ (M+Na) 523.3, found 523.3.

This compound was recrystallized from hexane to give a single crystal, which was submitted to the X-ray structure analysis (mp 115 °C).



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-9-isopropyl-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 4). The title compound was prepared according to General Procedure A with 10% catalyst from (±)-isopropyl 5-methylhexa-2,3-dienoate (126 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (CH_2Cl_2, then 4:1 hexane/EtOAc), the title compound was isolated as a colorless oil (206 mg, 89% yield, rr: >20:1) with 75% ee.

$[\alpha]^{24}_D$ = +51 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% 2-PrOH in hexane; 1.0 mL/min; retention times: 25.5 min (minor), 29.2 min (major).

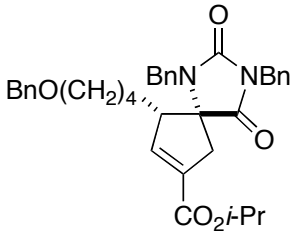
The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 50:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (218 mg, 95% yield, rr: >20:1) with 79% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.18-7.46 (m, 10H), 6.76-6.80 (m, 1H), 4.96 (d, *J* = 15.6 Hz, 1H), 4.88-4.97 (m, 1H), 4.72 (d, *J* = 14.4 Hz, 1H), 4.68 (d, *J* = 14.4 Hz, 1H), 3.88 (d, *J* = 15.6 Hz, 1H), 2.98 (d, *J* = 14.4 Hz, 1H), 2.93 (ddd, *J* = 16.6, 3.0, 3.0 Hz, 1H), 2.28 (d, *J* = 16.6 Hz, 1H), 1.52 (dqq, *J* = 14.4, 6.4, 6.4 Hz, 1H), 1.19 (d, *J* = 6.4 Hz, 3H), 1.12 (d, *J* = 6.4 Hz, 3H), 0.97 (d, *J* = 6.4 Hz, 3H), 0.39 (d, *J* = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.5, 163.0, 155.9, 141.7, 137.1, 135.3, 132.6, 129.0, 128.5, 128.4, 128.1, 127.9, 127.7, 73.5, 67.9, 60.4, 45.4, 42.9, 42.2, 26.4, 22.4, 21.71, 21.67, 20.6;

IR (film) 3854, 2978, 1768, 1709, 1653, 1636, 1559, 1540, 1497, 1441, 1418, 1370, 1267, 1237, 1173, 1136, 1110, 1090, 755, 700, 668 cm^{-1};

LRMS (APCI) calcd for $C_{28}H_{32}N_2O_4Na$ (M+Na) 483.2, found 483.2.



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-9-(4-(benzyloxy)butyl)-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 5). The title compound was prepared according to General Procedure A from (±)-isopropyl 8-(benzyloxy)octa-2,3-dienoate (216 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (2:1 → 3:2

hexane/Et_2O), the title compound was isolated as a colorless oil (262 mg, 90% yield, rr: >20:1) with 96% ee.

$[\alpha]^{24}_D$ = +63 (c = 1.0, $CHCl_3$).

SFC analysis of the product: Daicel CHIRALPAK IC-3 column; 20% 2-PrOH in CO_2; 3.0 mL/min; retention times: 7.3 min (major), 9.0 min (minor).

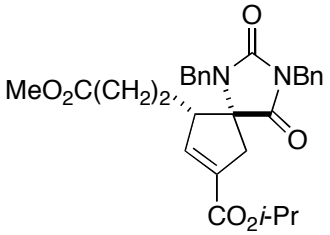
The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 11:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (271 mg, 94% yield, rr: >20:1) with 96% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.18-7.43 (m, 15H), 6.68-6.72 (m, 1H), 4.92-5.03 (m, 2H), 4.74 (d, *J* = 14.4 Hz, 1H), 4.72 (d, *J* = 14.4 Hz, 1H), 4.46 (d, *J* = 12.4 Hz, 1H), 4.43 (d, *J* = 12.4 Hz, 1H), 3.85 (d, *J* = 15.6 Hz, 1H), 3.28 (t, *J* = 6.0 Hz, 2H), 3.23-3.30 (br s, 1H), 3.00 (ddd, *J* = 17.0, 3.0, 3.0 Hz, 1H), 2.32 (d, *J* = 17.0 Hz, 1H), 1.25-1.50 (m, 4H), 1.23 (d, *J* = 6.0 Hz, 3H), 1.17 (d, *J* = 6.0 Hz, 3H), 1.02-1.15 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.4, 163.0, 155.9, 142.2, 138.4, 137.1, 136.0, 133.0, 128.62, 128.58, 128.5, 128.3, 128.1, 127.9, 127.8, 127.6, 127.5, 73.9, 72.8, 69.6, 68.0, 54.1, 45.3, 42.8, 40.4, 29.5, 26.4, 24.8, 21.8, 21.7;

IR (film) 2937, 2859, 1768, 1710, 1496, 1442, 1418, 1362, 1266, 1107, 738, 700 cm^{-1};

LRMS (APCI) calcd for $C_{36}H_{40}N_2NaO_5$ (M+Na) 603.3, found 603.3.



(5*R*,9*S*)-Isopropyl 1,3-dibenzyl-9-(3-methoxy-3-oxopropyl)-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 6). The title compound was prepared according to General Procedure A from (±)-1-isopropyl-7-methyl hepta-2,3-dienedioate (159 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (5:4 → 1:1 hexane/Et_2O), the title compound was isolated as a colorless oil (223 mg, 88% yield, rr: >20:1) with 94% ee.

$[\alpha]^{24}_D$ = +74 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% 2-PrOH in hexane; 1.0 mL/min; retention times: 14.9 min (minor), 16.7 min (major).

The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 13:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (220 mg, 87% yield, rr: >20:1) with 95% ee.

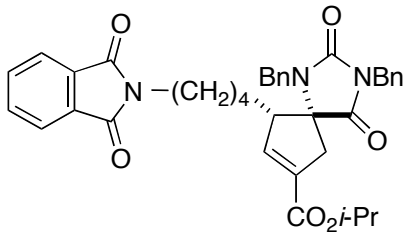
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.18-7.45 (m, 10H), 6.66-6.70 (m, 1H), 5.01 (d, *J* = 15.2 Hz, 1H), 4.97 (qq, *J* = 6.2, 6.2 Hz, 1H), 4.78 (d, *J* = 14.6 Hz, 1H), 4.73 (d, *J* = 14.6 Hz, 1H), 3.87 (d, *J* = 15.2 Hz, 1H), 3.62 (s, 3H), 3.25-3.30 (m, 1H), 2.99 (ddd, *J* = 16.8, 2.8, 2.8 Hz,

1H), 2.33 (d, *J* = 16.8 Hz, 1H), 2.08-2.28 (m, 2H), 1.60-1.70 (m, 1H), 1.42-1.52 (m, 1H), 1.23 (d, *J* = 6.2 Hz, 3H), 1.16 (d, *J* = 6.2 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.0, 172.4, 162.8, 155.8, 141.1, 136.9, 135.8, 133.5, 128.7, 128.6, 128.4, 128.0, 127.9, 127.8, 73.8, 68.0, 53.1, 51.6, 45.3, 42.9, 40.5, 32.2, 21.73 (2C), 21.69;

IR (film) 2981, 1769, 1737, 1710, 1632, 1496, 1442, 1418, 1372, 1267, 1172, 1136, 1107, 1074, 1029, 923, 877, 831, 752, 701, 623 cm^{-1};

LRMS (APCI) calcd for $C_{29}H_{32}N_2NaO_6$ (M+Na) 527.2, found 527.2.



(*5R,9S*)-Isopropyl 1,3-dibenzyl-9-(4-(1,3-dioxoisoindolin-2-yl)butyl)-2,4-dioxo-1,3-diazaspiro[4.4]non-7-ene-7-carboxylate (Table 2, entry 7). The title compound was prepared according to General Procedure A from (±)-isopropyl 8-(1,3-dioxoisoindolin-2-yl)octa-2,3-dienoate (264 mg, 0.75 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by column chromatography (5:2 → 2:1 hexane/EtOAc), the title compound was isolated as a colorless oil (251 mg, 81% yield, rr: >20:1) with 97% ee.

$[\alpha]^{24}_D$ = +69 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 25% 2-PrOH in hexane; 0.7 mL/min; retention times: 24.2 min (minor), 32.5 min (major).

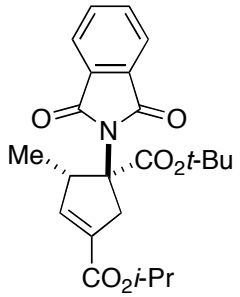
The second run was performed with (*R*)-**1**. The ratio of regioisomers was determined to be 9:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as white semi-solid (262 mg, 85% yield, rr: >20:1) with 98% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.85-7.89 (m, 2H), 7.70-7.76 (m, 2H), 7.18-7.43 (m, 10H), 6.66-6.70 (m, 1H), 4.97 (d, *J* = 15.4 Hz, 1H), 4.95-5.02 (m, 1H), 4.75 (d, *J* = 14.6 Hz, 1H), 4.71 (d, *J* = 14.6 Hz, 1H), 3.90 (d, *J* = 15.4 Hz, 1H), 3.52 (t, *J* = 7.0 Hz, 2H), 3.21-3.29 (m, 1H), 2.99 (ddd, *J* = 17.2, 3.0, 3.0 Hz, 1H), 2.33 (d, *J* = 17.2 Hz, 1H), 1.44-1.55 (m, 2H), 1.26-1.39 (m, 2H), 1.24 (d, *J* = 6.0 Hz, 3H), 1.17 (d, *J* = 5.6 Hz, 3H), 1.01-1.15 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.3, 168.2, 163.0, 155.8, 142.0, 137.1, 135.9, 133.9, 133.0, 132.0, 128.64, 128.58, 128.50, 128.06, 127.96, 127.8, 123.2, 73.9, 68.0, 54.0, 45.3, 42.9, 40.4, 37.2, 28.3, 26.0, 25.1, 21.8, 21.7;

IR (film) 2980, 2939, 1771, 1709, 1653, 1635, 1559, 1540, 1496, 1442, 1419, 1397, 1373, 1269, 1139, 1107, 1075, 924, 754, 721, 701, 668, 624 cm^{-1};

LRMS (APCI) calcd for $C_{37}H_{37}N_3NaO_6$ (M+Na) 642.3, found 642.3.



(*1S,5S*)-1-*tert*-Butyl 3-isopropyl 1-(1,3-dioxoisoindolin-2-yl)-5-methylcyclopent-3-ene-1,3-dicarboxylate (Table 3, entry 1). The title compound was prepared according to General Procedure B from (±)-isopropyl penta-2,3-dienoate (140 mg, 1.00 mmol) and *tert*-butyl 2-(1,3-dioxoisoindolin-2-yl)acrylate (137 mg, 0.50 mmol). After purification by column chromatography (3:1 hexane/Et_2O), the title compound was isolated as a colorless oil (175 mg, 85% yield) with 98% ee.

$[\alpha]^{24}_D$ = +241 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IC column; 30% 2-PrOH in hexane; 0.8 mL/min; retention times: 15.2 min (major), 24.1 min (minor).

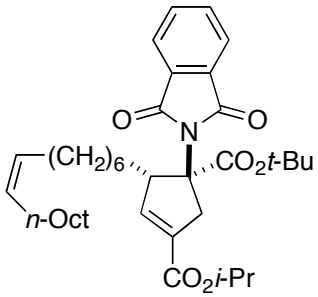
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be >20:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (163 mg, 79% yield) with 98% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80-7.87(m, 2H), 7.71-7.77 (m, 2H), 6.60-6.64 (m, 1H), 5.06 (qq, *J* = 6.4, 6.4 Hz, 1H), 4.62-4.71 (m, 1H), 3.92 (ddd, *J* = 17.2, 1.6, 0.8 Hz, 1H), 2.89 (ddd, *J* = 17.2, 2.0, 2.0 Hz, 1H), 1.41(s, 9H), 1.30 (d, *J* = 7.2 Hz, 3H), 1.27 (d, *J* = 6.4 Hz, 3H), 1.26 (d, *J* = 6.4 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.8, 168.7, 163.9, 144.2, 134.0, 132.9, 131.7, 123.0, 82.6, 72.9, 67.6, 44.3, 43.1, 27.7, 21.77, 21.76, 15.3;

IR (film) 2979, 1779, 1717, 1685, 1653, 1636, 1617, 1576, 1559, 1540, 1521, 1507, 1457, 1437, 1419, 1371, 1266, 1154, 1105, 871, 846, 752, 720, 668 cm^{-1};

LRMS (APCI) calcd for $C_{23}H_{27}NNaO_6$ (M+Na) 436.2, found 436.2.



(*1S,5S*)-(*Z*)-1-*tert*-Butyl 3-isopropyl 1-(1,3-dioxoisoindolin-2-yl)-5-(hexadec-7-en-1-yl)cyclopent-3-ene-1,3-dicarboxylate (Table 3, entry 2). The title compound was prepared according to General Procedure B from (±)-(*Z*)-isopropyl icosa-2,3,11-trienoate (349 mg, 1.00 mmol) and *tert*-butyl 2-(1,3-dioxoisoindolin-2-yl)acrylate (137

mg, 0.50 mmol). After purification by column chromatography (5:4 → 1:1 hexane/EtOAc), the ee of the mixture was determined to be 98%. In order to obtain pure product, the mixture was further purified by semi-preparative HPLC (Daicel CHIRALPAK IA column, 20 mm x 250 mm (5.0 μm); 1% 2-PrOH in hexane; 20.0 mL/min; retention times: 9-12 min (major), 14-15 min (minor)). The title compound was isolated as a colorless oil (236 mg, 76% yield) with 98% ee.

$[\alpha]^{24}_{D}$ = +168 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IA column; 2% 2-PrOH in hexane; 1.0 mL/min; retention times: 13.0 min (major), 17.1 min (minor).

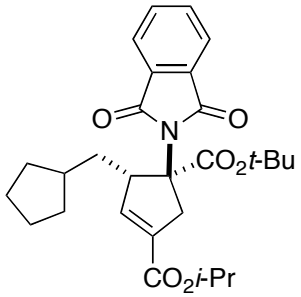
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be >20:1 by ^{1}H NMR analysis of the unpurified mixture. The ee of the unpurified mixture was 98%. The product was isolated as a colorless oil (212 mg, 68% yield) with >99% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80-7.86 (m, 2H), 7.70-7.76 (m, 2H), 6.75-6.80 (m, 1H), 5.30-5.42 (m, 2H), 5.07 (qq, *J* = 6.2, 6.2 Hz, 1H), 4.44 (d, *J* = 11.2 Hz, 1H), 3.93 (d, *J* = 17.0 Hz, 1H), 2.87 (ddd, *J* = 17.0, 2.0, 2.0 Hz, 1H), 2.00-2.08 (m, 4H), 1.80-1.90 (m, 1H), 1.50-1.68 (m, 2H), 1.40 (s, 9H), 1.28 (d, *J* = 6.2 Hz, 3H), 1.27 (d, *J* = 6.2 Hz, 3H), 1.22-1.46 (m, 19H), 0.88 (t, *J* = 6.8 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.0, 168.7, 164.0, 142.2, 134.0, 133.6, 131.7, 129.9, 129.7, 123.1, 82.5, 72.8, 67.6, 49.8, 43.3, 31.8, 30.4, 29.69, 29.65, 29.63, 29.4, 29.24 (2C), 29.18, 28.3, 27.7, 27.14, 27.13, 22.6, 21.82, 21.80, 14.0;

IR (film) 2978, 2926, 2855, 1778, 1719, 1653, 1616, 1559, 1540, 1507, 1467, 1371, 1324, 1263, 1154, 1106, 1037, 925, 871, 848, 792, 720, 666 cm^{-1};

LRMS (APCI) calcd for $C_{38}H_{55}NNaO_6$ (M+Na) 644.4, found 644.3.



(*1S,5S*)-1-*tert*-Butyl 3-isopropyl 5-(cyclopentylmethyl)-1-(1,3-dioxoisoindolin-2-yl)cyclopent-3-ene-1,3-dicarboxylate (Table 3, entry 3). The title compound was prepared according to General Procedure B from (±)-isopropyl 5-cyclopentylpenta-2,3-dienoate (208 mg, 1.00 mmol) and *tert*-butyl 2-(1,3-dioxoisoindolin-2-yl)acrylate (137 mg, 0.50 mmol). After purification by column chromatography (3:1 → 2:1 hexane/Et_2O), the ee of the mixture was determined to be 98%. In order to obtain pure product, the mixture was further purified by semi-preparative HPLC (Daicel CHIRALPAK IC column, 20 mm x 250 mm (5.0 μm); 20% 2-PrOH in hexane; 20.0 mL/min; retention

times: 10-15 min (major), 22-23 min (minor)). The title compound was isolated as a colorless oil (209 mg, 87% yield) with 98% ee.

$[\alpha]^{24}_{D}$ = +238 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IC column; 30% 2-PrOH in hexane; 1.0 mL/min; retention times: 12.8 min (major), 18.5 min (minor).

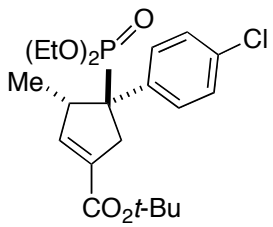
The second run was performed with (*R*)-**1**. The ee of the unpurified mixture was 98%. The ratio of diastereomers was determined to be >20:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (204 mg, 85% yield) with 98% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80-7.86 (m, 2H), 7.71-7.76 (m, 2H), 6.81-6.86 (m, 1H), 5.07 (qq, *J* = 6.0 Hz, 1H), 4.59 (d, *J* = 11.2 Hz, 1H), 3.93 (d, *J* = 17.0 Hz, 1H), 2.86 (d, *J* = 17.0 Hz, 1H), 1.12-2.05 (m, 11H), 1.40 (s, 9H), 1.28 (d, *J* = 6.0 Hz, 3H), 1.27 (d, *J* = 6.0 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.0, 168.7, 164.0, 142.5, 134.0, 133.4, 131.7, 123.0, 82.5, 73.1, 67.6, 48.6, 43.1, 38.7, 36.0, 33.7, 31.3, 27.7, 25.0, 24.9, 21.80, 21.78;

IR (film) 2978, 2946, 2869, 1778, 1717, 1653, 1616, 1469, 1456, 1371, 1326, 1267, 1155, 1104, 1041, 926, 871, 847, 793, 754, 720, 667 cm^{-1};

LRMS (APCI) calcd for $C_{28}H_{35}NNaO_6$ (M+Na) 504.2, found 504.2.



(*3S,4S*)-*tert*-Butyl 4-(4-chlorophenyl)-4-(diethoxyphosphoryl)-3-methylcyclopent-1-enecarboxylate (Table 4, entry 1). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl penta-2,3-dienoate (154 mg, 1.00 mmol) and diethyl (1-(4-chlorophenyl)vinyl)phosphonate (137 mg, 0.50 mmol). After purification by column chromatography (3:2 → 1:1 toluene/EtOAc), the title compound was isolated as a colorless oil (173 mg, 81% yield) with 99% ee.

$[\alpha]^{24}_{D}$ = +115 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% 2-PrOH in hexane; 1.0 mL/min; retention times: 8.9 min (minor), 24.1 min (major).

The second run was performed with (*R*)-**1**. The product was isolated as a colorless oil (177 mg, 83% yield) with 99% ee.

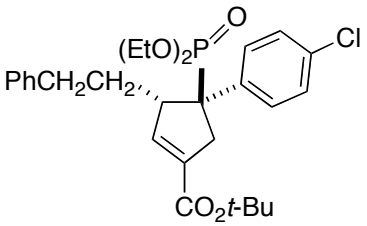
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 (dd, *J* = 8.8, 2.6 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 6.60-6.65 (m, 1H), 3.95-4.10 (m, 2H), 3.78-3.90 (m, 1H), 3.60-3.73 (m, 1H), 3.51-3.61 (m, 1H), 3.31 (dd, *J* = 17.0, 17.0 Hz, 1H), 3.13 (dddd, *J* = 24.0, 17.0, 2.0, 2.0 Hz, 1H), 1.52 (s,9H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.06 (t, *J* = 7.2 Hz, 3H), 0.76 (d, *J* = 7.2 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.0, 145.3 (d, *J* = 3 Hz), 136.0 (d, *J* = 5 Hz), 134.7 (d, *J* = 2 Hz), 132.7 (d, *J* = 3 Hz), 131.0 (d, *J* = 7 Hz), 127.8 (d, *J* = 2 Hz), 80.4, 62.7 (d, *J* = 8 Hz), 62.2 (d, *J* = 7 Hz), 53.9 (d, *J* = 135 Hz), 44.5 (d, *J* = 2 Hz), 36.7 (d, *J* = 4 Hz), 28.0, 16.14 (d, *J* = 3 Hz), 16.08 (d, *J* = 3 Hz), 15.8 (d, *J* = 10 Hz);

^{31}P NMR ($CDCl_3$, 162 MHz) δ 30.8;

IR (film) 2980, 2931, 1708, 1637, 1559, 1540, 1494, 1457, 1392, 1368, 1355, 1278, 1243, 1169, 1123, 1095, 1054, 1026, 965, 847, 793, 749, 668, 581 cm^{-1};

LRMS (APCI) calcd for $C_{21}H_{30}ClNaO_5P$ (M+Na) 451.1, found 451.1.



(*3S,4S*)-*tert*-Butyl 4-(4-chlorophenyl)-4-(diethoxyphosphoryl)-3-phenethylcyclopent-1-enecarboxylate (Table 4, entry 2). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl 6-phenylhexa-2,3-dienoate (244 mg, 1.00 mmol) and diethyl (1-(4-chlorophenyl)vinyl)phosphonate (137 mg, 0.50 mmol). After purification by column chromatography (1:5 → 1:6 hexane/Et_2O), the title compound was isolated as a colorless oil (212 mg, 82% yield) with 96% ee.

$[\alpha]^{23}_D$ = +93 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% 2-PrOH in hexane; 1.0 mL/min; retention times: 8.5 min (minor), 22.2 min (major).

The second run was performed with (*R*)-**1**. The product was isolated as a colorless oil (198 mg, 76% yield) with 97% ee.

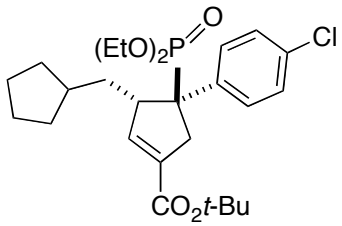
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.28 (d, *J* = 8.8 Hz, 2H), 7.23 (dd, *J* = 7.6, 7.2 Hz, 2H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 2H), 6.76-6.82 (m, 1H), 3.92-4.05 (m, 2H), 3.77-3.88 (m, 1H), 3.50-3.65 (m, 2H), 3.33 (dd, *J* = 17.2, 17.2 Hz, 1H), 3.15 (dd, *J* = 22.4, 16.8 Hz, 1H), 2.46-2.55 (m, 2H), 1.70-1.80 (m, 1H), 1.54 (s, 9H), 1.21 (t, *J* = 7.0 Hz, 3H), 1.10-1.20 (m, 1H), 1.04 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.8, 143.1 (d, *J* = 3 Hz), 141.3, 136.1 (d, *J* = 3 Hz), 135.9 (d, *J* = 4 Hz), 132.7 (d, *J* = 4 Hz), 130.8 (d, *J* = 7 Hz), 128.2, 128.1, 127.8 (d, *J* = 3 Hz), 125.8, 80.6, 62.7 (d, *J* = 7 Hz), 62.2 (d, *J* = 7 Hz), 53.9 (d, *J* = 135 Hz), 49.2 (d, *J* = 2 Hz), 37.8 (d, *J* = 4 Hz), 33.1, 32.6 (d, *J* = 8 Hz), 28.0, 16.1 (d, *J* = 3 Hz), 16.0 (d, *J* = 2 Hz);

^{31}P NMR ($CDCl_3$, 162 MHz) δ 30.6;

IR (film) 2979, 1772, 1734, 1706, 1685, 1653, 1636, 1617, 1576, 1559, 1540, 1521, 1507, 1495, 1457, 1393, 1368, 1243, 1168, 1096, 1052, 1026, 963, 848, 750, 700, 668, 578 cm^{-1};

LRMS (APCI) calcd for $C_{28}H_{36}ClNaO_5P$ (M+Na) 541.2, found 541.2.



(*3S,4S*)-*tert*-Butyl 4-(4-chlorophenyl)-3-(cyclopentylmethyl)-4-(diethoxyphosphoryl)cyclopent-1-enecarboxylate (Table 4, entry 3). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl 5-cyclopentylpenta-2,3-dienoate (222 mg, 1.00 mmol) and diethyl (1-(4-chlorophenyl)vinyl)phosphonate (137 mg, 0.50 mmol). After purification by column chromatography (1:4 hexane/Et_2O), the title compound was isolated as a colorless oil (215 mg, 86% yield) with 96% ee.

$[\alpha]^{23}_D$ = +118 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% 2-PrOH in hexane; 1.0 mL/min; retention times: 6.7 min (minor), 12.1 min (major).

The second run was performed with (*R*)-**1**. The product was isolated as a colorless oil (216 mg, 87% yield) with 97% ee.

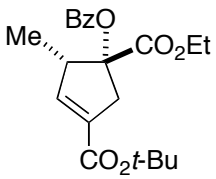
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 (dd, *J* = 8.8, 2.4 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 2H), 6.76-6.82 (m, 1H), 3.95-4.10 (m, 2H), 3.80-3.90 (m, 1H), 3.52-3.64 (m, 2H), 3.30 (dd, *J* = 17.0, 17.0 Hz, 1H), 3.11 (dd, *J* = 22.8, 16.4 Hz, 1H), 1.43-1.90 (m, 8H), 1.53 (s, 9H), 1.25 (t, *J* = 7.0 Hz, 3H), 1.05-1.15 (m, 1H), 1.07 (t, *J* = 7.0 Hz, 3H), 0.80-0.95 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.0, 144.2 (d, *J* = 3 Hz), 136.1 (d, *J* = 4 Hz), 135.5 (d, *J* = 3 Hz), 132.6 (d, *J* = 3 Hz), 131.0 (d, *J* = 6 Hz), 127.8 (d, *J* = 2 Hz), 80.5, 62.6 (d, *J* = 7 Hz), 62.2 (d, *J* = 7 Hz), 54.3 (d, *J* = 135 Hz), 48.8 (d, *J* = 1 Hz), 37.9, 37.4 (d, *J* = 4 Hz), 37.1 (d, *J* = 8 Hz), 33.7, 31.7, 28.1, 25.0, 24.9, 16.2 (d, *J* = 5 Hz), 16.1 (d, *J* = 4 Hz);

^{31}P NMR ($CDCl_3$, 162 MHz) δ 30.9;

IR (film) 2979, 2950, 2868, 1708, 1637, 1493, 1456, 1392, 1368, 1281, 1244, 1169, 1118, 1095, 1057, 1027, 963, 847, 791, 751, 668, 583 cm^{-1};

LRMS (APCI) calcd for $C_{26}H_{38}ClNaO_5P$ (M+Na) 519.2, found 519.2.



(*1R,5S*)-3-*tert*-butyl 1-ethyl 1-(benzoyloxy)-5-methylcyclopent-3-ene-1,3-dicarboxylate (Table 5, entry 1). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl penta-2,3-dienoate (154 mg, 1.00 mmol) and 3-ethoxy-3-oxoprop-1-en-2-yl benzoate (110 mg, 0.50 mmol). After purification by

column chromatography (6:1 hexane/Et_2O), the title compound was isolated as a colorless oil (145 mg, 78% yield, dr: 13:1) with 95% ee.

$[\alpha]^{23}_D = -23$ (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 1% 2-PrOH in hexane; 1.0 mL/min; retention times: 19.1 min (minor), 20.8 min (major).

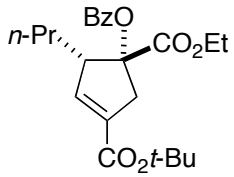
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 10:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (151 mg, 80% yield, dr: 11:1) with 96% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.04 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 7.6, 7.2 Hz, 2H), 6.49-6.54 (m, 1H), 4.23 (q, *J* = 7.0 Hz, 2H), 3.65 (ddd, *J* = 18.4, 2.0, 2.0 Hz, 1H), 3.33-3.43 (m, 1H), 3.06 (ddd, *J* = 18.4, 1.0, 1.0 Hz, 1H), 1.48 (s, 9H), 1.34 (d, *J* = 7.6 Hz, 3H), 1.23 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.0, 165.5, 163.6, 142.6, 134.0, 133.3, 129.72, 129.67, 128.4, 86.4, 80.7, 61.5, 48.5, 41.6, 28.0, 14.0, 13.0;

IR (film) 2979, 2937, 1745, 1720, 1637, 1602, 1452, 1393, 1368, 1316, 1284, 1175, 1138, 1113, 1037, 849, 746, 713 cm^{-1};

LRMS (APCI) calcd for $C_{21}H_{26}NaO_6$ (M+Na) 397.2, found 397.1.



(*1R,5S*)-3-*tert*-Butyl 1-ethyl 1-(benzoyloxy)-5-propylcyclopent-3-ene-1,3-dicarboxylate (Table 5, entry 2). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl hepta-2,3-dienoate (182 mg, 1.00 mmol) and 3-ethoxy-3-oxoprop-1-en-2-yl benzoate (110 mg, 0.50 mmol). After purification by column chromatography (7:1 hexane/Et_2O), the title compound was isolated as a colorless oil (160 mg, 80% yield, dr: 14:1) with 90% ee.

$[\alpha]^{23}_D = -35$ (c = 1.0, $CHCl_3$).

HPLC analysis of the product after deprotection of the *tert*-Bu ester with trifluoroacetic acid: Daicel CHIRALPAK IC column; 10% 2-PrOH in hexane; 1.0 mL/min; retention times: 21.6 min (minor), 39.1 min (major).

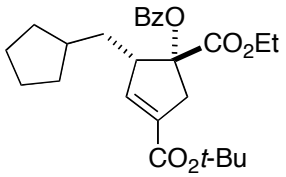
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 11:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (180 mg, 90% yield, dr: 14:1) with 88% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.02 (d, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.46 (dd, *J* = 8.0, 7.6 Hz, 2H), 6.60-6.65 (m, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 3.70 (ddd, *J* = 18.0, 2.0, 2.0 Hz, 1H), 3.16-3.22 (m, 1H), 3.04 (ddd, *J* = 18.0, 1.5, 1.5 Hz, 1H), 1.81-1.91 (m, 1H), 1.65-1.75 (m, 1H), 1.53-1.64 (m, 1H), 1.41-1.52 (m, 1H), 1.48 (s, 9H), 1.23 (t, *J* = 7.0 Hz, 3H), 0.99 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.2, 165.4, 163.7, 140.8, 134.6, 133.3, 129.8, 129.7, 128.4, 86.6, 80.7, 61.6, 53.9, 41.9, 30.2, 28.0, 21.0, 14.1, 14.0;

IR (film) 2977, 2935, 2873, 1744, 1722, 1641, 1602, 1585, 1452, 1393, 1368, 1316, 1285, 1175, 1138, 1112, 1097, 1069, 1048, 1026, 902, 849, 798, 740, 712, 687 cm^{-1};

LRMS (APCI) calcd for $C_{23}H_{30}NaO_6$ (M+Na) 425.2, found 425.2.



(*1R,5S*)-3-*tert*-Butyl 1-ethyl 1-(benzoyloxy)-5-(cyclopentylmethyl)cyclopent-3-ene-1,3-dicarboxylate (Table 5, entry 3). The title compound was prepared according to General Procedure B from (±)-*tert*-butyl 5-cyclopentylpenta-2,3-dienoate (222 mg, 1.00 mmol) and 3-ethoxy-3-oxoprop-1-en-2-yl benzoate (110 mg, 0.50 mmol). After purification by column chromatography (7:1 hexane/Et_2O), the title compound was isolated as a colorless oil (182 mg, 82% yield, dr: 17:1) with 85% ee.

$[\alpha]^{24}_D$ = –43 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IA column; 1% 2-PrOH in hexane; 1.0 mL/min; retention times: 9.1 min (major), 12.8 min (minor).

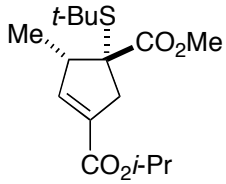
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 12:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (186 mg, 84% yield, dr: 17:1) with 87% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.02 (d, *J* = 7.4 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (dd, *J* = 7.4, 7.4 Hz, 2H), 6.62-6.67 (m, 1H), 4.18-4.32 (m, 2H), 3.71 (d, *J* = 18.0 Hz, 1H), 3.17-3.25 (m, 1H), 3.05 (d, *J* = 18.0 Hz, 1H), 1.50-2.05 (m, 9H), 1.48 (s, 9H), 1.24 (t, *J* = 7.0 Hz, 3H), 1.05-1.20 (m, 2H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.0, 165.3, 163.6, 141.0, 134.5, 133.2, 129.8, 129.6, 128.3, 86.8, 80.6, 61.5, 53.4, 41.8, 38.1, 34.2, 33.4, 32.2, 28.0, 25.1, 25.0, 14.0;

IR (film) 2946, 2868, 1744, 1723, 1638, 1602, 1452, 1392, 1368, 1316, 1285, 1175, 1116, 1069, 1027, 850, 736, 712 cm^{-1};

LRMS (APCI) calcd for $C_{26}H_{34}NaO_6$ (M+Na) 465.2, found 465.2.



(*1R,5S*)-3-Isopropyl 1-methyl 1-(*tert*-butylthio)-5-methylcyclopent-3-ene-1,3-dicarboxylate (Table 6, entry 1). The title compound was prepared according to

General Procedure B from (±)-isopropyl penta-2,3-dienoate (140 mg, 1.00 mmol) and methyl 2-(*tert*-butylthio)acrylate (87 mg, 0.50 mmol). After purification by column chromatography (6:1 hexane/Et_2O), the title compound was isolated as a colorless oil (102 mg, 65% yield, dr: 8:1) with 98% ee.

$[\alpha]^{25}_D$ = +182 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IA column; 1% 2-PrOH in hexane; 1.0 mL/min; retention times: 7.1 min (major), 8.4 min (minor).

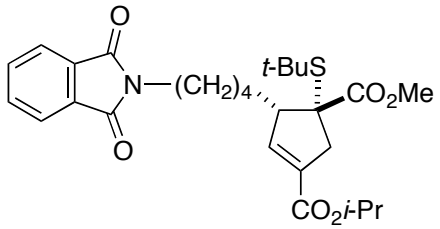
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 7:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (112 mg, 71% yield, dr: 9:1) with 98% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.57-6.62 (m, 1H), 5.07 (qq, *J* = 6.4, 6.4 Hz, 1H), 3.78 (s, 3H), 3.57 (ddd, *J* = 17.3, 2.0, 2.0 Hz, 1H), 3.12 (d, *J* = 17.3 Hz, 1H), 2.88-2.97 (m, 1H), 1.36 (s, 9H), 1.28 (d, *J* = 6.4 Hz, 3H), 1.27 (d, *J* = 6.4 Hz, 3H), 1.00 (d, *J* = 7.2 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 173.4, 164.1, 144.0, 133.1, 67.6, 61.5, 52.0, 51.4, 46.6, 40.1, 31.9, 21.78, 21.76, 14.6;

IR (film) 2980, 1717, 1685, 1653, 1636, 1559, 1540, 1521, 1507, 1457, 1365, 1261, 1159, 1097, 936, 744, 668 cm^{-1};

LRMS (APCI) calcd for $C_{16}H_{26}O_4SNa$ (M+Na) 337.2, found 337.2.



(*1R,5S*)-3-Isopropyl 1-methyl 1-(*tert*-butylthio)-5-(4-(1,3-dioxoisoindolin-2-yl)butyl)cyclopent-3-ene-1,3-dicarboxylate (Table 6, entry 2). The title compound was prepared according to General Procedure B from (±)-isopropyl 8-(1,3-dioxoisoindolin-2-yl)octa-2,3-dienoate (327 mg, 1.00 mmol) and methyl 2-(*tert*-butylthio)acrylate (87 mg, 0.50 mmol). After purification by column chromatography (5:2 hexane/Et_2O), the title compound was isolated as a colorless oil (187 mg, 75% yield, dr: 14:1) with 96% ee.

$[\alpha]^{24}_D$ = +113 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IA column; 4% 2-PrOH in hexane; 1.0 mL/min; retention times: 17.8 min (major), 23.7 min (minor).

The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 6:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (203 mg, 81% yield, dr: 14:1) with 97% ee.

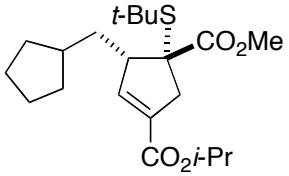
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81-7.86 (m, 2H), 7.70-7.75 (m, 2H), 6.70 (s, 1H), 5.07 (qq, *J* = 6.0, 6.0 Hz, 1H), 3.76 (s, 3H), 3.66 (t, *J* = 7.2 Hz, 2H), 3.52 (d, *J* = 17.2 Hz, 1H), 3.09

(d, J = 17.2 Hz, 1H), 2.76-2.85 (m, 1H), 1.58-1.73 (m, 3H), 1.34 (s, 9H), 1.28 (d, J = 6.0 Hz, 3H), 1.27 (d, J = 6.0 Hz, 3H), 1.18-1.41 (m, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 173.3, 168.2, 164.0, 142.3, 134.5, 133.8, 132.0, 123.1, 67.7, 61.8, 56.3, 52.1, 46.7, 40.7, 37.6, 31.9, 29.4, 28.5, 24.7, 21.79, 21.78;

IR (film) 2947, 1773, 1713, 1636, 1559, 1466, 1437, 1397, 1373, 1261, 1161, 1104, 753, 721, 668 cm^{-1};

LRMS (APCI) calcd for $C_{27}H_{35}NNaO_6S$ (M+Na) 524.2, found 524.2.



(*1R,5S*)-3-Isopropyl 1-methyl 1-(*tert*-butylthio)-5-(cyclopentylmethyl)cyclopent-3-ene-1,3-dicarboxylate (Table 6, entry 3). The title compound was prepared according to General Procedure B from (±)-isopropyl 5-cyclopentylpenta-2,3-dienoate (208 mg, 1.00 mmol) and methyl 2-(*tert*-butylthio)acrylate (87 mg, 0.50 mmol). After purification by column chromatography (7:1 hexane/Et_2O), the title compound was isolated as a colorless oil (170 mg, 89% yield, dr: 8:1) with 97% ee.

$[\alpha]^{24}_D$ = +187 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 1% 2-PrOH in hexane; 1.0 mL/min; retention times: 6.2 min (major), 7.4 min (minor).

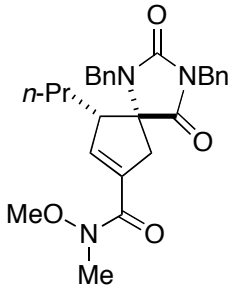
The second run was performed with (*R*)-**1**. The ratio of diastereomers was determined to be 7:1 by ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (174 mg, 91% yield, dr: 8:1) with 97% ee.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.76 (s, 1H), 5.07 (qq, J = 6.0, 6.0 Hz, 1H), 3.76 (s, 3H), 3.53 (ddd, J = 16.8, 2.0, 2.0 Hz, 1H), 3.10 (d, J = 16.8 Hz, 1H), 2.79-2.88 (m, 1H), 1.38-1.85 (m, 8H), 1.35 (s, 9H), 1.28 (d, J = 6.0 Hz, 3H), 1.27 (d, J = 6.0 Hz, 3H), 1.08-1.33 (m, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 173.4, 164.1, 143.0, 134.1, 67.7, 62.2, 55.6, 52.0, 46.6, 40.4, 37.9, 35.8, 33.7, 32.0, 31.5, 25.0, 24.9, 21.82, 21.80;

IR (film) 2949, 2868, 1726, 1712, 1640, 1461, 1452, 1366, 1260, 1231, 1160, 1107, 938, 739 cm^{-1};

LRMS (APCI) calcd for $C_{21}H_{34}NaO_4S$ (M+Na) 405.2, found 405.2.



(5*R*,9*S*)-1,3-dibenzyl-*N*-methoxy-*N*-methyl-2,4-dioxo-9-propyl-1,3-diazaspiro[4.4]non-7-ene-7-carboxamide (eq 3). The title compound was prepared according to General Procedure B from (±)-*N*-methoxy-*N*-methylhepta-2,3-dienamide (169 mg, 1.00 mmol) and 1,3-dibenzyl-5-methyleneimidazolidine-2,4-dione (146 mg, 0.50 mmol). After purification by reverse-phase column chromatography using gradient elution (10% to 90% MeCN/water), the title compound was isolated as a colorless oil (195 mg, 84% yield, rr: >20:1, dr: >20:1) with 94% ee.

$[\alpha]^{24}_{D}$ = +45 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IB-3 column; 15% 2-PrOH in hexane; 0.9 mL/min; retention times: 10.9 min (major), 18.2 min (minor).

The second run was performed with (*R*)-**1**. The ratios of regioisomers and diastereomers were both 17:1, according to ^{1}H NMR analysis of the unpurified mixture. The product was isolated as a colorless oil (200 mg, 86% yield, rr: >20:1, dr: >20:1) with 94% ee.

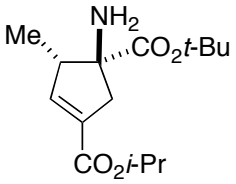
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.21-7.45 (m, 10H), 6.62-6.67 (m, 1H), 4.93 (d, *J* = 15.2 Hz, 1H), 4.77 (d, *J* = 14.4 Hz, 1H), 4.72 (d, *J* = 14.4 Hz, 1H), 3.98 (d, *J* = 15.2 Hz, 1H), 3.39 (s, 3H), 3.15-3.28 (m, 2H), 3.16 (s, 3H), 2.42 (d, *J* = 16.8 Hz, 1H), 0.98-1.30 (m, 4H), 0.71 (t, *J* = 6.8 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 174.6, 164.8, 155.9, 142.0, 137.4, 135.9, 133.5, 128.6 (2C), 128.4, 128.3, 127.9, 127.6, 74.3, 61.2, 53.1, 45.2, 42.8, 42.1, 32.7, 28.8, 21.1, 13.8;

IR (film) 2959, 2933, 2872, 1766, 1709, 1637, 1607, 1496, 1443, 1418, 1381, 1359, 1205, 1136, 1075, 977, 752, 701, 624, 565 cm^{-1};

LRMS (APCI) calcd for $C_{27}H_{31}N_3NaO_4$ (M) 484.2, found 484.2.

V. Functionalizations of the Cycloaddition Products



(1*S*,5*S*)-1-*tert*-Butyl 3-isopropyl 1-amino-5-methylcyclopent-3-ene-1,3-dicarboxylate (eq 4). An aqueous solution of methylamine (3.6 mL, 42 mmol; 40%)

was added to a solution of (*1S,5S*)-1-*tert*-butyl 3-isopropyl 1-(1,3-dioxoisoindolin-2-yl)-5-methylcyclopent-3-ene-1,3-dicarboxylate (300 mg, 0.726 mmol; 99% ee) in THF (30 mL), and the resulting mixture was stirred at r.t. for 24 h. Then, the volatiles were removed under reduced pressure, the residue was added to 2-propanol (20 mL), and the volatiles were evaporated under reduced pressure (to remove the residual methylamine). The resulting residue was dissolved in 2-propanol (10 mL), trifluoromethanesulfonimide (1.02 g, 3.63 mmol) was added, and the resulting solution was allowed to stand at r.t. for 2 days. Then, the reaction was quenched by the addition of an aqueous solution of Na_2CO_3 (4 mL; 10%). The 2-propanol was removed under reduced pressure, the resulting aqueous phase was extracted with EtOAc (4 mL x3), and the combined organic extracts were washed with brine (4 mL). The solvent was removed under reduced pressure, and then toluene (10 mL) was added to the residue. The toluene solution was washed successively with aqueous sodium hydroxide (1%), water, and brine, and then it was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography (100:100:1 CH_2Cl_2/EtOAc/NEt_3), which furnished the title compound as a colorless oil (156 mg, 76% yield) with 98% ee.

$[\alpha]^{24}_D$ = +137 (c = 1.0, $CHCl_3$).

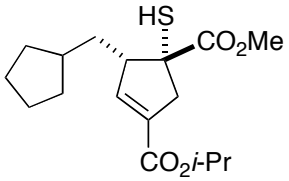
HPLC analysis of the product: Daicel CHIRALPAK IC column; 65% 2-PrOH in hexane; 0.5 mL/min; retention times for major isomers: 16.3 min (major), 26.6 min (minor).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.55-6.59 (m, 1H), 5.06 (qq, *J* = 6.4, 6.4 Hz, 1H), 3.34 (ddd, *J* = 16.8, 2.2, 2.2 Hz, 1H), 2.68-2.76 (m, 1H), 2.44 (d, *J* = 16.8 Hz, 1H), 1.77 (s, 2H), 1.49 (s, 9H), 1.27 (d, *J* = 6.4 Hz, 3H), 1.26 (d, *J* = 6.4 Hz, 3H), 1.03 (d, *J* = 7.2 Hz, 3H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 173.8, 164.4, 144.1, 133.7, 81.4, 67.6, 67.5, 53.6, 41.7, 27.9, 21.8 (2C), 15.2;

IR (film) 3397, 2979, 2935, 1710, 1636, 1457, 1369, 1238, 1161, 1103, 1032, 847, 744 cm^{-1};

LRMS (APCI) calcd for $C_{15}H_{26}NO_4$ (M+H) 284.2, found 284.2.



(1*R*,5*S*)-3-Isopropyl 1-methyl 5-(cyclopentylmethyl)-1-mercaptocyclopent-3-ene-1,3-dicarboxylate (eq 5). Hg(TFA)$_2$ (280 mg, 0.656 mmol) and water (0.8 mL) were added to a solution of (1*R*,5*S*)-3-isopropyl 1-methyl 1-(*tert*-butylthio)-5-(cyclopentylmethyl)cyclopent-3-ene-1,3-dicarboxylate (147 mg, 0.384 mmol; 97% ee, dr: 8:1) in acetic acid (3.4 mL). The reaction mixture was stirred at r.t. for 1 h, and then 2-mercaptoethanol (123 μL, 1.76 mmol) was added. The resulting mixture was stirred for an additional 3 h, and then it was filtered through a plug of silica gel (10 g) and

washed with Et_2O (100 mL). The filtrate was concentrated under reduced pressure, and the residue was suspended in water (10 mL). The mixture was extracted with Et_2O (10 mL x4), and the combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography (6:1 hexane/Et_2O), which furnished the title compound as a colorless oil (88 mg, 70% yield; 98% ee, dr: 8:1).

$[\alpha]^{24}_D$ = +151 (c = 1.0, $CHCl_3$).

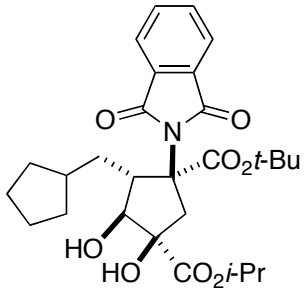
SFC analysis of the product: Daicel CHIRALPAK IC-3 column; 5% MeOH in CO_2; 3.0 mL/min; retention times: 3.8 min (major), 7.2 min (minor).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.76-6.81 (m, 1H), 5.07 (qq, *J* = 6.2, 6.2 Hz, 1H), 3.78 (s, 3H), 3.49 (d, *J* = 17.8 Hz, 1H), 2.98-3.05 (m, 1H), 2.66 (d, *J* = 17.8 Hz, 1H), 2.63 (s, 1H), 1.29 (d, *J* = 6.2 Hz, 3H), 1.28 (d, *J* = 6.2 Hz, 3H), 0.87-1.93 (m, 11H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 172.6, 164.0, 143.2, 134.0, 67.9, 58.7, 57.4, 52.6, 41.9, 37.9, 36.8, 33.7, 31.7, 25.1, 24.9, 21.84, 21.82;

IR (film) 3421, 2950, 2868, 1734, 1715, 1653, 1636, 1559, 1540, 1507, 1457, 1437, 1374, 1263, 1233, 1180, 1108, 740 cm^{-1};

LRMS (ESI) calcd for $C_{17}H_{26}NaO_4S$ (M+Na) 349.2, found 349.1.



(*1S,3R,4S,5R*)-1-*tert*-Butyl 3-isopropyl 5-(cyclopentylmethyl)-1-(1,3-dioxoisoindolin-2-yl)-3,4-dihydroxycyclopentane-1,3-dicarboxylate (eq 6). A solution of *N*-methylmorpholine *N*-oxide (155 μL, 0.748 mmol; 50%), potassium osmate dihydrate (13.7 mg, 0.0373 mmol), and acetic acid (1 drop) in water (6 mL) was added to a solution of (*1S,5S*)-1-*tert*-butyl 3-isopropyl 5-(cyclopentylmethyl)-1-(1,3-dioxoisoindolin-2-yl)cyclopent-3-ene-1,3-dicarboxylate (180 mg, 0.374 mmol; 98% ee) in acetonitrile (12 mL), and the resulting mixture was stirred at r.t. for 4 h. Next, aqueous solutions of $Na_2S_2O_3$ (5 mL; 10%) and $NaHCO_3$ (5 mL; saturated) were added, followed by EtOAc (10 mL). The organic phase was separated, and the aqueous phase was extracted with EtOAc (10 mL x3). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The ratio of diastereomers of this unpurified mixture was determined by ^{1}H NMR spectroscopy to be 16:1. The residue was purified by column chromatography (3:1 → 2:1 hexane/EtOAc), which furnished the title compound as a colorless oil (182 mg, 94% yield; dr: 20:1, 99% ee).

$[\alpha]^{24}_D$ = +162 (c = 1.0, $CHCl_3$).

HPLC analysis of the product: Daicel CHIRALPAK IB-3 column; 10% 2-PrOH in hexane; 0.9 mL/min; retention times for major isomers: 7.8 min (minor), 8.3 min (major).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.79-7.85 (m, 2H), 7.68-7.76 (m, 2H), 5.12 (qq, *J* = 6.0, 6.0 Hz, 1H), 4.28 (dd, *J* = 11.0, 10.0 Hz, 1H), 3.96 (ddd, *J* = 10.6, 10.6, 3.6 Hz, 1H), 3.82 (s, 1H), 3.43 (d, *J* = 15.6 Hz, 1H), 2.78 (d, *J* = 11.0 Hz, 1H), 2.37 (d, *J* = 15.6 Hz, 1H), 2.25-2.38 (br s, 1H), 1.10-1.95 (m, 10H), 1.44 (s, 9H), 1.32 (d, *J* = 6.0 Hz, 3H), 1.31 (d, *J* = 6.0 Hz, 3H);

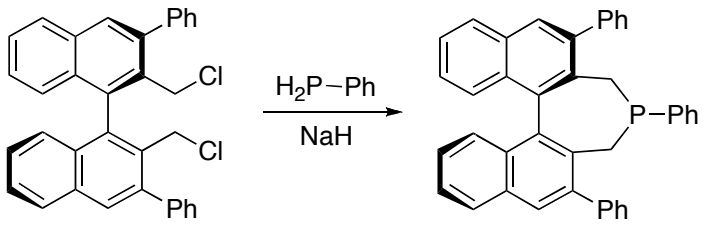
^{13}C NMR ($CDCl_3$, 100 MHz) δ 173.8, 169.6, 168.8, 134.0, 131.7, 123.0, 83.0, 81.1, 79.8, 70.4, 70.2, 45.5, 44.9, 37.1, 36.7, 34.2, 31.3, 27.8, 25.2, 24.9, 21.7, 21.6;

IR (film) 3448, 2979, 2945, 2868, 1779, 1716, 1653, 1468, 1456, 1371, 1320, 1259, 1154, 1134, 1107, 1042, 1007, 878, 846, 755, 722 cm^{-1};

LRMS (APCI) calcd for $C_{28}H_{37}NNaO_8$ (M) 538.2, found 538.2.

This compound was recrystallized from hexane to give a single crystal (mp 130–131 °C), which was analyzed by X-ray crystallography.

VI. Preparation of Catalyst 1



(*R*)-**1**

Phosphepine (*R*)-1. (*R*)-2,2'-Bis(chloromethyl)-3,3'-diphenyl-1,1'-binaphthalene[4,5] (1.20 g, 2.38 mmol) and a stir bar were added to an oven-dried 300-mL flask, which was then evacuated and back-filled with nitrogen three times. THF (96 mL; degassed, anhydrous) was added via syringe, and the flask was moved into a glovebox. Phenylphosphine (275 μL, 2.50 mmol) and sodium hydride (72 mg, 2.9 mmol) were added in turn, and the resulting mixture was stirred vigorously at r.t. for 2 days. Additional sodium hydride (108 mg, 4.28 mmol) was then added, and the reaction mixture was stirred for an additional 3 days (the disappearance of starting material was monitored by TLC). Next, the flask was removed from the glovebox, and the reaction mixture was worked up and outside of the glovebox with degassed solvents. First, the THF was removed under reduced pressure, and then the flask was backfilled with nitrogen. Toluene (15 mL) was added, and then water (15 mL) was cautiously added. The phases were separated, and the aqueous phase was extracted with toluene (10 mL).

(4) Ooi, T.; Kameda, M.; Maruoka, K. *J. Am. Chem. Soc*. **2003**, *125*, 5139–5151.

(5) Zhou, Y.-G.; Zhang, X. *Chem. Commun*. **2002**, 1124–1125.

The combined organic phases were washed with water (10 mL), dried (Na_2SO_4), filtered through a pad of celite, and concentrated under reduced pressure. The flask was back-filled with nitrogen, and then toluene (3 mL) and 2-propanol (4 mL) were added to the residue under nitrogen. The mixture was heated at 50 °C until all of the solids had dissolved. Next, the stirred solution was cooled to r.t. over 1 h (during which time seed crystals were added). After a significant amount of solid had precipitated, additional 2-propanol (20 mL) was added dropwise, and stirring was continued for another 2 h. The solid was then isolated by filtration, washed with 2-propanol (twice), and dried under reduced pressure to provide phosphepine (*R*)-**1** (1.11 g) as a white powder, contaminated with a small amount of 2-propanol (according to ^{1}H NMR spectroscopy).

In order to remove the 2-propanol, this white solid was dissolved in toluene (12 mL), and then the toluene was removed under reduced pressure. The flask was back-filled with nitrogen, toluene (1.25 mL) was added, and the resulting mixture was heated with stirring at 50 °C. After all of the solid had dissolved, hexane (2.5 mL) was added, and the mixture was allowed to cool to r.t., resulting in the precipitation of a significant quantity of a white solid. Additional hexane (5.5 mL) was added dropwise over 5 min. After 3 h of stirring, the white solid was collected by filtration, washed with pentane (1.5 mL), and dried under reduced pressure to afford phosphepine (*R*)-**1** (0.81 g, 63%) as a white powder.

Mp 219–220 °C (decomp.);

$[\alpha]^{24}_D$ = +148 (c = 1.0, $CHCl_3$);

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.93 (d, *J* = 8.0 Hz, 1H), 7.90 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 7.2 Hz, 2H), 7.64 (s, 1H), 7.33-7.48 (m, 5H), 7.03-7.28 (m, 11H), 6.80-6.86 (m, 2H), 6.50-6.90 (br s, 1H), 3.21 (dd, *J* = 14.4, 4.4 Hz, 1H), 2.96 (dd, *J* = 14.8, 11.6 Hz, 1H), 2.80 (dd, *J* = 11.6, 2.4 Hz, 1H), 2.76 (dd, *J* = 14.4, 11.6 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 141.3 (*J* = 33 Hz), 140.14 (*J* = 5 Hz), 140.12 (*J* = 8 Hz), 136.1 (*J* = 23 Hz), 134.7 (*J* = 5 Hz), 134.0 (*J* = 1 Hz), 132.2, 132.1 (*J* = 2 Hz), 131.66 (*J* = 1 Hz), 131.64 (2C), 131.62, 131.56, 131.4, 131.2, 129.8 (*J* = 5 Hz), 129.5, 129.2 (*J* = 2 Hz), 128.7, 128.23, 128.18, 128.14, 128.12, 128.10, 127.2, 126.63, 126.60, 126.2, 125.9, 125.8, 125.5 (*J* = 1 Hz), 125.2, 28.0 (*J* = 25 Hz), 25.6 (*J* = 16 Hz);

^{31}P NMR ($CDCl_3$, 162 MHz) δ 5.2;

IR (film) 3054, 1587, 1494, 1433, 1328, 1214, 1072, 1026, 1001 cm^{-1};

LRMS (ESI) calcd for $C_{40}H_{30}P$ (M+H) 541.21, found 541.21.

The enantiomeric excess of the phosphepine was determined after oxidation to the phosphine oxide. *tert*-Butyl hydroperoxide (3.7 μL, 11.1 mmol; 3.0 M solution in isooctane) was added to a solution of phosphephine (*R*)-**1** (3.0 mg, 5.5 μmol) in CH_2Cl_2 (1.0 mL). After 5 min of stirring at r.t., an aqueous solution of $Na_2S_2O_3$ (1 mL; 20%) was added, and the resulting mixture was stirred at r.t. for 5 min. The organic phase was separated and then concentrated under reduced pressure. The enantiomeric excess of the phosphine oxide was determined by HPLC analysis [Daicel CHIRALCEL OD-H column; 30% 2-propanol/hexane; 0.8 mL/min; retention times: 6.27 min (*R*), 8.10 min (*S*)].

Mp 281–282 °C;

$[\alpha]^{24}_{D}$ = –64 (c = 1.0, $CHCl_3$);

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.77 (s, 1H), 7.60-8.10 (br s, 1H), 7.43-7.52 (m, 5H), 7.34-7.38 (m, 1H), 7.05-7.31 (m, 12H), 6.77 (br s, 2H), 3.62 (t, *J* = 14.2 Hz, 1H), 3.50 (dd, *J* = 14.6 Hz, 1H), 3.35 (dd, *J* = 22.4, 14.2 Hz, 1H), 3.27 (dd, *J* = 14.6, 9.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 140.9 (*J* = 4 Hz), 140.6, 140.4 (*J* = 5 Hz), 140.0, 135.2 (*J* = 5 Hz), 134.9 (*J* = 4 Hz), 132.3 (*J* = 2 Hz), 132.2 (*J* = 2 Hz), 132.1, 131.7 (*J* = 3 Hz), 131.64 (*J* = 2 Hz), 131.62, 131.2, 130.7 (*J* = 8 Hz), 130.0 (*J* = 2 Hz), 129.32, 129.31 (*J* = 3 Hz), 128.3 (*J* = 11 Hz), 128.23 (*J* = 1 Hz), 128.22 (2C), 128.03 (*J* = 7 Hz), 127.98, 127.94 (*J* = 1 Hz), 127.2, 126.9, 126.65 (*J* = 1 Hz), 126.56 (*J* = 1 Hz), 126.4 (*J* = 1 Hz), 126.3 (*J* = 1 Hz), 126.2 (*J* = 1 Hz), 126.0 (*J* = 1 Hz), 33.1 (*J* = 65 Hz), 29.9 (*J* = 64 Hz);

^{31}P NMR ($CDCl_3$, 162 MHz) δ 53.9;

IR (film) 3054, 1957, 1589, 1493, 1449, 1435, 1418, 1402, 1357, 1331, 1275, 1246, 1230, 1211, 1190, 1161, 1151, 1103, 1078, 1024 cm^{-1};

LRMS (APCI) calcd for $C_{40}H_{29}OP$ (M) 556.63, found 556.70.

X-ray crystal structure of phosphepine (*R*)-**1** (for the sake of simplicity, a solvent molecule (CH_2Cl_2) has been omitted).

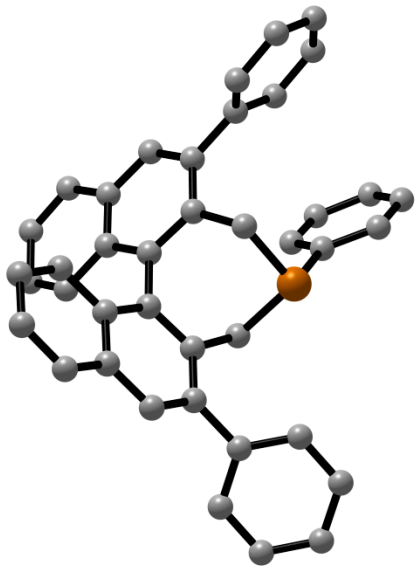


Table 1. Crystal data and structure refinement for d10050.

Identification code	d10050	
Empirical formula	C41 H31 Cl2 P	
Formula weight	625.53	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.2234(2) Å	α= 90°.
	b = 17.7084(5) Å	β= 100.953(2)°.
	c = 9.9464(3) Å	γ = 90°.
Volume	1594.97(7) $Å^3$	
Z	2	
Density (calculated)	1.302 Mg/m^3	
Absorption coefficient	2.516 mm^{-1}	
F(000)	652	
Crystal size	0.45 x 0.20 x 0.15 mm^3	
Theta range for data collection	4.53 to 68.25°.	
Index ranges	-11<=h<=11, -17<=k<=21, -11<=l<=11	
Reflections collected	30883	
Independent reflections	5255 [R(int) = 0.0302]	
Completeness to theta = 68.25°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7040 and 0.3972	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5255 / 1 / 397	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0836	
R indices (all data)	R1 = 0.0330, wR2 = 0.0844	
Absolute structure parameter	0.035(12)	
Largest diff. peak and hole	0.222 and -0.381 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d10050. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	4560(1)	365(1)	6162(1)	18(1)
C(1)	4705(2)	1404(1)	6247(2)	20(1)
C(2)	4827(2)	1831(1)	7444(2)	25(1)
C(3)	4931(3)	2609(1)	7401(2)	30(1)
C(4)	4934(3)	2979(1)	6177(2)	30(1)
C(5)	4807(3)	2561(2)	4978(2)	32(1)
C(6)	4677(2)	1780(1)	5014(2)	28(1)
C(11)	6512(2)	45(1)	6803(2)	18(1)
C(12)	7109(2)	251(1)	8268(2)	18(1)
C(13)	8129(2)	858(1)	8608(2)	18(1)
C(14)	8478(2)	1105(1)	9939(2)	20(1)
C(15)	7844(2)	778(1)	10993(2)	20(1)
C(16)	8136(2)	1060(1)	12352(2)	22(1)
C(17)	7437(2)	764(1)	13333(2)	25(1)
C(18)	6443(2)	161(1)	13002(2)	24(1)
C(19)	6184(2)	-149(1)	11718(2)	22(1)
C(20)	6870(2)	156(1)	10670(2)	19(1)
C(21)	6547(2)	-118(1)	9291(2)	19(1)
C(22)	8865(2)	1212(1)	7547(2)	21(1)
C(23)	8625(2)	1966(1)	7183(2)	27(1)
C(24)	9352(3)	2296(2)	6234(3)	33(1)
C(25)	10327(2)	1877(1)	5625(2)	30(1)
C(26)	10549(2)	1126(1)	5957(2)	26(1)
C(27)	9816(2)	794(1)	6907(2)	22(1)
C(31)	3740(2)	118(1)	7691(2)	19(1)
C(32)	4172(2)	-680(1)	8125(2)	19(1)
C(33)	3230(2)	-1314(1)	7726(2)	21(1)
C(34)	3737(2)	-2027(1)	8096(2)	23(1)
C(35)	5183(2)	-2161(1)	8841(2)	22(1)
C(36)	5741(2)	-2903(1)	9131(2)	26(1)
C(37)	7144(3)	-3016(1)	9841(2)	30(1)

C(38)	8055(2)	-2390(1)	10308(2)	29(1)
C(39)	7562(2)	-1669(1)	10029(2)	24(1)
C(40)	6114(2)	-1528(1)	9281(2)	20(1)
C(41)	5566(2)	-788(1)	8913(2)	18(1)
C(42)	1692(2)	-1230(1)	6913(2)	23(1)
C(43)	1406(2)	-883(1)	5637(2)	25(1)
C(44)	-25(3)	-850(1)	4875(2)	27(1)
C(45)	-1183(2)	-1175(1)	5382(2)	31(1)
C(46)	-914(3)	-1522(1)	6651(3)	31(1)
C(47)	513(2)	-1551(1)	7419(2)	28(1)
C(1S)	1578(4)	9774(2)	868(3)	55(1)
Cl(2S)	2076(1)	10346(1)	2336(1)	58(1)
Cl(1S)	1754(1)	8815(1)	1272(1)	65(1)

Table 3. Bond lengths [Å] and angles [°] for d10050.

P(1)-C(1)	1.845(2)
P(1)-C(31)	1.874(2)
P(1)-C(11)	1.8802(19)
C(1)-C(6)	1.391(3)
C(1)-C(2)	1.397(3)
C(2)-C(3)	1.382(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(11)-C(12)	1.501(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(21)	1.390(3)
C(12)-C(13)	1.425(3)
C(13)-C(14)	1.374(3)
C(13)-C(22)	1.496(3)
C(14)-C(15)	1.417(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.418(3)
C(15)-C(20)	1.420(3)
C(16)-C(17)	1.372(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.405(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.369(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.424(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.433(3)

C(21)-C(41)	1.496(3)
C(22)-C(23)	1.390(3)
C(22)-C(27)	1.392(3)
C(23)-C(24)	1.387(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.389(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.376(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(31)-C(32)	1.508(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(41)	1.386(3)
C(32)-C(33)	1.429(3)
C(33)-C(34)	1.373(3)
C(33)-C(42)	1.500(3)
C(34)-C(35)	1.418(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.421(3)
C(35)-C(40)	1.429(3)
C(36)-C(37)	1.365(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.414(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.366(3)
C(38)-H(38)	0.9500
C(39)-C(40)	1.422(3)
C(39)-H(39)	0.9500
C(40)-C(41)	1.427(3)
C(42)-C(43)	1.390(3)
C(42)-C(47)	1.403(3)
C(43)-C(44)	1.393(3)
C(43)-H(43)	0.9500

C(44)-C(45)	1.390(4)
C(44)-H(44)	0.9500
C(45)-C(46)	1.383(4)
C(45)-H(45)	0.9500
C(46)-C(47)	1.391(3)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(1S)-Cl(1S)	1.747(3)
C(1S)-Cl(2S)	1.765(3)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900

C(1)-P(1)-C(31)	103.50(9)
C(1)-P(1)-C(11)	103.20(9)
C(31)-P(1)-C(11)	99.36(9)
C(6)-C(1)-C(2)	118.5(2)
C(6)-C(1)-P(1)	116.59(16)
C(2)-C(1)-P(1)	124.87(16)
C(3)-C(2)-C(1)	120.5(2)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(2)-C(3)-C(4)	120.7(2)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	119.3(2)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.1(2)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.8(2)
C(5)-C(6)-H(6)	119.6
C(1)-C(6)-H(6)	119.6
C(12)-C(11)-P(1)	114.00(13)
C(12)-C(11)-H(11A)	108.8
P(1)-C(11)-H(11A)	108.8

C(12)-C(11)-H(11B)	108.8
P(1)-C(11)-H(11B)	108.8
H(11A)-C(11)-H(11B)	107.6
C(21)-C(12)-C(13)	120.17(17)
C(21)-C(12)-C(11)	118.46(17)
C(13)-C(12)-C(11)	121.13(17)
C(14)-C(13)-C(12)	119.45(18)
C(14)-C(13)-C(22)	119.43(19)
C(12)-C(13)-C(22)	121.09(17)
C(13)-C(14)-C(15)	121.93(19)
C(13)-C(14)-H(14)	119.0
C(15)-C(14)-H(14)	119.0
C(14)-C(15)-C(16)	122.08(19)
C(14)-C(15)-C(20)	118.84(18)
C(16)-C(15)-C(20)	119.07(18)
C(17)-C(16)-C(15)	120.9(2)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	119.86(19)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(19)-C(18)-C(17)	120.93(19)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(18)-C(19)-C(20)	120.5(2)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(15)-C(20)-C(19)	118.63(18)
C(15)-C(20)-C(21)	119.13(18)
C(19)-C(20)-C(21)	122.15(19)
C(12)-C(21)-C(20)	120.19(18)
C(12)-C(21)-C(41)	118.78(17)
C(20)-C(21)-C(41)	121.00(17)
C(23)-C(22)-C(27)	118.37(19)
C(23)-C(22)-C(13)	121.04(19)
C(27)-C(22)-C(13)	120.59(19)

C(24)-C(23)-C(22)	120.5(2)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	120.6(2)
C(23)-C(24)-H(24)	119.7
C(25)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	119.3(2)
C(26)-C(25)-H(25)	120.3
C(24)-C(25)-H(25)	120.3
C(25)-C(26)-C(27)	120.2(2)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(22)-C(27)-C(26)	121.0(2)
C(22)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(32)-C(31)-P(1)	109.03(13)
C(32)-C(31)-H(31A)	109.9
P(1)-C(31)-H(31A)	109.9
C(32)-C(31)-H(31B)	109.9
P(1)-C(31)-H(31B)	109.9
H(31A)-C(31)-H(31B)	108.3
C(41)-C(32)-C(33)	119.87(19)
C(41)-C(32)-C(31)	117.27(18)
C(33)-C(32)-C(31)	122.83(18)
C(34)-C(33)-C(32)	119.33(19)
C(34)-C(33)-C(42)	118.29(19)
C(32)-C(33)-C(42)	122.39(19)
C(33)-C(34)-C(35)	122.20(19)
C(33)-C(34)-H(34)	118.9
C(35)-C(34)-H(34)	118.9
C(34)-C(35)-C(36)	122.0(2)
C(34)-C(35)-C(40)	118.68(19)
C(36)-C(35)-C(40)	119.34(19)
C(37)-C(36)-C(35)	120.7(2)
C(37)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6

C(36)-C(37)-C(38)	120.1(2)
C(36)-C(37)-H(37)	120.0
C(38)-C(37)-H(37)	120.0
C(39)-C(38)-C(37)	120.8(2)
C(39)-C(38)-H(38)	119.6
C(37)-C(38)-H(38)	119.6
C(38)-C(39)-C(40)	120.9(2)
C(38)-C(39)-H(39)	119.6
C(40)-C(39)-H(39)	119.6
C(39)-C(40)-C(41)	123.14(19)
C(39)-C(40)-C(35)	118.21(19)
C(41)-C(40)-C(35)	118.62(18)
C(32)-C(41)-C(40)	121.18(19)
C(32)-C(41)-C(21)	118.91(18)
C(40)-C(41)-C(21)	119.76(17)
C(43)-C(42)-C(47)	118.8(2)
C(43)-C(42)-C(33)	122.12(19)
C(47)-C(42)-C(33)	119.0(2)
C(42)-C(43)-C(44)	120.7(2)
C(42)-C(43)-H(43)	119.6
C(44)-C(43)-H(43)	119.6
C(45)-C(44)-C(43)	120.0(2)
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.0
C(46)-C(45)-C(44)	119.8(2)
C(46)-C(45)-H(45)	120.1
C(44)-C(45)-H(45)	120.1
C(45)-C(46)-C(47)	120.3(2)
C(45)-C(46)-H(46)	119.8
C(47)-C(46)-H(46)	119.8
C(46)-C(47)-C(42)	120.3(2)
C(46)-C(47)-H(47)	119.8
C(42)-C(47)-H(47)	119.8
Cl(1S)-C(1S)-Cl(2S)	111.67(17)
Cl(1S)-C(1S)-H(1S1)	109.3
Cl(2S)-C(1S)-H(1S1)	109.3

Cl(1S)-C(1S)-H(1S2)	109.3
Cl(2S)-C(1S)-H(1S2)	109.3
H(1S1)-C(1S)-H(1S2)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d10050. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	18(1)	20(1)	16(1)	-2(1)	2(1)	-1(1)
C(1)	16(1)	19(1)	23(1)	1(1)	2(1)	2(1)
C(2)	32(1)	23(1)	21(1)	0(1)	6(1)	0(1)
C(3)	36(1)	26(1)	30(1)	-4(1)	10(1)	1(1)
C(4)	31(1)	19(1)	41(1)	7(1)	11(1)	5(1)
C(5)	36(1)	31(1)	28(1)	10(1)	8(1)	4(1)
C(6)	29(1)	31(1)	23(1)	2(1)	6(1)	4(1)
C(11)	17(1)	18(1)	19(1)	0(1)	3(1)	0(1)
C(12)	16(1)	19(1)	18(1)	0(1)	2(1)	4(1)
C(13)	18(1)	16(1)	20(1)	2(1)	2(1)	4(1)
C(14)	18(1)	17(1)	24(1)	-1(1)	1(1)	0(1)
C(15)	18(1)	20(1)	21(1)	1(1)	0(1)	5(1)
C(16)	21(1)	21(1)	22(1)	-3(1)	0(1)	2(1)
C(17)	28(1)	28(1)	17(1)	-3(1)	-1(1)	6(1)
C(18)	28(1)	27(1)	17(1)	2(1)	4(1)	3(1)
C(19)	22(1)	22(1)	21(1)	1(1)	1(1)	0(1)
C(20)	18(1)	19(1)	20(1)	2(1)	1(1)	4(1)
C(21)	18(1)	17(1)	21(1)	0(1)	2(1)	2(1)
C(22)	19(1)	21(1)	20(1)	-1(1)	-2(1)	-4(1)
C(23)	28(1)	20(1)	31(1)	1(1)	4(1)	-1(1)
C(24)	38(1)	21(1)	40(1)	10(1)	4(1)	-4(1)
C(25)	28(1)	35(1)	25(1)	9(1)	3(1)	-10(1)
C(26)	21(1)	35(1)	23(1)	2(1)	3(1)	-2(1)
C(27)	20(1)	22(1)	25(1)	5(1)	1(1)	-1(1)
C(31)	19(1)	20(1)	20(1)	-2(1)	4(1)	-2(1)
C(32)	21(1)	19(1)	18(1)	-4(1)	7(1)	-1(1)
C(33)	19(1)	23(1)	22(1)	-4(1)	6(1)	-3(1)
C(34)	25(1)	19(1)	26(1)	-3(1)	7(1)	-6(1)
C(35)	28(1)	20(1)	20(1)	0(1)	8(1)	-1(1)
C(36)	33(1)	20(1)	27(1)	0(1)	6(1)	-3(1)
C(37)	38(1)	21(1)	33(1)	4(1)	8(1)	6(1)

C(38)	27(1)	30(1)	28(1)	4(1)	3(1)	4(1)
C(39)	25(1)	24(1)	23(1)	0(1)	4(1)	-2(1)
C(40)	23(1)	22(1)	17(1)	0(1)	8(1)	-1(1)
C(41)	21(1)	20(1)	15(1)	-1(1)	6(1)	-2(1)
C(42)	20(1)	17(1)	30(1)	-9(1)	4(1)	-3(1)
C(43)	23(1)	21(1)	31(1)	-10(1)	4(1)	-1(1)
C(44)	27(1)	20(1)	33(1)	-11(1)	-1(1)	3(1)
C(45)	21(1)	26(1)	43(1)	-15(1)	-2(1)	4(1)
C(46)	22(1)	27(1)	46(1)	-11(1)	9(1)	-3(1)
C(47)	26(1)	24(1)	33(1)	-6(1)	6(1)	-2(1)
C(1S)	70(2)	47(2)	44(2)	7(1)	2(1)	14(2)
Cl(2S)	60(1)	53(1)	60(1)	-3(1)	11(1)	-12(1)
Cl(1S)	85(1)	42(1)	59(1)	5(1)	-7(1)	10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d10050.

	x	y	z	U(eq)
H(2)	4839	1585	8295	30
H(3)	5000	2893	8222	36
H(4)	5023	3513	6156	36
H(5)	4809	2810	4132	38
H(6)	4568	1499	4187	33
H(11A)	6557	-510	6706	21
H(11B)	7155	271	6219	21
H(14)	9164	1507	10160	24
H(16)	8824	1460	12587	26
H(17)	7625	965	14235	30
H(18)	5944	-34	13679	29
H(19)	5542	-571	11524	27
H(23)	7957	2258	7588	32
H(24)	9183	2812	5997	40
H(25)	10835	2107	4986	36
H(26)	11204	834	5538	32
H(27)	9968	274	7121	27
H(31A)	4106	471	8451	23
H(31B)	2651	161	7458	23
H(34)	3097	-2445	7844	28
H(36)	5132	-3326	8827	32
H(37)	7508	-3514	10022	36
H(38)	9021	-2473	10821	35
H(39)	8196	-1256	10338	29
H(43)	2196	-665	5280	30
H(44)	-210	-606	4009	33
H(45)	-2158	-1159	4859	37
H(46)	-1706	-1742	7000	38
H(47)	689	-1789	8291	33
H(1S1)	542	9883	430	66

H(1S2)	2215	9899	202	66

VII. Determination of the Absolute Configurations of the Products

Absolute configuration of the products from cycloaddition of 5-methylenehydantoin: Product of Table 2, entry 3, derived from catalyst (*S*)-**1**.

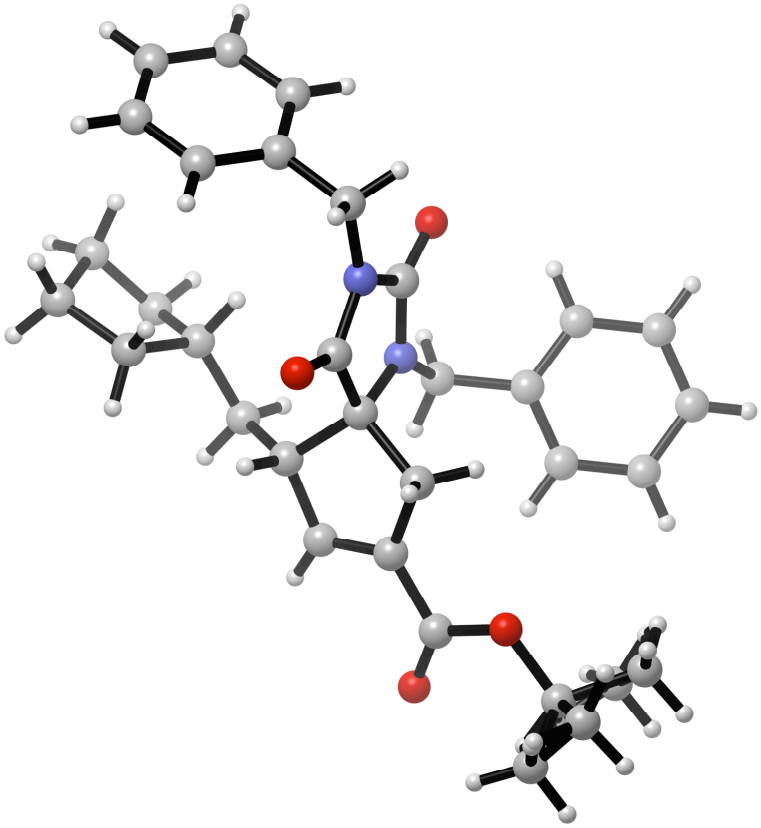


Table 1. Crystal data and structure refinement for x11029.

Identification code	x11029	
Empirical formula	C31 H36 N2 O4	
Formula weight	500.62	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.3572(3) Å	a= 90°.
	b = 12.4724(4) Å	b= 90°.
	c = 26.0754(8) Å	g = 90°.
Volume	2717.95(16) Å^3	
Z	4	

Density (calculated)	1.223 Mg/m^3
Absorption coefficient	0.643 mm^{-1}
F(000)	1072
Crystal size	0.25 x 0.20 x 0.15 mm^3
Theta range for data collection	3.39 to 67.73°.
Index ranges	-9<=h<=10, -14<=k<=14, -30<=l<=31
Reflections collected	29588
Independent reflections	4852 [R(int) = 0.0298]
Completeness to theta = 67.73°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9096 and 0.8557
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4852 / 31 / 355
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0653
R indices (all data)	R1 = 0.0256, wR2 = 0.0657
Absolute structure parameter	-0.02(12)
Largest diff. peak and hole	0.188 and -0.131 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for x11029. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	11748(1)	-1619(1)	369(1)	21(1)
O(2)	9906(1)	1077(1)	1392(1)	26(1)
O(4)	6882(1)	-16(1)	-1362(1)	27(1)
N(1)	11117(1)	-343(1)	973(1)	16(1)
N(2)	8980(1)	417(1)	621(1)	16(1)
C(1)	9458(1)	-414(1)	257(1)	15(1)
C(2)	8148(1)	-1287(1)	151(1)	17(1)
C(3)	7481(1)	-943(1)	-358(1)	19(1)
C(4)	8404(1)	-231(1)	-595(1)	18(1)
C(5)	9873(1)	37(1)	-284(1)	17(1)
C(6)	10918(1)	-891(1)	526(1)	16(1)
C(7)	9956(1)	466(1)	1032(1)	18(1)
C(8)	6898(1)	-1487(1)	568(1)	19(1)
C(9)	7520(1)	-1986(1)	1064(1)	19(1)
C(10)	6166(2)	-2197(1)	1449(1)	27(1)
C(11)	6867(2)	-3021(1)	1812(1)	30(1)
C(12)	7736(2)	-3792(1)	1452(1)	30(1)
C(13)	8311(2)	-3102(1)	999(1)	21(1)
C(14)	8050(1)	209(1)	-1111(1)	20(1)
O(3)	9186(1)	906(1)	-1259(1)	25(1)
C(15)	8961(2)	1434(1)	-1755(1)	28(1)
C(16)	9504(3)	718(2)	-2176(1)	40(1)
C(17)	9935(2)	2474(1)	-1719(1)	39(1)
C(16A)	10536(15)	1320(14)	-2025(5)	58(5)
C(17A)	8264(19)	2430(9)	-1658(4)	53(4)
C(18)	12371(1)	-543(1)	1353(1)	20(1)
C(19)	11779(1)	-1180(1)	1807(1)	19(1)
C(20)	11146(2)	-664(1)	2235(1)	25(1)
C(21)	10578(2)	-1249(1)	2648(1)	32(1)
C(22)	10651(2)	-2362(1)	2638(1)	32(1)
C(23)	11283(2)	-2879(1)	2216(1)	29(1)

C(24)	11840(2)	-2296(1)	1801(1)	23(1)
C(25)	7629(1)	1161(1)	565(1)	19(1)
C(26)	8071(1)	2271(1)	378(1)	19(1)
C(27)	8659(1)	3045(1)	713(1)	22(1)
C(28)	9037(2)	4064(1)	538(1)	27(1)
C(29)	8837(2)	4318(1)	25(1)	29(1)
C(30)	8252(2)	3556(1)	-311(1)	29(1)
C(31)	7866(2)	2536(1)	-136(1)	24(1)

Table 3. Bond lengths [Å] and angles [°] for x11029.

O(1)-C(6)	1.2134(14)
O(2)-C(7)	1.2114(14)
O(4)-C(14)	1.2090(15)
N(1)-C(6)	1.3614(14)
N(1)-C(7)	1.4081(15)
N(1)-C(18)	1.4638(14)
N(2)-C(7)	1.3487(15)
N(2)-C(1)	1.4605(14)
N(2)-C(25)	1.4689(14)
C(1)-C(6)	1.5276(15)
C(1)-C(5)	1.5576(15)
C(1)-C(2)	1.5681(15)
C(2)-C(3)	1.5022(15)
C(2)-C(8)	1.5296(16)
C(2)-H(2)	1.0000
C(3)-C(4)	1.3288(17)
C(3)-H(3)	0.9500
C(4)-C(14)	1.4823(16)
C(4)-C(5)	1.5084(15)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(8)-C(9)	1.5255(16)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.5349(16)
C(9)-C(13)	1.5492(16)
C(9)-H(9)	1.0000
C(10)-C(11)	1.5159(18)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5284(19)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5382(16)

C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-O(3)	1.3439(15)
O(3)-C(15)	1.4644(14)
C(15)-C(17A)	1.395(10)
C(15)-C(16)	1.485(2)
C(15)-C(16A)	1.499(10)
C(15)-C(17)	1.534(2)
C(15)-H(15A)	1.0000
C(15)-H(15B)	1.0000
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(16A)-H(16D)	0.9800
C(16A)-H(16E)	0.9800
C(16A)-H(16F)	0.9800
C(17A)-H(17D)	0.9800
C(17A)-H(17E)	0.9800
C(17A)-H(17F)	0.9800
C(18)-C(19)	1.5094(16)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.3919(17)
C(19)-C(24)	1.3931(18)
C(20)-C(21)	1.3844(18)
C(20)-H(20)	0.9500
C(21)-C(22)	1.390(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.381(2)
C(22)-H(22)	0.9500
C(23)-C(24)	1.3841(18)

C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.5133(16)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(31)	1.3909(17)
C(26)-C(27)	1.3932(17)
C(27)-C(28)	1.3875(18)
C(27)-H(27)	0.9500
C(28)-C(29)	1.383(2)
C(28)-H(28)	0.9500
C(29)-C(30)	1.382(2)
C(29)-H(29)	0.9500
C(30)-C(31)	1.3900(18)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500

C(6)-N(1)-C(7)	111.61(9)
C(6)-N(1)-C(18)	125.58(9)
C(7)-N(1)-C(18)	122.80(9)
C(7)-N(2)-C(1)	112.50(9)
C(7)-N(2)-C(25)	121.01(9)
C(1)-N(2)-C(25)	126.47(9)
N(2)-C(1)-C(6)	101.34(9)
N(2)-C(1)-C(5)	113.07(9)
C(6)-C(1)-C(5)	112.23(9)
N(2)-C(1)-C(2)	114.63(9)
C(6)-C(1)-C(2)	111.64(9)
C(5)-C(1)-C(2)	104.23(8)
C(3)-C(2)-C(8)	114.98(10)
C(3)-C(2)-C(1)	102.57(9)
C(8)-C(2)-C(1)	117.62(9)
C(3)-C(2)-H(2)	107.0
C(8)-C(2)-H(2)	107.0
C(1)-C(2)-H(2)	107.0
C(4)-C(3)-C(2)	112.65(10)

C(4)-C(3)-H(3)	123.7
C(2)-C(3)-H(3)	123.7
C(3)-C(4)-C(14)	123.53(11)
C(3)-C(4)-C(5)	111.78(10)
C(14)-C(4)-C(5)	124.65(10)
C(4)-C(5)-C(1)	103.05(9)
C(4)-C(5)-H(5A)	111.2
C(1)-C(5)-H(5A)	111.2
C(4)-C(5)-H(5B)	111.2
C(1)-C(5)-H(5B)	111.2
H(5A)-C(5)-H(5B)	109.1
O(1)-C(6)-N(1)	126.41(11)
O(1)-C(6)-C(1)	126.39(10)
N(1)-C(6)-C(1)	107.20(9)
O(2)-C(7)-N(2)	128.67(11)
O(2)-C(7)-N(1)	124.00(10)
N(2)-C(7)-N(1)	107.33(9)
C(9)-C(8)-C(2)	115.93(10)
C(9)-C(8)-H(8A)	108.3
C(2)-C(8)-H(8A)	108.3
C(9)-C(8)-H(8B)	108.3
C(2)-C(8)-H(8B)	108.3
H(8A)-C(8)-H(8B)	107.4
C(8)-C(9)-C(10)	111.87(10)
C(8)-C(9)-C(13)	114.78(9)
C(10)-C(9)-C(13)	103.44(9)
C(8)-C(9)-H(9)	108.8
C(10)-C(9)-H(9)	108.8
C(13)-C(9)-H(9)	108.8
C(11)-C(10)-C(9)	103.88(10)
C(11)-C(10)-H(10A)	111.0
C(9)-C(10)-H(10A)	111.0
C(11)-C(10)-H(10B)	111.0
C(9)-C(10)-H(10B)	111.0
H(10A)-C(10)-H(10B)	109.0
C(10)-C(11)-C(12)	103.03(10)

C(10)-C(11)-H(11A)	111.2
C(12)-C(11)-H(11A)	111.2
C(10)-C(11)-H(11B)	111.2
C(12)-C(11)-H(11B)	111.2
H(11A)-C(11)-H(11B)	109.1
C(11)-C(12)-C(13)	105.57(10)
C(11)-C(12)-H(12A)	110.6
C(13)-C(12)-H(12A)	110.6
C(11)-C(12)-H(12B)	110.6
C(13)-C(12)-H(12B)	110.6
H(12A)-C(12)-H(12B)	108.8
C(12)-C(13)-C(9)	106.57(10)
C(12)-C(13)-H(13A)	110.4
C(9)-C(13)-H(13A)	110.4
C(12)-C(13)-H(13B)	110.4
C(9)-C(13)-H(13B)	110.4
H(13A)-C(13)-H(13B)	108.6
O(4)-C(14)-O(3)	124.35(10)
O(4)-C(14)-C(4)	124.59(11)
O(3)-C(14)-C(4)	111.05(10)
C(14)-O(3)-C(15)	117.04(9)
C(17A)-C(15)-O(3)	107.1(5)
C(17A)-C(15)-C(16)	142.9(5)
O(3)-C(15)-C(16)	110.01(11)
C(17A)-C(15)-C(16A)	122.5(9)
O(3)-C(15)-C(16A)	105.0(4)
C(16)-C(15)-C(16A)	47.8(7)
C(17A)-C(15)-C(17)	57.2(7)
O(3)-C(15)-C(17)	104.94(11)
C(16)-C(15)-C(17)	113.10(14)
C(16A)-C(15)-C(17)	69.1(7)
C(17A)-C(15)-H(15A)	54.8
O(3)-C(15)-H(15A)	109.6
C(16)-C(15)-H(15A)	109.6
C(16A)-C(15)-H(15A)	144.2
C(17)-C(15)-H(15A)	109.6

C(17A)-C(15)-H(15B)	107.2
O(3)-C(15)-H(15B)	107.2
C(16)-C(15)-H(15B)	60.1
C(16A)-C(15)-H(15B)	107.2
C(17)-C(15)-H(15B)	147.4
H(15A)-C(15)-H(15B)	53.7
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
C(15)-C(16A)-H(16D)	109.5
C(15)-C(16A)-H(16E)	109.5
H(16D)-C(16A)-H(16E)	109.5
C(15)-C(16A)-H(16F)	109.5
H(16D)-C(16A)-H(16F)	109.5
H(16E)-C(16A)-H(16F)	109.5
C(15)-C(17A)-H(17D)	109.5
C(15)-C(17A)-H(17E)	109.5
H(17D)-C(17A)-H(17E)	109.5
C(15)-C(17A)-H(17F)	109.5
H(17D)-C(17A)-H(17F)	109.5
H(17E)-C(17A)-H(17F)	109.5
N(1)-C(18)-C(19)	112.73(10)
N(1)-C(18)-H(18A)	109.0
C(19)-C(18)-H(18A)	109.0
N(1)-C(18)-H(18B)	109.0
C(19)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
C(20)-C(19)-C(24)	119.01(11)
C(20)-C(19)-C(18)	120.65(11)
C(24)-C(19)-C(18)	120.34(11)
C(21)-C(20)-C(19)	120.65(12)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7

C(20)-C(21)-C(22)	119.83(13)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	119.84(12)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.40(12)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	120.26(12)
C(23)-C(24)-H(24)	119.9
C(19)-C(24)-H(24)	119.9
N(2)-C(25)-C(26)	114.96(9)
N(2)-C(25)-H(25A)	108.5
C(26)-C(25)-H(25A)	108.5
N(2)-C(25)-H(25B)	108.5
C(26)-C(25)-H(25B)	108.5
H(25A)-C(25)-H(25B)	107.5
C(31)-C(26)-C(27)	118.94(11)
C(31)-C(26)-C(25)	119.88(11)
C(27)-C(26)-C(25)	121.17(11)
C(28)-C(27)-C(26)	120.53(12)
C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(29)-C(28)-C(27)	120.04(12)
C(29)-C(28)-H(28)	120.0
C(27)-C(28)-H(28)	120.0
C(30)-C(29)-C(28)	119.96(12)
C(30)-C(29)-H(29)	120.0
C(28)-C(29)-H(29)	120.0
C(29)-C(30)-C(31)	120.16(12)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(30)-C(31)-C(26)	120.37(12)
C(30)-C(31)-H(31)	119.8
C(26)-C(31)-H(31)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for x11029. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	18(1)	21(1)	0(1)	1(1)	5(1)
O(2)	38(1)	21(1)	18(1)	-6(1)	-4(1)	5(1)
O(4)	29(1)	33(1)	20(1)	3(1)	-8(1)	-4(1)
N(1)	19(1)	16(1)	15(1)	2(1)	-1(1)	2(1)
N(2)	19(1)	13(1)	17(1)	-1(1)	-1(1)	2(1)
C(1)	18(1)	13(1)	15(1)	-1(1)	1(1)	0(1)
C(2)	20(1)	13(1)	18(1)	-1(1)	-1(1)	-1(1)
C(3)	20(1)	17(1)	19(1)	-4(1)	-3(1)	0(1)
C(4)	20(1)	16(1)	17(1)	-2(1)	0(1)	1(1)
C(5)	19(1)	16(1)	16(1)	1(1)	-1(1)	0(1)
C(6)	19(1)	13(1)	15(1)	3(1)	2(1)	-2(1)
C(7)	22(1)	15(1)	15(1)	2(1)	1(1)	-1(1)
C(8)	18(1)	17(1)	22(1)	0(1)	1(1)	-2(1)
C(9)	21(1)	17(1)	19(1)	0(1)	3(1)	-1(1)
C(10)	27(1)	30(1)	24(1)	4(1)	7(1)	5(1)
C(11)	33(1)	34(1)	23(1)	6(1)	6(1)	-1(1)
C(12)	40(1)	23(1)	26(1)	6(1)	3(1)	2(1)
C(13)	23(1)	19(1)	21(1)	0(1)	2(1)	3(1)
C(14)	21(1)	20(1)	17(1)	-2(1)	-1(1)	2(1)
O(3)	24(1)	32(1)	18(1)	8(1)	-2(1)	-2(1)
C(15)	30(1)	36(1)	20(1)	11(1)	-2(1)	0(1)
C(16)	55(1)	46(1)	21(1)	8(1)	4(1)	4(1)
C(17)	47(1)	38(1)	31(1)	14(1)	-2(1)	-8(1)
C(16A)	53(8)	84(11)	38(7)	38(7)	9(6)	25(8)
C(17A)	75(9)	51(7)	34(6)	19(5)	8(6)	27(7)
C(18)	19(1)	22(1)	18(1)	3(1)	-4(1)	-1(1)
C(19)	18(1)	22(1)	17(1)	3(1)	-5(1)	-2(1)
C(20)	32(1)	23(1)	21(1)	1(1)	-1(1)	0(1)
C(21)	38(1)	39(1)	18(1)	0(1)	3(1)	-2(1)
C(22)	36(1)	38(1)	23(1)	13(1)	-2(1)	-8(1)
C(23)	32(1)	24(1)	32(1)	10(1)	-4(1)	-2(1)

C(24)	22(1)	24(1)	22(1)	1(1)	-3(1)	2(1)
C(25)	17(1)	17(1)	22(1)	-1(1)	0(1)	2(1)
C(26)	16(1)	16(1)	25(1)	0(1)	2(1)	5(1)
C(27)	20(1)	20(1)	27(1)	0(1)	-2(1)	3(1)
C(28)	19(1)	18(1)	44(1)	-3(1)	-1(1)	2(1)
C(29)	20(1)	18(1)	49(1)	10(1)	10(1)	6(1)
C(30)	29(1)	28(1)	28(1)	10(1)	7(1)	12(1)
C(31)	26(1)	21(1)	25(1)	0(1)	0(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for x11029.

	x	y	z	U(eq)
H(2)	8721	-1980	93	20
H(3)	6504	-1207	-496	23
H(5A)	10054	821	-271	20
H(5B)	10836	-316	-427	20
H(8A)	6384	-795	654	23
H(8B)	6060	-1962	426	23
H(9)	8312	-1486	1223	23
H(10A)	5873	-1533	1634	32
H(10B)	5205	-2483	1274	32
H(11A)	6016	-3394	2006	36
H(11B)	7621	-2684	2057	36
H(12A)	7002	-4362	1331	36
H(12B)	8656	-4131	1627	36
H(13A)	7985	-3430	669	25
H(13B)	9492	-3035	1003	25
H(15A)	7804	1611	-1804	34
H(15B)	8162	1001	-1951	34
H(16A)	10635	538	-2125	61
H(16B)	9371	1083	-2506	61
H(16C)	8865	59	-2173	61
H(17A)	9572	2891	-1422	58
H(17B)	9783	2896	-2032	58
H(17C)	11072	2300	-1679	58
H(16D)	10720	563	-2108	87
H(16E)	11396	1578	-1801	87
H(16F)	10521	1743	-2342	87
H(17D)	7223	2326	-1492	80
H(17E)	8118	2816	-1982	80
H(17F)	8962	2846	-1431	80
H(18A)	12797	152	1475	24

H(18B)	13259	-938	1188	24
H(20)	11104	97	2244	30
H(21)	10139	-890	2937	38
H(22)	10267	-2766	2922	39
H(23)	11335	-3640	2210	35
H(24)	12266	-2659	1511	27
H(25A)	7088	1230	901	23
H(25B)	6850	846	322	23
H(27)	8801	2875	1065	27
H(28)	9435	4588	769	32
H(29)	9101	5014	-95	35
H(30)	8113	3731	-663	34
H(31)	7459	2017	-369	28

Absolute configuration of the products from cycloaddition of the phthalimide-substituted olefin: Product of eq 6, derived from catalyst (*S*)-**1**.

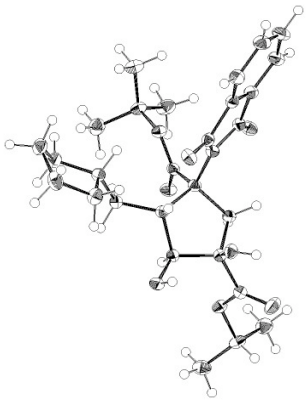


Table 1. Crystal data and structure refinement for D11023.

Identification code	d11023	
Empirical formula	C28 H37.25 N O8.12	
Formula weight	517.84	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 12.00440(10) Å	α= 65.2090(10)°.
	b = 15.5921(2) Å	β= 76.5250(10)°.
	c = 16.7986(2) Å	γ = 89.3110(10)°.
Volume	2762.81(5) $Å^3$	
Z	4	
Density (calculated)	1.245 Mg/m^3	
Absorption coefficient	0.751 mm^{-1}	
F(000)	1109	
Crystal size	0.35 x 0.30 x 0.25 mm^3	
Theta range for data collection	2.99 to 69.31°.	
Index ranges	-14<=h<=14, -15<=k<=18, -20<=l<=20	
Reflections collected	65881	
Independent reflections	17035 [R(int) = 0.0221]	
Completeness to theta = 69.31°	97.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8345 and 0.7791	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17035 / 660 / 1523
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0807
R indices (all data)	R1 = 0.0307, wR2 = 0.0810
Absolute structure parameter	0.06(6)
Largest diff. peak and hole	0.372 and -0.286 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for D11023. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2785(1)	8360(1)	4187(1)	18(1)
C(6)	3794(1)	9015(1)	3415(1)	19(1)
O(1)	4416(1)	8752(1)	2908(1)	24(1)
O(2)	3800(1)	9894(1)	3358(1)	20(1)
C(7)	4710(1)	10648(1)	2688(1)	23(1)
C(8)	4464(2)	11440(1)	2982(1)	33(1)
C(9)	4558(2)	10936(1)	1742(1)	31(1)
C(10)	5893(1)	10319(1)	2775(1)	32(1)
N(1)	2520(1)	8691(1)	4909(1)	19(1)
C(11)	3419(1)	8812(1)	5272(1)	20(1)
O(3)	4394(1)	8637(1)	5046(1)	25(1)
C(12)	2922(1)	9177(1)	5950(1)	22(1)
C(13)	3433(2)	9423(1)	6497(1)	26(1)
C(14)	2725(2)	9756(1)	7071(1)	30(1)
C(15)	1564(2)	9832(1)	7094(1)	29(1)
C(16)	1054(1)	9567(1)	6552(1)	25(1)
C(17)	1766(1)	9242(1)	5984(1)	22(1)
C(18)	1476(1)	8909(1)	5337(1)	20(1)
O(4)	535(1)	8843(1)	5215(1)	25(1)
C(2)	1758(1)	8332(1)	3756(1)	18(1)
C(19)	1682(1)	9184(1)	2874(1)	20(1)
C(20)	872(1)	9892(1)	3027(1)	22(1)
C(21)	913(2)	10806(1)	2170(1)	26(1)
C(22)	-205(2)	11211(1)	2425(1)	31(1)
C(23)	-1092(2)	10337(1)	2902(1)	31(1)
C(24)	-411(1)	9497(1)	3358(1)	28(1)
C(3)	1828(1)	7399(1)	3661(1)	19(1)
O(5)	765(1)	7087(1)	3586(1)	24(1)
C(4)	2142(1)	6718(1)	4530(1)	19(1)
O(6)	1141(1)	6574(1)	5224(1)	23(1)
C(25)	2520(1)	5776(1)	4560(1)	22(1)

O(7)	2303(1)	5046(1)	5247(1)	39(1)
O(8)	3146(1)	5858(1)	3761(1)	22(1)
C(26)	3588(1)	4988(1)	3714(1)	24(1)
C(27)	3567(2)	5066(1)	2792(1)	29(1)
C(28)	4779(2)	4927(1)	3884(1)	30(1)
C(5)	3114(1)	7316(1)	4574(1)	20(1)
C(101)	2049(1)	3578(1)	7845(1)	19(1)
C(106)	2779(1)	2967(1)	8485(1)	21(1)
O(101)	3226(1)	3259(1)	8909(1)	26(1)
O(102)	2771(1)	2089(1)	8542(1)	21(1)
C(107)	3465(1)	1387(1)	9074(1)	23(1)
C(108)	3364(2)	596(1)	8784(1)	29(1)
C(109)	2895(2)	1059(1)	10077(1)	32(1)
C(110)	4711(1)	1790(1)	8812(1)	29(1)
N(101)	2086(1)	3235(1)	7145(1)	18(1)
C(111)	3172(1)	3167(1)	6649(1)	20(1)
O(103)	4079(1)	3387(1)	6752(1)	23(1)
C(112)	2974(1)	2804(1)	6006(1)	20(1)
C(113)	3752(1)	2582(1)	5388(1)	23(1)
C(114)	3301(1)	2282(1)	4844(1)	26(1)
C(115)	2125(2)	2212(1)	4920(1)	27(1)
C(116)	1345(1)	2441(1)	5544(1)	25(1)
C(117)	1803(1)	2727(1)	6091(1)	20(1)
C(118)	1204(1)	3020(1)	6812(1)	20(1)
O(104)	187(1)	3047(1)	7062(1)	27(1)
C(102)	813(1)	3553(1)	8443(1)	20(1)
C(119)	364(1)	2680(1)	9354(1)	22(1)
C(120)	-281(2)	1870(1)	9313(1)	27(1)
C(121)	-632(7)	998(6)	10244(6)	37(2)
C(122)	-1569(8)	437(5)	10135(7)	44(2)
C(123)	-2267(4)	1180(4)	9603(4)	42(1)
C(124)	-1502(5)	2128(6)	9154(6)	30(1)
C(21B)	-459(14)	934(10)	10179(11)	28(2)
C(22B)	-1656(13)	480(10)	10304(13)	36(3)
C(23B)	-2301(7)	1339(7)	9911(9)	44(2)
C(24B)	-1426(10)	2042(13)	9066(12)	35(3)

C(103)	887(1)	4472(1)	8560(1)	21(1)
O(105)	-242(1)	4693(1)	8832(1)	24(1)
C(104)	1562(1)	5189(1)	7612(1)	20(1)
O(106)	895(1)	5357(1)	6982(1)	22(1)
O(107)	1798(1)	6902(1)	7062(1)	32(1)
C(125)	1986(1)	6128(1)	7576(1)	22(1)
O(108)	2592(1)	5982(1)	8186(1)	29(1)
C(126)	3114(13)	6837(8)	8180(8)	32(2)
C(127)	4284(15)	7095(17)	7523(13)	38(2)
C(128)	3170(20)	6577(12)	9146(9)	55(3)
C(26B)	3260(30)	6789(17)	8146(15)	32(3)
C(27B)	4350(30)	7040(30)	7410(20)	36(4)
C(28B)	3450(20)	6450(20)	9087(14)	45(4)
C(105)	2553(1)	4640(1)	7392(1)	21(1)
C(201)	7247(1)	8072(1)	8568(1)	20(1)
C(206)	6276(1)	7697(1)	9453(1)	20(1)
O(201)	5862(1)	6884(1)	9823(1)	27(1)
O(202)	6044(1)	8358(1)	9755(1)	22(1)
C(207)	5248(1)	8126(1)	10659(1)	25(1)
C(208)	5256(2)	9075(1)	10706(1)	36(1)
C(209)	5739(2)	7402(1)	11403(1)	31(1)
C(210)	4057(2)	7789(2)	10675(1)	36(1)
N(201)	7250(1)	9109(1)	8061(1)	20(1)
C(211)	6293(1)	9480(1)	7724(1)	20(1)
O(203)	5440(1)	9004(1)	7820(1)	24(1)
C(212)	6548(1)	10530(1)	7274(1)	20(1)
C(213)	5926(1)	11236(1)	6804(1)	22(1)
C(214)	6382(1)	12173(1)	6484(1)	25(1)
C(215)	7429(2)	12389(1)	6616(1)	27(1)
C(216)	8055(1)	11671(1)	7081(1)	24(1)
C(217)	7586(1)	10746(1)	7407(1)	21(1)
C(218)	8038(1)	9842(1)	7940(1)	20(1)
O(204)	8895(1)	9767(1)	8213(1)	26(1)
C(202)	8415(1)	7762(1)	8827(1)	20(1)
C(219)	8445(1)	7655(1)	9775(1)	23(1)
C(220)	9578(1)	7416(1)	10043(1)	27(1)

C(221)	9482(2)	7299(2)	11010(1)	36(1)
C(222)	10689(5)	7467(6)	11053(4)	49(1)
C(223)	11161(8)	8318(6)	10153(4)	67(2)
C(22C)	11390(10)	8050(12)	10059(8)	49(1)
C(23C)	10746(13)	7360(20)	11013(13)	67(2)
C(224)	10587(2)	8191(2)	9469(1)	42(1)
C(203)	8568(1)	6854(1)	8688(1)	22(1)
O(205)	9714(1)	6593(1)	8606(1)	26(1)
C(204)	8164(1)	7079(1)	7822(1)	23(1)
O(206)	9025(1)	7736(1)	7086(1)	31(1)
C(225)	8065(6)	6232(5)	7641(5)	23(1)
O(207)	8771(4)	6112(5)	7062(4)	31(1)
O(208)	7162(6)	5627(4)	8208(5)	28(1)
C(226)	7057(7)	4699(3)	8174(5)	36(1)
C(227)	6211(8)	4077(3)	9059(5)	51(2)
C(228)	6637(7)	4809(6)	7354(5)	51(2)
C(25C)	7878(17)	6041(14)	7815(15)	21(2)
O(07C)	8556(10)	5785(10)	7341(10)	28(2)
O(08C)	6894(17)	5582(12)	8362(15)	31(2)
C(26C)	6641(15)	4607(8)	8450(9)	32(2)
C(27C)	5709(16)	4136(9)	9313(9)	51(3)
C(28C)	6290(20)	4704(16)	7615(11)	56(4)
C(205)	7073(1)	7556(1)	7976(1)	22(1)
C(301)	8365(1)	3891(1)	3516(1)	18(1)
C(306)	7838(1)	4274(1)	2690(1)	18(1)
O(301)	7511(1)	5053(1)	2414(1)	23(1)
O(302)	7875(1)	3670(1)	2313(1)	19(1)
C(307)	7346(1)	3880(1)	1546(1)	21(1)
C(308)	7515(2)	2992(1)	1390(1)	27(1)
C(309)	7994(2)	4749(1)	720(1)	27(1)
C(310)	6080(1)	4008(1)	1823(1)	26(1)
N(301)	8177(1)	2838(1)	3962(1)	18(1)
C(311)	7059(1)	2399(1)	4196(1)	19(1)
O(303)	6224(1)	2827(1)	4047(1)	22(1)
C(312)	7122(1)	1359(1)	4648(1)	19(1)
C(313)	6295(1)	601(1)	4970(1)	22(1)

C(314)	6632(1)	-308(1)	5366(1)	24(1)
C(315)	7762(1)	-448(1)	5446(1)	25(1)
C(316)	8588(1)	321(1)	5122(1)	23(1)
C(317)	8244(1)	1216(1)	4719(1)	19(1)
C(318)	8940(1)	2157(1)	4282(1)	20(1)
O(304)	9951(1)	2288(1)	4217(1)	25(1)
C(302)	9661(1)	4305(1)	3185(1)	19(1)
C(319)	10295(1)	4552(1)	2196(1)	21(1)
C(320)	10699(1)	3715(1)	1994(1)	22(1)
C(321)	11095(1)	4016(1)	953(1)	28(1)
C(322)	12283(2)	3666(1)	774(1)	33(1)
C(323)	12789(1)	3720(1)	1511(1)	32(1)
C(324)	11770(1)	3325(1)	2350(1)	25(1)
C(303)	9632(1)	5170(1)	3391(1)	19(1)
O(305)	10746(1)	5408(1)	3423(1)	24(1)
C(304)	8734(1)	4835(1)	4319(1)	20(1)
O(306)	9187(1)	4175(1)	5019(1)	23(1)
O(307)	8734(1)	5861(1)	5054(1)	31(1)
C(325)	8382(1)	5675(1)	4524(1)	21(1)
O(308)	7718(1)	6201(1)	4013(1)	31(1)
C(326)	7397(6)	7079(3)	4093(3)	38(1)
C(327)	7226(11)	7745(4)	3191(4)	75(2)
C(328)	6336(5)	6839(7)	4867(4)	62(1)
C(26D)	7110(60)	6970(40)	4180(30)	38(1)
C(27D)	6750(110)	7550(60)	3320(50)	75(2)
C(28D)	6130(50)	6510(80)	5010(40)	62(1)
C(305)	7779(1)	4304(1)	4190(1)	20(1)
O(1W)	8833(4)	7435(3)	5561(3)	72(1)

Table 3. Bond lengths [Å] and angles [°] for D11023.

C(1)-N(1)	1.477(2)
C(1)-C(6)	1.5423(19)
C(1)-C(5)	1.564(2)
C(1)-C(2)	1.5780(19)
C(6)-O(1)	1.200(2)
C(6)-O(2)	1.3335(19)
O(2)-C(7)	1.4796(18)
C(7)-C(8)	1.514(3)
C(7)-C(9)	1.515(2)
C(7)-C(10)	1.523(2)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
N(1)-C(18)	1.407(2)
N(1)-C(11)	1.4073(19)
C(11)-O(3)	1.209(2)
C(11)-C(12)	1.482(2)
C(12)-C(17)	1.380(2)
C(12)-C(13)	1.390(2)
C(13)-C(14)	1.396(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.390(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.399(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.492(2)

C(18)-O(4)	1.2080(19)
C(2)-C(3)	1.528(2)
C(2)-C(19)	1.542(2)
C(2)-H(2)	1.0000
C(19)-C(20)	1.525(2)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.535(2)
C(20)-C(24)	1.549(2)
C(20)-H(20)	1.0000
C(21)-C(22)	1.524(2)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.535(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.547(2)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(3)-O(5)	1.4217(17)
C(3)-C(4)	1.5322(19)
C(3)-H(3)	1.0000
O(5)-H(5)	0.845(16)
C(4)-O(6)	1.4090(18)
C(4)-C(25)	1.518(2)
C(4)-C(5)	1.535(2)
O(6)-H(6)	0.824(16)
C(25)-O(7)	1.208(2)
C(25)-O(8)	1.331(2)
O(8)-C(26)	1.476(2)
C(26)-C(27)	1.508(2)
C(26)-C(28)	1.516(2)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800

C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(101)-N(101)	1.472(2)
C(101)-C(106)	1.547(2)
C(101)-C(105)	1.562(2)
C(101)-C(102)	1.577(2)
C(106)-O(101)	1.207(2)
C(106)-O(102)	1.332(2)
O(102)-C(107)	1.4821(18)
C(107)-C(108)	1.519(2)
C(107)-C(110)	1.519(2)
C(107)-C(109)	1.522(2)
C(108)-H(10D)	0.9800
C(108)-H(10E)	0.9800
C(108)-H(10F)	0.9800
C(109)-H(10G)	0.9800
C(109)-H(10H)	0.9800
C(109)-H(10I)	0.9800
C(110)-H(11A)	0.9800
C(110)-H(11B)	0.9800
C(110)-H(11C)	0.9800
N(101)-C(111)	1.4028(19)
N(101)-C(118)	1.4109(19)
C(111)-O(103)	1.2163(19)
C(111)-C(112)	1.476(2)
C(112)-C(117)	1.380(2)
C(112)-C(113)	1.382(2)
C(113)-C(114)	1.395(2)
C(113)-H(113)	0.9500
C(114)-C(115)	1.389(2)
C(114)-H(114)	0.9500

C(115)-C(116)	1.397(2)
C(115)-H(115)	0.9500
C(116)-C(117)	1.390(2)
C(116)-H(116)	0.9500
C(117)-C(118)	1.498(2)
C(118)-O(104)	1.2014(19)
C(102)-C(103)	1.532(2)
C(102)-C(119)	1.539(2)
C(102)-H(102)	1.0000
C(119)-C(120)	1.523(2)
C(119)-H(11D)	0.9900
C(119)-H(11E)	0.9900
C(120)-C(24B)	1.515(12)
C(120)-C(21B)	1.542(11)
C(120)-C(121)	1.548(7)
C(120)-C(124)	1.568(6)
C(120)-H(20A)	1.0000
C(120)-H(20B)	1.0000
C(121)-C(122)	1.523(9)
C(121)-H(12A)	0.9900
C(121)-H(12B)	0.9900
C(122)-C(123)	1.517(8)
C(122)-H(12C)	0.9900
C(122)-H(12D)	0.9900
C(123)-C(124)	1.540(8)
C(123)-H(12E)	0.9900
C(123)-H(12F)	0.9900
C(124)-H(12G)	0.9900
C(124)-H(12H)	0.9900
C(21B)-C(22B)	1.539(12)
C(21B)-H(21C)	0.9900
C(21B)-H(21D)	0.9900
C(22B)-C(23B)	1.517(13)
C(22B)-H(22C)	0.9900
C(22B)-H(22D)	0.9900
C(23B)-C(24B)	1.532(12)

C(23B)-H(23C)	0.9900
C(23B)-H(23D)	0.9900
C(24B)-H(24C)	0.9900
C(24B)-H(24D)	0.9900
C(103)-O(105)	1.4127(19)
C(103)-C(104)	1.539(2)
C(103)-H(103)	1.0000
O(105)-H(105)	0.817(17)
C(104)-O(106)	1.4102(17)
C(104)-C(105)	1.525(2)
C(104)-C(125)	1.529(2)
O(106)-H(106)	0.834(16)
O(107)-C(125)	1.210(2)
C(125)-O(108)	1.332(2)
O(108)-C(26B)	1.467(13)
O(108)-C(126)	1.476(7)
C(126)-C(127)	1.508(8)
C(126)-C(128)	1.515(7)
C(126)-H(126)	1.0000
C(127)-H(12I)	0.9800
C(127)-H(12J)	0.9800
C(127)-H(12K)	0.9800
C(128)-H(12L)	0.9800
C(128)-H(12M)	0.9800
C(128)-H(12N)	0.9800
C(26B)-C(27B)	1.499(13)
C(26B)-C(28B)	1.516(13)
C(26B)-H(26B)	1.0000
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(28B)-H(28D)	0.9800
C(28B)-H(28E)	0.9800
C(28B)-H(28F)	0.9800
C(105)-H(10J)	0.9900
C(105)-H(10K)	0.9900

C(201)-N(201)	1.477(2)
C(201)-C(206)	1.547(2)
C(201)-C(205)	1.565(2)
C(201)-C(202)	1.575(2)
C(206)-O(201)	1.2043(19)
C(206)-O(202)	1.329(2)
O(202)-C(207)	1.4903(18)
C(207)-C(208)	1.515(3)
C(207)-C(210)	1.520(2)
C(207)-C(209)	1.525(2)
C(208)-H(20C)	0.9800
C(208)-H(20D)	0.9800
C(208)-H(20E)	0.9800
C(209)-H(20F)	0.9800
C(209)-H(20G)	0.9800
C(209)-H(20H)	0.9800
C(210)-H(21E)	0.9800
C(210)-H(21F)	0.9800
C(210)-H(21G)	0.9800
N(201)-C(218)	1.409(2)
N(201)-C(211)	1.410(2)
C(211)-O(203)	1.2109(19)
C(211)-C(212)	1.488(2)
C(212)-C(213)	1.385(2)
C(212)-C(217)	1.386(2)
C(213)-C(214)	1.396(2)
C(213)-H(213)	0.9500
C(214)-C(215)	1.395(2)
C(214)-H(214)	0.9500
C(215)-C(216)	1.395(2)
C(215)-H(215)	0.9500
C(216)-C(217)	1.382(2)
C(216)-H(216)	0.9500
C(217)-C(218)	1.495(2)
C(218)-O(204)	1.2052(19)
C(202)-C(203)	1.530(2)

C(202)-C(219)	1.539(2)
C(202)-H(202)	1.0000
C(219)-C(220)	1.524(2)
C(219)-H(21H)	0.9900
C(219)-H(21I)	0.9900
C(220)-C(221)	1.535(2)
C(220)-C(224)	1.541(2)
C(220)-H(220)	1.0000
C(221)-C(222)	1.500(5)
C(221)-C(23C)	1.523(14)
C(221)-H(21J)	0.9900
C(221)-H(21K)	0.9900
C(221)-H(21L)	0.9900
C(221)-H(21M)	0.9900
C(222)-C(223)	1.518(6)
C(222)-H(22E)	0.9900
C(222)-H(22F)	0.9900
C(223)-C(224)	1.548(6)
C(223)-H(22G)	0.9900
C(223)-H(22H)	0.9900
C(22C)-C(224)	1.489(9)
C(22C)-C(23C)	1.522(14)
C(22C)-H(22I)	0.9900
C(22C)-H(22J)	0.9900
C(23C)-H(23E)	0.9900
C(23C)-H(23F)	0.9900
C(224)-H(24I)	0.9900
C(224)-H(24J)	0.9900
C(224)-H(24K)	0.9900
C(224)-H(24L)	0.9900
C(203)-O(205)	1.4227(19)
C(203)-C(204)	1.540(2)
C(203)-H(203)	1.0000
O(205)-H(205)	0.829(16)
C(204)-O(206)	1.4196(19)
C(204)-C(225)	1.486(7)

C(204)-C(205)	1.521(2)
C(204)-C(25C)	1.663(17)
O(206)-H(206)	0.831(17)
C(225)-O(207)	1.210(5)
C(225)-O(208)	1.327(4)
O(208)-C(226)	1.479(5)
C(226)-C(227)	1.514(5)
C(226)-C(228)	1.519(5)
C(226)-H(226)	1.0000
C(227)-H(22K)	0.9800
C(227)-H(22L)	0.9800
C(227)-H(22M)	0.9800
C(228)-H(22N)	0.9800
C(228)-H(22O)	0.9800
C(228)-H(22P)	0.9800
C(25C)-O(07C)	1.189(13)
C(25C)-O(08C)	1.310(12)
O(08C)-C(26C)	1.491(13)
C(26C)-C(28C)	1.502(12)
C(26C)-C(27C)	1.505(10)
C(26C)-H(26C)	1.0000
C(27C)-H(27G)	0.9800
C(27C)-H(27H)	0.9800
C(27C)-H(27I)	0.9800
C(28C)-H(28G)	0.9800
C(28C)-H(28H)	0.9800
C(28C)-H(28I)	0.9800
C(205)-H(20I)	0.9900
C(205)-H(20J)	0.9900
C(301)-N(301)	1.4860(19)
C(301)-C(306)	1.5454(19)
C(301)-C(305)	1.556(2)
C(301)-C(302)	1.5708(19)
C(306)-O(301)	1.2014(19)
C(306)-O(302)	1.331(2)
O(302)-C(307)	1.4815(17)

C(307)-C(308)	1.516(2)
C(307)-C(310)	1.520(2)
C(307)-C(309)	1.521(2)
C(308)-H(30A)	0.9800
C(308)-H(30B)	0.9800
C(308)-H(30C)	0.9800
C(309)-H(30D)	0.9800
C(309)-H(30E)	0.9800
C(309)-H(30F)	0.9800
C(310)-H(31A)	0.9800
C(310)-H(31B)	0.9800
C(310)-H(31C)	0.9800
N(301)-C(311)	1.4053(18)
N(301)-C(318)	1.409(2)
C(311)-O(303)	1.2133(19)
C(311)-C(312)	1.484(2)
C(312)-C(313)	1.385(2)
C(312)-C(317)	1.386(2)
C(313)-C(314)	1.392(2)
C(313)-H(313)	0.9500
C(314)-C(315)	1.399(2)
C(314)-H(314)	0.9500
C(315)-C(316)	1.396(2)
C(315)-H(315)	0.9500
C(316)-C(317)	1.379(2)
C(316)-H(316)	0.9500
C(317)-C(318)	1.493(2)
C(318)-O(304)	1.2053(19)
C(302)-C(303)	1.525(2)
C(302)-C(319)	1.539(2)
C(302)-H(302)	1.0000
C(319)-C(320)	1.528(2)
C(319)-H(31D)	0.9900
C(319)-H(31E)	0.9900
C(320)-C(324)	1.554(2)
C(320)-C(321)	1.559(2)

C(320)-H(320)	1.0000
C(321)-C(322)	1.530(2)
C(321)-H(32A)	0.9900
C(321)-H(32B)	0.9900
C(322)-C(323)	1.532(3)
C(322)-H(32C)	0.9900
C(322)-H(32D)	0.9900
C(323)-C(324)	1.533(2)
C(323)-H(32E)	0.9900
C(323)-H(32F)	0.9900
C(324)-H(32G)	0.9900
C(324)-H(32H)	0.9900
C(303)-O(305)	1.4110(17)
C(303)-C(304)	1.553(2)
C(303)-H(303)	1.0000
O(305)-H(305)	0.821(16)
C(304)-O(306)	1.4159(18)
C(304)-C(325)	1.520(2)
C(304)-C(305)	1.528(2)
O(306)-H(306)	0.781(16)
O(307)-C(325)	1.205(2)
C(325)-O(308)	1.326(2)
O(308)-C(326)	1.468(3)
O(308)-C(26D)	1.478(19)
C(326)-C(327)	1.496(3)
C(326)-C(328)	1.512(4)
C(326)-H(326)	1.0000
C(327)-H(32I)	0.9800
C(327)-H(32J)	0.9800
C(327)-H(32K)	0.9800
C(328)-H(32L)	0.9800
C(328)-H(32M)	0.9800
C(328)-H(32N)	0.9800
C(26D)-C(28D)	1.508(17)
C(26D)-C(27D)	1.510(17)
C(26D)-H(26D)	1.0000

C(27D)-H(27J)	0.9800
C(27D)-H(27K)	0.9800
C(27D)-H(27L)	0.9800
C(28D)-H(28J)	0.9800
C(28D)-H(28K)	0.9800
C(28D)-H(28L)	0.9800
C(305)-H(30G)	0.9900
C(305)-H(30H)	0.9900
O(1W)-H(1W)	0.90(2)
O(1W)-H(2W)	0.89(2)

N(1)-C(1)-C(6)	109.26(12)
N(1)-C(1)-C(5)	110.10(11)
C(6)-C(1)-C(5)	109.86(12)
N(1)-C(1)-C(2)	115.09(12)
C(6)-C(1)-C(2)	107.53(11)
C(5)-C(1)-C(2)	104.85(12)
O(1)-C(6)-O(2)	126.65(13)
O(1)-C(6)-C(1)	122.13(14)
O(2)-C(6)-C(1)	110.99(12)
C(6)-O(2)-C(7)	121.27(12)
O(2)-C(7)-C(8)	101.57(13)
O(2)-C(7)-C(9)	110.07(12)
C(8)-C(7)-C(9)	111.04(15)
O(2)-C(7)-C(10)	110.14(13)
C(8)-C(7)-C(10)	111.17(14)
C(9)-C(7)-C(10)	112.34(15)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5

C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(18)-N(1)-C(11)	110.72(12)
C(18)-N(1)-C(1)	130.91(12)
C(11)-N(1)-C(1)	118.37(12)
O(3)-C(11)-N(1)	124.01(15)
O(3)-C(11)-C(12)	129.19(14)
N(1)-C(11)-C(12)	106.80(13)
C(17)-C(12)-C(13)	121.65(16)
C(17)-C(12)-C(11)	107.82(14)
C(13)-C(12)-C(11)	130.52(15)
C(12)-C(13)-C(14)	116.77(16)
C(12)-C(13)-H(13)	121.6
C(14)-C(13)-H(13)	121.6
C(15)-C(14)-C(13)	121.37(16)
C(15)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(14)-C(15)-C(16)	121.38(16)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	116.69(15)
C(17)-C(16)-H(16)	121.7
C(15)-C(16)-H(16)	121.7
C(12)-C(17)-C(16)	122.13(15)
C(12)-C(17)-C(18)	108.83(14)
C(16)-C(17)-C(18)	129.04(15)
O(4)-C(18)-N(1)	127.70(14)
O(4)-C(18)-C(17)	126.57(14)
N(1)-C(18)-C(17)	105.73(12)

C(3)-C(2)-C(19)	112.74(12)
C(3)-C(2)-C(1)	103.73(11)
C(19)-C(2)-C(1)	118.81(12)
C(3)-C(2)-H(2)	107.0
C(19)-C(2)-H(2)	107.0
C(1)-C(2)-H(2)	107.0
C(20)-C(19)-C(2)	113.66(13)
C(20)-C(19)-H(19A)	108.8
C(2)-C(19)-H(19A)	108.8
C(20)-C(19)-H(19B)	108.8
C(2)-C(19)-H(19B)	108.8
H(19A)-C(19)-H(19B)	107.7
C(19)-C(20)-C(21)	114.10(13)
C(19)-C(20)-C(24)	112.95(13)
C(21)-C(20)-C(24)	103.49(12)
C(19)-C(20)-H(20)	108.7
C(21)-C(20)-H(20)	108.7
C(24)-C(20)-H(20)	108.7
C(22)-C(21)-C(20)	102.97(13)
C(22)-C(21)-H(21A)	111.2
C(20)-C(21)-H(21A)	111.2
C(22)-C(21)-H(21B)	111.2
C(20)-C(21)-H(21B)	111.2
H(21A)-C(21)-H(21B)	109.1
C(21)-C(22)-C(23)	103.27(14)
C(21)-C(22)-H(22A)	111.1
C(23)-C(22)-H(22A)	111.1
C(21)-C(22)-H(22B)	111.1
C(23)-C(22)-H(22B)	111.1
H(22A)-C(22)-H(22B)	109.1
C(22)-C(23)-C(24)	105.09(13)
C(22)-C(23)-H(23A)	110.7
C(24)-C(23)-H(23A)	110.7
C(22)-C(23)-H(23B)	110.7
C(24)-C(23)-H(23B)	110.7
H(23A)-C(23)-H(23B)	108.8

C(23)-C(24)-C(20)	106.49(13)
C(23)-C(24)-H(24A)	110.4
C(20)-C(24)-H(24A)	110.4
C(23)-C(24)-H(24B)	110.4
C(20)-C(24)-H(24B)	110.4
H(24A)-C(24)-H(24B)	108.6
O(5)-C(3)-C(2)	111.49(12)
O(5)-C(3)-C(4)	112.14(12)
C(2)-C(3)-C(4)	103.07(12)
O(5)-C(3)-H(3)	110.0
C(2)-C(3)-H(3)	110.0
C(4)-C(3)-H(3)	110.0
C(3)-O(5)-H(5)	105.3(16)
O(6)-C(4)-C(25)	110.54(12)
O(6)-C(4)-C(3)	104.46(12)
C(25)-C(4)-C(3)	116.21(13)
O(6)-C(4)-C(5)	111.68(13)
C(25)-C(4)-C(5)	111.56(12)
C(3)-C(4)-C(5)	101.97(11)
C(4)-O(6)-H(6)	108.0(16)
O(7)-C(25)-O(8)	124.72(16)
O(7)-C(25)-C(4)	122.80(15)
O(8)-C(25)-C(4)	112.43(13)
C(25)-O(8)-C(26)	117.21(12)
O(8)-C(26)-C(27)	106.41(13)
O(8)-C(26)-C(28)	108.06(13)
C(27)-C(26)-C(28)	113.97(14)
O(8)-C(26)-H(26)	109.4
C(27)-C(26)-H(26)	109.4
C(28)-C(26)-H(26)	109.4
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(4)-C(5)-C(1)	105.47(12)
C(4)-C(5)-H(5A)	110.6
C(1)-C(5)-H(5A)	110.6
C(4)-C(5)-H(5B)	110.6
C(1)-C(5)-H(5B)	110.6
H(5A)-C(5)-H(5B)	108.8
N(101)-C(101)-C(106)	108.51(12)
N(101)-C(101)-C(105)	109.95(11)
C(106)-C(101)-C(105)	109.51(12)
N(101)-C(101)-C(102)	115.69(12)
C(106)-C(101)-C(102)	107.92(11)
C(105)-C(101)-C(102)	105.11(12)
O(101)-C(106)-O(102)	126.16(14)
O(101)-C(106)-C(101)	122.48(15)
O(102)-C(106)-C(101)	111.21(12)
C(106)-O(102)-C(107)	121.18(12)
O(102)-C(107)-C(108)	101.35(12)
O(102)-C(107)-C(110)	111.18(13)
C(108)-C(107)-C(110)	110.92(14)
O(102)-C(107)-C(109)	108.62(13)
C(108)-C(107)-C(109)	111.12(15)
C(110)-C(107)-C(109)	113.04(14)
C(107)-C(108)-H(10D)	109.5
C(107)-C(108)-H(10E)	109.5
H(10D)-C(108)-H(10E)	109.5
C(107)-C(108)-H(10F)	109.5
H(10D)-C(108)-H(10F)	109.5
H(10E)-C(108)-H(10F)	109.5
C(107)-C(109)-H(10G)	109.5
C(107)-C(109)-H(10H)	109.5

H(10G)-C(109)-H(10H)	109.5
C(107)-C(109)-H(10I)	109.5
H(10G)-C(109)-H(10I)	109.5
H(10H)-C(109)-H(10I)	109.5
C(107)-C(110)-H(11A)	109.5
C(107)-C(110)-H(11B)	109.5
H(11A)-C(110)-H(11B)	109.5
C(107)-C(110)-H(11C)	109.5
H(11A)-C(110)-H(11C)	109.5
H(11B)-C(110)-H(11C)	109.5
C(111)-N(101)-C(118)	110.84(12)
C(111)-N(101)-C(101)	117.68(12)
C(118)-N(101)-C(101)	131.28(12)
O(103)-C(111)-N(101)	124.07(14)
O(103)-C(111)-C(112)	128.88(14)
N(101)-C(111)-C(112)	107.04(12)
C(117)-C(112)-C(113)	122.02(14)
C(117)-C(112)-C(111)	107.83(13)
C(113)-C(112)-C(111)	130.13(14)
C(112)-C(113)-C(114)	116.86(14)
C(112)-C(113)-H(113)	121.6
C(114)-C(113)-H(113)	121.6
C(115)-C(114)-C(113)	121.38(15)
C(115)-C(114)-H(114)	119.3
C(113)-C(114)-H(114)	119.3
C(114)-C(115)-C(116)	121.40(15)
C(114)-C(115)-H(115)	119.3
C(116)-C(115)-H(115)	119.3
C(117)-C(116)-C(115)	116.66(15)
C(117)-C(116)-H(116)	121.7
C(115)-C(116)-H(116)	121.7
C(112)-C(117)-C(116)	121.66(15)
C(112)-C(117)-C(118)	108.85(13)
C(116)-C(117)-C(118)	129.47(14)
O(104)-C(118)-N(101)	127.70(15)
O(104)-C(118)-C(117)	127.07(14)

N(101)-C(118)-C(117)	105.21(12)
C(103)-C(102)-C(119)	112.30(12)
C(103)-C(102)-C(101)	102.85(12)
C(119)-C(102)-C(101)	118.59(13)
C(103)-C(102)-H(102)	107.5
C(119)-C(102)-H(102)	107.5
C(101)-C(102)-H(102)	107.5
C(120)-C(119)-C(102)	115.58(13)
C(120)-C(119)-H(11D)	108.4
C(102)-C(119)-H(11D)	108.4
C(120)-C(119)-H(11E)	108.4
C(102)-C(119)-H(11E)	108.4
H(11D)-C(119)-H(11E)	107.4
C(24B)-C(120)-C(119)	117.9(8)
C(24B)-C(120)-C(21B)	107.6(7)
C(119)-C(120)-C(21B)	113.5(6)
C(24B)-C(120)-C(121)	101.3(6)
C(119)-C(120)-C(121)	112.2(4)
C(119)-C(120)-C(124)	111.2(4)
C(21B)-C(120)-C(124)	107.1(6)
C(121)-C(120)-C(124)	99.9(4)
C(24B)-C(120)-H(20A)	105.6
C(119)-C(120)-H(20A)	105.6
C(21B)-C(120)-H(20A)	105.6
C(121)-C(120)-H(20A)	114.4
C(124)-C(120)-H(20A)	113.8
C(24B)-C(120)-H(20B)	102.6
C(119)-C(120)-H(20B)	111.0
C(21B)-C(120)-H(20B)	102.5
C(121)-C(120)-H(20B)	111.0
C(124)-C(120)-H(20B)	111.0
C(122)-C(121)-C(120)	103.2(6)
C(122)-C(121)-H(12A)	111.1
C(120)-C(121)-H(12A)	111.1
C(122)-C(121)-H(12B)	111.1
C(120)-C(121)-H(12B)	111.1

H(12A)-C(121)-H(12B)	109.1
C(123)-C(122)-C(121)	104.9(5)
C(123)-C(122)-H(12C)	110.8
C(121)-C(122)-H(12C)	110.8
C(123)-C(122)-H(12D)	110.8
C(121)-C(122)-H(12D)	110.8
H(12C)-C(122)-H(12D)	108.8
C(122)-C(123)-C(124)	106.2(4)
C(122)-C(123)-H(12E)	110.5
C(124)-C(123)-H(12E)	110.5
C(122)-C(123)-H(12F)	110.5
C(124)-C(123)-H(12F)	110.5
H(12E)-C(123)-H(12F)	108.7
C(123)-C(124)-C(120)	105.9(5)
C(123)-C(124)-H(12G)	110.5
C(120)-C(124)-H(12G)	110.5
C(123)-C(124)-H(12H)	110.5
C(120)-C(124)-H(12H)	110.5
H(12G)-C(124)-H(12H)	108.7
C(22B)-C(21B)-C(120)	105.0(8)
C(22B)-C(21B)-H(21C)	110.7
C(120)-C(21B)-H(21C)	110.7
C(22B)-C(21B)-H(21D)	110.7
C(120)-C(21B)-H(21D)	110.7
H(21C)-C(21B)-H(21D)	108.8
C(23B)-C(22B)-C(21B)	102.6(10)
C(23B)-C(22B)-H(22C)	111.3
C(21B)-C(22B)-H(22C)	111.3
C(23B)-C(22B)-H(22D)	111.3
C(21B)-C(22B)-H(22D)	111.3
H(22C)-C(22B)-H(22D)	109.2
C(22B)-C(23B)-C(24B)	104.8(9)
C(22B)-C(23B)-H(23C)	110.8
C(24B)-C(23B)-H(23C)	110.8
C(22B)-C(23B)-H(23D)	110.8
C(24B)-C(23B)-H(23D)	110.8

H(23C)-C(23B)-H(23D)	108.9
C(120)-C(24B)-C(23B)	104.3(8)
C(120)-C(24B)-H(24C)	110.9
C(23B)-C(24B)-H(24C)	110.9
C(120)-C(24B)-H(24D)	110.9
C(23B)-C(24B)-H(24D)	110.9
H(24C)-C(24B)-H(24D)	108.9
O(105)-C(103)-C(102)	108.63(12)
O(105)-C(103)-C(104)	113.93(12)
C(102)-C(103)-C(104)	102.70(12)
O(105)-C(103)-H(103)	110.4
C(102)-C(103)-H(103)	110.4
C(104)-C(103)-H(103)	110.4
C(103)-O(105)-H(105)	110.3(17)
O(106)-C(104)-C(105)	107.83(12)
O(106)-C(104)-C(125)	110.21(12)
C(105)-C(104)-C(125)	112.08(12)
O(106)-C(104)-C(103)	110.16(12)
C(105)-C(104)-C(103)	102.04(12)
C(125)-C(104)-C(103)	114.12(13)
C(104)-O(106)-H(106)	108.3(15)
O(107)-C(125)-O(108)	124.48(16)
O(107)-C(125)-C(104)	124.46(15)
O(108)-C(125)-C(104)	111.05(13)
C(125)-O(108)-C(26B)	119.3(10)
C(125)-O(108)-C(126)	116.4(5)
O(108)-C(126)-C(127)	107.5(9)
O(108)-C(126)-C(128)	106.3(8)
C(127)-C(126)-C(128)	113.1(8)
O(108)-C(126)-H(126)	109.9
C(127)-C(126)-H(126)	109.9
C(128)-C(126)-H(126)	109.9
C(126)-C(127)-H(12I)	109.5
C(126)-C(127)-H(12J)	109.5
H(12I)-C(127)-H(12J)	109.5
C(126)-C(127)-H(12K)	109.5

H(12I)-C(127)-H(12K)	109.5
H(12J)-C(127)-H(12K)	109.5
C(126)-C(128)-H(12L)	109.5
C(126)-C(128)-H(12M)	109.5
H(12L)-C(128)-H(12M)	109.5
C(126)-C(128)-H(12N)	109.5
H(12L)-C(128)-H(12N)	109.5
H(12M)-C(128)-H(12N)	109.5
O(108)-C(26B)-C(27B)	109.7(17)
O(108)-C(26B)-C(28B)	104.4(15)
C(27B)-C(26B)-C(28B)	113.5(16)
O(108)-C(26B)-H(26B)	109.7
C(27B)-C(26B)-H(26B)	109.7
C(28B)-C(26B)-H(26B)	109.7
C(26B)-C(27B)-H(27D)	109.5
C(26B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(26B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(26B)-C(28B)-H(28D)	109.5
C(26B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(26B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(104)-C(105)-C(101)	105.75(12)
C(104)-C(105)-H(10J)	110.6
C(101)-C(105)-H(10J)	110.6
C(104)-C(105)-H(10K)	110.6
C(101)-C(105)-H(10K)	110.6
H(10J)-C(105)-H(10K)	108.7
N(201)-C(201)-C(206)	110.23(13)
N(201)-C(201)-C(205)	110.37(12)
C(206)-C(201)-C(205)	109.55(12)
N(201)-C(201)-C(202)	113.57(12)

C(206)-C(201)-C(202)	107.91(12)
C(205)-C(201)-C(202)	105.04(13)
O(201)-C(206)-O(202)	126.67(14)
O(201)-C(206)-C(201)	121.86(15)
O(202)-C(206)-C(201)	111.32(12)
C(206)-O(202)-C(207)	121.00(12)
O(202)-C(207)-C(208)	102.07(13)
O(202)-C(207)-C(210)	109.57(13)
C(208)-C(207)-C(210)	111.45(16)
O(202)-C(207)-C(209)	109.96(13)
C(208)-C(207)-C(209)	110.34(15)
C(210)-C(207)-C(209)	112.92(15)
C(207)-C(208)-H(20C)	109.5
C(207)-C(208)-H(20D)	109.5
H(20C)-C(208)-H(20D)	109.5
C(207)-C(208)-H(20E)	109.5
H(20C)-C(208)-H(20E)	109.5
H(20D)-C(208)-H(20E)	109.5
C(207)-C(209)-H(20F)	109.5
C(207)-C(209)-H(20G)	109.5
H(20F)-C(209)-H(20G)	109.5
C(207)-C(209)-H(20H)	109.5
H(20F)-C(209)-H(20H)	109.5
H(20G)-C(209)-H(20H)	109.5
C(207)-C(210)-H(21E)	109.5
C(207)-C(210)-H(21F)	109.5
H(21E)-C(210)-H(21F)	109.5
C(207)-C(210)-H(21G)	109.5
H(21E)-C(210)-H(21G)	109.5
H(21F)-C(210)-H(21G)	109.5
C(218)-N(201)-C(211)	110.96(13)
C(218)-N(201)-C(201)	128.99(13)
C(211)-N(201)-C(201)	119.56(12)
O(203)-C(211)-N(201)	124.51(15)
O(203)-C(211)-C(212)	129.04(15)
N(201)-C(211)-C(212)	106.43(12)

C(213)-C(212)-C(217)	121.38(15)
C(213)-C(212)-C(211)	130.70(14)
C(217)-C(212)-C(211)	107.91(13)
C(212)-C(213)-C(214)	116.99(14)
C(212)-C(213)-H(213)	121.5
C(214)-C(213)-H(213)	121.5
C(215)-C(214)-C(213)	121.53(15)
C(215)-C(214)-H(214)	119.2
C(213)-C(214)-H(214)	119.2
C(214)-C(215)-C(216)	120.92(16)
C(214)-C(215)-H(215)	119.5
C(216)-C(215)-H(215)	119.5
C(217)-C(216)-C(215)	117.07(15)
C(217)-C(216)-H(216)	121.5
C(215)-C(216)-H(216)	121.5
C(216)-C(217)-C(212)	122.10(15)
C(216)-C(217)-C(218)	129.19(14)
C(212)-C(217)-C(218)	108.71(13)
O(204)-C(218)-N(201)	127.81(15)
O(204)-C(218)-C(217)	126.52(14)
N(201)-C(218)-C(217)	105.66(13)
C(203)-C(202)-C(219)	114.96(13)
C(203)-C(202)-C(201)	103.11(12)
C(219)-C(202)-C(201)	114.13(13)
C(203)-C(202)-H(202)	108.1
C(219)-C(202)-H(202)	108.1
C(201)-C(202)-H(202)	108.1
C(220)-C(219)-C(202)	116.65(14)
C(220)-C(219)-H(21H)	108.1
C(202)-C(219)-H(21H)	108.1
C(220)-C(219)-H(21I)	108.1
C(202)-C(219)-H(21I)	108.1
H(21H)-C(219)-H(21I)	107.3
C(219)-C(220)-C(221)	111.43(15)
C(219)-C(220)-C(224)	114.58(14)
C(221)-C(220)-C(224)	103.41(15)

C(219)-C(220)-H(220)	109.1
C(221)-C(220)-H(220)	109.1
C(224)-C(220)-H(220)	109.1
C(222)-C(221)-C(220)	105.6(3)
C(23C)-C(221)-C(220)	101.1(9)
C(222)-C(221)-H(21J)	110.6
C(23C)-C(221)-H(21J)	118.4
C(220)-C(221)-H(21J)	110.6
C(222)-C(221)-H(21K)	110.6
C(23C)-C(221)-H(21K)	107.0
C(220)-C(221)-H(21K)	110.6
H(21J)-C(221)-H(21K)	108.8
C(222)-C(221)-H(21L)	103.8
C(23C)-C(221)-H(21L)	111.5
C(220)-C(221)-H(21L)	111.5
H(21K)-C(221)-H(21L)	114.1
C(222)-C(221)-H(21M)	114.7
C(23C)-C(221)-H(21M)	111.5
C(220)-C(221)-H(21M)	111.5
H(21J)-C(221)-H(21M)	103.8
H(21L)-C(221)-H(21M)	109.4
C(221)-C(222)-C(223)	101.6(4)
C(221)-C(222)-H(22E)	111.5
C(223)-C(222)-H(22E)	111.5
C(221)-C(222)-H(22F)	111.5
C(223)-C(222)-H(22F)	111.5
H(22E)-C(222)-H(22F)	109.3
C(222)-C(223)-C(224)	106.1(3)
C(222)-C(223)-H(22G)	110.5
C(224)-C(223)-H(22G)	110.5
C(222)-C(223)-H(22H)	110.5
C(224)-C(223)-H(22H)	110.5
H(22G)-C(223)-H(22H)	108.7
C(224)-C(22C)-C(23C)	106.8(9)
C(224)-C(22C)-H(22I)	110.4
C(23C)-C(22C)-H(22I)	110.4

C(224)-C(22C)-H(22J)	110.4
C(23C)-C(22C)-H(22J)	110.4
H(22I)-C(22C)-H(22J)	108.6
C(22C)-C(23C)-C(221)	106.7(10)
C(22C)-C(23C)-H(23E)	110.4
C(221)-C(23C)-H(23E)	110.4
C(22C)-C(23C)-H(23F)	110.4
C(221)-C(23C)-H(23F)	110.4
H(23E)-C(23C)-H(23F)	108.6
C(22C)-C(224)-C(220)	105.5(5)
C(220)-C(224)-C(223)	105.9(2)
C(22C)-C(224)-H(24I)	127.7
C(220)-C(224)-H(24I)	110.6
C(223)-C(224)-H(24I)	110.6
C(22C)-C(224)-H(24J)	91.9
C(220)-C(224)-H(24J)	110.6
C(223)-C(224)-H(24J)	110.6
H(24I)-C(224)-H(24J)	108.7
C(22C)-C(224)-H(24K)	110.6
C(220)-C(224)-H(24K)	110.6
C(223)-C(224)-H(24K)	127.4
H(24I)-C(224)-H(24K)	90.6
C(22C)-C(224)-H(24L)	110.6
C(220)-C(224)-H(24L)	110.6
C(223)-C(224)-H(24L)	91.7
H(24J)-C(224)-H(24L)	124.7
H(24K)-C(224)-H(24L)	108.8
O(205)-C(203)-C(202)	113.77(13)
O(205)-C(203)-C(204)	112.09(13)
C(202)-C(203)-C(204)	103.69(12)
O(205)-C(203)-H(203)	109.0
C(202)-C(203)-H(203)	109.0
C(204)-C(203)-H(203)	109.0
C(203)-O(205)-H(205)	109.9(17)
O(206)-C(204)-C(225)	106.6(3)
O(206)-C(204)-C(205)	110.41(13)

C(225)-C(204)-C(205)	117.4(3)
O(206)-C(204)-C(203)	106.96(12)
C(225)-C(204)-C(203)	112.6(4)
C(205)-C(204)-C(203)	102.52(13)
O(206)-C(204)-C(25C)	117.5(6)
C(205)-C(204)-C(25C)	111.6(7)
C(203)-C(204)-C(25C)	106.5(9)
C(204)-O(206)-H(206)	109.5(19)
O(207)-C(225)-O(208)	125.5(5)
O(207)-C(225)-C(204)	122.2(4)
O(208)-C(225)-C(204)	112.2(4)
C(225)-O(208)-C(226)	117.2(4)
O(208)-C(226)-C(227)	104.4(3)
O(208)-C(226)-C(228)	110.4(5)
C(227)-C(226)-C(228)	112.5(3)
O(208)-C(226)-H(226)	109.8
C(227)-C(226)-H(226)	109.8
C(228)-C(226)-H(226)	109.8
C(226)-C(227)-H(22K)	109.5
C(226)-C(227)-H(22L)	109.5
H(22K)-C(227)-H(22L)	109.5
C(226)-C(227)-H(22M)	109.5
H(22K)-C(227)-H(22M)	109.5
H(22L)-C(227)-H(22M)	109.5
C(226)-C(228)-H(22N)	109.5
C(226)-C(228)-H(22O)	109.5
H(22N)-C(228)-H(22O)	109.5
C(226)-C(228)-H(22P)	109.5
H(22N)-C(228)-H(22P)	109.5
H(22O)-C(228)-H(22P)	109.5
O(07C)-C(25C)-O(08C)	126.6(13)
O(07C)-C(25C)-C(204)	119.3(12)
O(08C)-C(25C)-C(204)	114.1(11)
C(25C)-O(08C)-C(26C)	116.5(11)
O(08C)-C(26C)-C(28C)	107.8(12)
O(08C)-C(26C)-C(27C)	105.1(9)

C(28C)-C(26C)-C(27C)	114.2(10)
O(08C)-C(26C)-H(26C)	109.9
C(28C)-C(26C)-H(26C)	109.9
C(27C)-C(26C)-H(26C)	109.9
C(26C)-C(27C)-H(27G)	109.5
C(26C)-C(27C)-H(27H)	109.5
H(27G)-C(27C)-H(27H)	109.5
C(26C)-C(27C)-H(27I)	109.5
H(27G)-C(27C)-H(27I)	109.5
H(27H)-C(27C)-H(27I)	109.5
C(26C)-C(28C)-H(28G)	109.5
C(26C)-C(28C)-H(28H)	109.5
H(28G)-C(28C)-H(28H)	109.5
C(26C)-C(28C)-H(28I)	109.5
H(28G)-C(28C)-H(28I)	109.5
H(28H)-C(28C)-H(28I)	109.5
C(204)-C(205)-C(201)	106.54(12)
C(204)-C(205)-H(20I)	110.4
C(201)-C(205)-H(20I)	110.4
C(204)-C(205)-H(20J)	110.4
C(201)-C(205)-H(20J)	110.4
H(20I)-C(205)-H(20J)	108.6
N(301)-C(301)-C(306)	109.32(12)
N(301)-C(301)-C(305)	110.16(11)
C(306)-C(301)-C(305)	109.03(12)
N(301)-C(301)-C(302)	114.67(12)
C(306)-C(301)-C(302)	108.22(11)
C(305)-C(301)-C(302)	105.26(12)
O(301)-C(306)-O(302)	126.41(14)
O(301)-C(306)-C(301)	121.67(14)
O(302)-C(306)-C(301)	111.76(12)
C(306)-O(302)-C(307)	120.06(12)
O(302)-C(307)-C(308)	101.74(12)
O(302)-C(307)-C(310)	109.88(12)
C(308)-C(307)-C(310)	111.87(13)
O(302)-C(307)-C(309)	110.28(12)

C(308)-C(307)-C(309)	110.87(14)
C(310)-C(307)-C(309)	111.76(14)
C(307)-C(308)-H(30A)	109.5
C(307)-C(308)-H(30B)	109.5
H(30A)-C(308)-H(30B)	109.5
C(307)-C(308)-H(30C)	109.5
H(30A)-C(308)-H(30C)	109.5
H(30B)-C(308)-H(30C)	109.5
C(307)-C(309)-H(30D)	109.5
C(307)-C(309)-H(30E)	109.5
H(30D)-C(309)-H(30E)	109.5
C(307)-C(309)-H(30F)	109.5
H(30D)-C(309)-H(30F)	109.5
H(30E)-C(309)-H(30F)	109.5
C(307)-C(310)-H(31A)	109.5
C(307)-C(310)-H(31B)	109.5
H(31A)-C(310)-H(31B)	109.5
C(307)-C(310)-H(31C)	109.5
H(31A)-C(310)-H(31C)	109.5
H(31B)-C(310)-H(31C)	109.5
C(311)-N(301)-C(318)	110.54(12)
C(311)-N(301)-C(301)	118.94(12)
C(318)-N(301)-C(301)	130.26(12)
O(303)-C(311)-N(301)	124.04(14)
O(303)-C(311)-C(312)	128.77(14)
N(301)-C(311)-C(312)	107.19(12)
C(313)-C(312)-C(317)	121.17(15)
C(313)-C(312)-C(311)	131.39(14)
C(317)-C(312)-C(311)	107.44(13)
C(312)-C(313)-C(314)	117.53(14)
C(312)-C(313)-H(313)	121.2
C(314)-C(313)-H(313)	121.2
C(313)-C(314)-C(315)	121.04(14)
C(313)-C(314)-H(314)	119.5
C(315)-C(314)-H(314)	119.5
C(316)-C(315)-C(314)	120.97(15)

C(316)-C(315)-H(315)	119.5
C(314)-C(315)-H(315)	119.5
C(317)-C(316)-C(315)	117.18(14)
C(317)-C(316)-H(316)	121.4
C(315)-C(316)-H(316)	121.4
C(316)-C(317)-C(312)	122.09(14)
C(316)-C(317)-C(318)	129.06(14)
C(312)-C(317)-C(318)	108.82(13)
O(304)-C(318)-N(301)	128.01(14)
O(304)-C(318)-C(317)	126.11(14)
N(301)-C(318)-C(317)	105.87(12)
C(303)-C(302)-C(319)	112.03(12)
C(303)-C(302)-C(301)	103.46(12)
C(319)-C(302)-C(301)	117.80(12)
C(303)-C(302)-H(302)	107.7
C(319)-C(302)-H(302)	107.7
C(301)-C(302)-H(302)	107.7
C(320)-C(319)-C(302)	115.93(13)
C(320)-C(319)-H(31D)	108.3
C(302)-C(319)-H(31D)	108.3
C(320)-C(319)-H(31E)	108.3
C(302)-C(319)-H(31E)	108.3
H(31D)-C(319)-H(31E)	107.4
C(319)-C(320)-C(324)	112.65(13)
C(319)-C(320)-C(321)	111.17(13)
C(324)-C(320)-C(321)	104.59(13)
C(319)-C(320)-H(320)	109.4
C(324)-C(320)-H(320)	109.4
C(321)-C(320)-H(320)	109.4
C(322)-C(321)-C(320)	106.53(14)
C(322)-C(321)-H(32A)	110.4
C(320)-C(321)-H(32A)	110.4
C(322)-C(321)-H(32B)	110.4
C(320)-C(321)-H(32B)	110.4
H(32A)-C(321)-H(32B)	108.6
C(321)-C(322)-C(323)	102.86(14)

C(321)-C(322)-H(32C)	111.2
C(323)-C(322)-H(32C)	111.2
C(321)-C(322)-H(32D)	111.2
C(323)-C(322)-H(32D)	111.2
H(32C)-C(322)-H(32D)	109.1
C(322)-C(323)-C(324)	102.78(13)
C(322)-C(323)-H(32E)	111.2
C(324)-C(323)-H(32E)	111.2
C(322)-C(323)-H(32F)	111.2
C(324)-C(323)-H(32F)	111.2
H(32E)-C(323)-H(32F)	109.1
C(323)-C(324)-C(320)	105.08(13)
C(323)-C(324)-H(32G)	110.7
C(320)-C(324)-H(32G)	110.7
C(323)-C(324)-H(32H)	110.7
C(320)-C(324)-H(32H)	110.7
H(32G)-C(324)-H(32H)	108.8
O(305)-C(303)-C(302)	108.55(12)
O(305)-C(303)-C(304)	113.16(12)
C(302)-C(303)-C(304)	103.72(12)
O(305)-C(303)-H(303)	110.4
C(302)-C(303)-H(303)	110.4
C(304)-C(303)-H(303)	110.4
C(303)-O(305)-H(305)	108.3(16)
O(306)-C(304)-C(325)	109.96(12)
O(306)-C(304)-C(305)	108.11(12)
C(325)-C(304)-C(305)	115.43(12)
O(306)-C(304)-C(303)	110.38(12)
C(325)-C(304)-C(303)	110.68(12)
C(305)-C(304)-C(303)	101.99(12)
C(304)-O(306)-H(306)	110.2(16)
O(307)-C(325)-O(308)	124.71(16)
O(307)-C(325)-C(304)	122.77(14)
O(308)-C(325)-C(304)	112.37(13)
C(325)-O(308)-C(326)	117.7(2)
C(325)-O(308)-C(26D)	122.8(18)

O(308)-C(326)-C(327)	106.1(2)
O(308)-C(326)-C(328)	108.4(2)
C(327)-C(326)-C(328)	114.0(3)
O(308)-C(326)-H(326)	109.4
C(327)-C(326)-H(326)	109.4
C(328)-C(326)-H(326)	109.4
C(326)-C(327)-H(32I)	109.5
C(326)-C(327)-H(32J)	109.5
H(32I)-C(327)-H(32J)	109.5
C(326)-C(327)-H(32K)	109.5
H(32I)-C(327)-H(32K)	109.5
H(32J)-C(327)-H(32K)	109.5
C(326)-C(328)-H(32L)	109.5
C(326)-C(328)-H(32M)	109.5
H(32L)-C(328)-H(32M)	109.5
C(326)-C(328)-H(32N)	109.5
H(32L)-C(328)-H(32N)	109.5
H(32M)-C(328)-H(32N)	109.5
O(308)-C(26D)-C(28D)	108(2)
O(308)-C(26D)-C(27D)	105(2)
C(28D)-C(26D)-C(27D)	114(3)
O(308)-C(26D)-H(26D)	109.8
C(28D)-C(26D)-H(26D)	109.8
C(27D)-C(26D)-H(26D)	109.8
C(26D)-C(27D)-H(27J)	109.5
C(26D)-C(27D)-H(27K)	109.5
H(27J)-C(27D)-H(27K)	109.5
C(26D)-C(27D)-H(27L)	109.5
H(27J)-C(27D)-H(27L)	109.5
H(27K)-C(27D)-H(27L)	109.5
C(26D)-C(28D)-H(28J)	109.5
C(26D)-C(28D)-H(28K)	109.5
H(28J)-C(28D)-H(28K)	109.5
C(26D)-C(28D)-H(28L)	109.5
H(28J)-C(28D)-H(28L)	109.5
H(28K)-C(28D)-H(28L)	109.5

C(304)-C(305)-C(301)	106.93(12)
C(304)-C(305)-H(30G)	110.3
C(301)-C(305)-H(30G)	110.3
C(304)-C(305)-H(30H)	110.3
C(301)-C(305)-H(30H)	110.3
H(30G)-C(305)-H(30H)	108.6
H(1W)-O(1W)-H(2W)	103(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D11023. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(1)	19(1)	20(1)	-10(1)	-5(1)	3(1)
C(6)	18(1)	20(1)	21(1)	-10(1)	-8(1)	3(1)
O(1)	23(1)	25(1)	24(1)	-15(1)	-1(1)	1(1)
O(2)	20(1)	19(1)	23(1)	-11(1)	-2(1)	1(1)
C(7)	22(1)	18(1)	27(1)	-9(1)	-3(1)	-3(1)
C(8)	35(1)	23(1)	41(1)	-16(1)	-7(1)	-2(1)
C(9)	34(1)	27(1)	26(1)	-8(1)	-4(1)	-1(1)
C(10)	23(1)	26(1)	47(1)	-14(1)	-8(1)	-2(1)
N(1)	18(1)	19(1)	20(1)	-10(1)	-5(1)	2(1)
C(11)	22(1)	19(1)	19(1)	-8(1)	-5(1)	0(1)
O(3)	20(1)	32(1)	30(1)	-18(1)	-7(1)	3(1)
C(12)	25(1)	20(1)	20(1)	-9(1)	-3(1)	-1(1)
C(13)	28(1)	28(1)	25(1)	-14(1)	-4(1)	-4(1)
C(14)	35(1)	32(1)	25(1)	-18(1)	-3(1)	-7(1)
C(15)	35(1)	28(1)	24(1)	-16(1)	0(1)	-1(1)
C(16)	27(1)	27(1)	22(1)	-12(1)	-4(1)	4(1)
C(17)	26(1)	18(1)	18(1)	-7(1)	-4(1)	0(1)
C(18)	22(1)	18(1)	16(1)	-6(1)	-3(1)	3(1)
O(4)	20(1)	35(1)	24(1)	-16(1)	-6(1)	6(1)
C(2)	18(1)	18(1)	20(1)	-9(1)	-5(1)	2(1)
C(19)	22(1)	19(1)	21(1)	-9(1)	-7(1)	3(1)
C(20)	25(1)	21(1)	21(1)	-10(1)	-6(1)	3(1)
C(21)	31(1)	22(1)	24(1)	-9(1)	-9(1)	6(1)
C(22)	40(1)	26(1)	30(1)	-12(1)	-14(1)	14(1)
C(23)	26(1)	41(1)	30(1)	-17(1)	-12(1)	14(1)
C(24)	24(1)	28(1)	30(1)	-10(1)	-6(1)	4(1)
C(3)	20(1)	20(1)	20(1)	-9(1)	-6(1)	3(1)
O(5)	25(1)	23(1)	27(1)	-12(1)	-10(1)	0(1)
C(4)	21(1)	19(1)	19(1)	-7(1)	-6(1)	1(1)
O(6)	24(1)	22(1)	19(1)	-7(1)	-4(1)	3(1)
C(25)	26(1)	21(1)	22(1)	-10(1)	-8(1)	3(1)

O(7)	68(1)	20(1)	21(1)	-7(1)	-4(1)	9(1)
O(8)	24(1)	18(1)	25(1)	-10(1)	-4(1)	4(1)
C(26)	24(1)	18(1)	32(1)	-13(1)	-4(1)	4(1)
C(27)	26(1)	32(1)	36(1)	-22(1)	-5(1)	4(1)
C(28)	28(1)	28(1)	38(1)	-16(1)	-11(1)	7(1)
C(5)	22(1)	19(1)	22(1)	-10(1)	-8(1)	3(1)
C(101)	20(1)	20(1)	20(1)	-11(1)	-6(1)	2(1)
C(106)	20(1)	26(1)	19(1)	-12(1)	-4(1)	3(1)
O(101)	31(1)	31(1)	28(1)	-20(1)	-14(1)	8(1)
O(102)	24(1)	21(1)	21(1)	-11(1)	-9(1)	5(1)
C(107)	27(1)	23(1)	21(1)	-10(1)	-10(1)	8(1)
C(108)	34(1)	24(1)	30(1)	-12(1)	-10(1)	5(1)
C(109)	37(1)	37(1)	22(1)	-11(1)	-10(1)	12(1)
C(110)	28(1)	31(1)	34(1)	-17(1)	-14(1)	9(1)
N(101)	18(1)	21(1)	18(1)	-10(1)	-5(1)	3(1)
C(111)	21(1)	18(1)	19(1)	-8(1)	-6(1)	4(1)
O(103)	18(1)	30(1)	26(1)	-14(1)	-8(1)	4(1)
C(112)	23(1)	18(1)	17(1)	-6(1)	-6(1)	4(1)
C(113)	21(1)	26(1)	22(1)	-11(1)	-6(1)	6(1)
C(114)	29(1)	30(1)	24(1)	-18(1)	-7(1)	10(1)
C(115)	31(1)	34(1)	28(1)	-21(1)	-12(1)	6(1)
C(116)	23(1)	32(1)	24(1)	-16(1)	-9(1)	4(1)
C(117)	22(1)	19(1)	19(1)	-9(1)	-5(1)	2(1)
C(118)	20(1)	22(1)	18(1)	-9(1)	-6(1)	2(1)
O(104)	18(1)	42(1)	28(1)	-22(1)	-4(1)	2(1)
C(102)	20(1)	23(1)	20(1)	-11(1)	-5(1)	3(1)
C(119)	24(1)	24(1)	19(1)	-10(1)	-4(1)	3(1)
C(120)	31(1)	26(1)	22(1)	-8(1)	-7(1)	-3(1)
C(121)	38(3)	36(3)	29(2)	-4(2)	-12(2)	-2(2)
C(122)	53(3)	34(2)	38(4)	-8(2)	-13(2)	-15(2)
C(123)	38(2)	48(2)	36(2)	-14(2)	-7(2)	-11(1)
C(124)	28(2)	33(2)	29(3)	-12(2)	-9(2)	1(2)
C(21B)	36(4)	17(3)	28(4)	-10(2)	-5(3)	-13(3)
C(22B)	35(4)	38(4)	26(5)	-7(3)	-2(3)	-12(3)
C(23B)	29(3)	47(4)	42(5)	-11(3)	3(3)	-8(2)
C(24B)	36(4)	43(5)	19(4)	-6(4)	-7(3)	-12(4)

C(103)	22(1)	23(1)	20(1)	-11(1)	-6(1)	4(1)
O(105)	25(1)	23(1)	26(1)	-14(1)	-1(1)	4(1)
C(104)	21(1)	23(1)	18(1)	-10(1)	-6(1)	3(1)
O(106)	20(1)	26(1)	20(1)	-10(1)	-5(1)	2(1)
O(107)	39(1)	22(1)	36(1)	-11(1)	-15(1)	4(1)
C(125)	22(1)	24(1)	22(1)	-12(1)	-3(1)	3(1)
O(108)	38(1)	23(1)	31(1)	-13(1)	-15(1)	0(1)
C(126)	38(3)	24(3)	41(3)	-18(2)	-17(2)	1(2)
C(127)	33(3)	31(3)	60(5)	-25(4)	-21(3)	4(2)
C(128)	89(7)	46(3)	50(3)	-29(3)	-36(4)	5(5)
C(26B)	38(5)	29(5)	45(4)	-27(4)	-18(4)	8(4)
C(27B)	31(5)	37(10)	43(5)	-19(5)	-10(4)	-2(5)
C(28B)	52(8)	51(9)	41(4)	-29(5)	-10(5)	-12(6)
C(105)	21(1)	20(1)	22(1)	-10(1)	-4(1)	1(1)
C(201)	22(1)	18(1)	20(1)	-9(1)	-5(1)	2(1)
C(206)	21(1)	20(1)	21(1)	-10(1)	-7(1)	2(1)
O(201)	29(1)	22(1)	26(1)	-10(1)	-2(1)	-3(1)
O(202)	24(1)	22(1)	19(1)	-10(1)	-3(1)	1(1)
C(207)	25(1)	30(1)	19(1)	-11(1)	-2(1)	2(1)
C(208)	47(1)	35(1)	26(1)	-18(1)	-2(1)	8(1)
C(209)	34(1)	34(1)	20(1)	-8(1)	-4(1)	2(1)
C(210)	24(1)	50(1)	30(1)	-17(1)	-1(1)	1(1)
N(201)	19(1)	19(1)	20(1)	-8(1)	-4(1)	2(1)
C(211)	22(1)	22(1)	18(1)	-10(1)	-4(1)	3(1)
O(203)	21(1)	24(1)	29(1)	-11(1)	-8(1)	1(1)
C(212)	21(1)	23(1)	16(1)	-9(1)	-2(1)	2(1)
C(213)	21(1)	24(1)	19(1)	-9(1)	-4(1)	4(1)
C(214)	27(1)	24(1)	20(1)	-6(1)	-4(1)	6(1)
C(215)	30(1)	22(1)	22(1)	-7(1)	-2(1)	-1(1)
C(216)	24(1)	23(1)	24(1)	-10(1)	-3(1)	-1(1)
C(217)	22(1)	23(1)	18(1)	-9(1)	-2(1)	1(1)
C(218)	21(1)	22(1)	19(1)	-11(1)	-3(1)	2(1)
O(204)	24(1)	23(1)	34(1)	-11(1)	-12(1)	2(1)
C(202)	20(1)	20(1)	20(1)	-7(1)	-5(1)	1(1)
C(219)	26(1)	22(1)	22(1)	-9(1)	-8(1)	2(1)
C(220)	29(1)	26(1)	26(1)	-8(1)	-11(1)	1(1)

C(221)	45(1)	36(1)	30(1)	-10(1)	-20(1)	-1(1)
C(222)	55(2)	43(3)	54(2)	-13(1)	-37(1)	4(1)
C(223)	66(3)	50(3)	71(2)	0(2)	-41(2)	-21(2)
C(22C)	55(2)	43(3)	54(2)	-13(1)	-37(1)	4(1)
C(23C)	66(3)	50(3)	71(2)	0(2)	-41(2)	-21(2)
C(224)	30(1)	41(1)	41(1)	-1(1)	-13(1)	-5(1)
C(203)	24(1)	20(1)	21(1)	-8(1)	-6(1)	3(1)
O(205)	26(1)	26(1)	30(1)	-14(1)	-10(1)	8(1)
C(204)	25(1)	26(1)	20(1)	-11(1)	-6(1)	3(1)
O(206)	26(1)	42(1)	21(1)	-12(1)	-2(1)	2(1)
C(225)	23(2)	24(2)	21(2)	-8(2)	-9(1)	7(2)
O(207)	31(2)	43(2)	34(2)	-28(2)	-12(1)	13(2)
O(208)	38(3)	22(1)	30(2)	-15(2)	-9(2)	1(2)
C(226)	49(3)	23(2)	47(3)	-20(2)	-23(2)	2(2)
C(227)	76(4)	29(2)	49(3)	-12(2)	-27(3)	-13(2)
C(228)	70(4)	54(3)	55(3)	-39(3)	-34(3)	8(3)
C(25C)	26(6)	22(6)	24(7)	-16(5)	-8(4)	4(3)
O(07C)	28(4)	28(5)	33(5)	-17(4)	-6(3)	7(3)
O(08C)	33(5)	24(3)	32(5)	-13(3)	-3(3)	-2(3)
C(26C)	38(6)	20(3)	35(5)	-11(4)	-3(4)	0(4)
C(27C)	58(7)	42(5)	44(5)	-21(4)	10(5)	-16(5)
C(28C)	85(11)	43(6)	46(5)	-24(6)	-18(6)	-8(7)
C(205)	24(1)	21(1)	22(1)	-11(1)	-7(1)	2(1)
C(301)	18(1)	17(1)	20(1)	-8(1)	-3(1)	1(1)
C(306)	15(1)	18(1)	20(1)	-8(1)	-1(1)	0(1)
O(301)	27(1)	18(1)	25(1)	-9(1)	-9(1)	4(1)
O(302)	20(1)	18(1)	18(1)	-8(1)	-5(1)	1(1)
C(307)	24(1)	20(1)	21(1)	-9(1)	-9(1)	1(1)
C(308)	33(1)	26(1)	27(1)	-14(1)	-11(1)	2(1)
C(309)	33(1)	25(1)	19(1)	-5(1)	-7(1)	-1(1)
C(310)	23(1)	29(1)	32(1)	-15(1)	-11(1)	3(1)
N(301)	17(1)	18(1)	18(1)	-8(1)	-3(1)	2(1)
C(311)	18(1)	23(1)	15(1)	-10(1)	-2(1)	0(1)
O(303)	18(1)	21(1)	23(1)	-7(1)	-4(1)	3(1)
C(312)	21(1)	21(1)	16(1)	-10(1)	-4(1)	2(1)
C(313)	22(1)	23(1)	20(1)	-9(1)	-4(1)	0(1)

C(314)	27(1)	20(1)	24(1)	-9(1)	-2(1)	-2(1)
C(315)	31(1)	20(1)	22(1)	-7(1)	-4(1)	4(1)
C(316)	22(1)	24(1)	22(1)	-8(1)	-6(1)	6(1)
C(317)	22(1)	20(1)	17(1)	-9(1)	-4(1)	2(1)
C(318)	21(1)	20(1)	18(1)	-9(1)	-4(1)	2(1)
O(304)	19(1)	24(1)	32(1)	-10(1)	-10(1)	2(1)
C(302)	17(1)	18(1)	22(1)	-9(1)	-4(1)	1(1)
C(319)	20(1)	22(1)	22(1)	-10(1)	-3(1)	-2(1)
C(320)	21(1)	25(1)	22(1)	-12(1)	-3(1)	-1(1)
C(321)	27(1)	36(1)	24(1)	-18(1)	-4(1)	2(1)
C(322)	30(1)	39(1)	30(1)	-19(1)	-1(1)	5(1)
C(323)	21(1)	42(1)	32(1)	-18(1)	-4(1)	4(1)
C(324)	22(1)	28(1)	27(1)	-14(1)	-6(1)	4(1)
C(303)	18(1)	20(1)	20(1)	-10(1)	-5(1)	1(1)
O(305)	19(1)	23(1)	34(1)	-17(1)	-6(1)	-1(1)
C(304)	20(1)	20(1)	20(1)	-9(1)	-7(1)	3(1)
O(306)	23(1)	24(1)	21(1)	-8(1)	-7(1)	2(1)
O(307)	34(1)	35(1)	35(1)	-24(1)	-14(1)	7(1)
C(325)	18(1)	24(1)	21(1)	-10(1)	-2(1)	0(1)
O(308)	40(1)	29(1)	38(1)	-22(1)	-21(1)	15(1)
C(326)	46(2)	32(1)	53(1)	-29(1)	-26(1)	18(1)
C(327)	134(5)	47(2)	73(2)	-34(2)	-64(2)	51(3)
C(328)	56(2)	59(3)	85(2)	-45(2)	-14(2)	29(2)
C(26D)	46(2)	32(1)	53(1)	-29(1)	-26(1)	18(1)
C(27D)	134(5)	47(2)	73(2)	-34(2)	-64(2)	51(3)
C(28D)	56(2)	59(3)	85(2)	-45(2)	-14(2)	29(2)
C(305)	18(1)	21(1)	23(1)	-13(1)	-4(1)	3(1)
O(1W)	85(3)	66(3)	59(2)	-23(2)	-16(2)	-16(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D11023.

	x	y	z	U(eq)
H(8A)	3669	11589	2984	49
H(8B)	4992	12005	2560	49
H(8C)	4574	11238	3593	49
H(9A)	4685	10402	1578	47
H(9B)	5115	11478	1311	47
H(9C)	3775	11115	1725	47
H(10A)	5918	10064	3412	49
H(10B)	6482	10857	2411	49
H(10C)	6041	9824	2560	49
H(13)	4226	9367	6481	32
H(14)	3044	9935	7453	36
H(15)	1108	10069	7487	35
H(16)	258	9608	6574	30
H(2)	1030	8262	4222	22
H(19A)	2462	9518	2547	24
H(19B)	1418	8945	2482	24
H(20)	1072	10063	3491	26
H(21A)	1590	11250	2028	31
H(21B)	938	10667	1643	31
H(22A)	-405	11691	1879	37
H(22B)	-149	11504	2837	37
H(23A)	-1428	10236	2460	38
H(23B)	-1720	10413	3361	38
H(24A)	-525	8980	3180	34
H(24B)	-673	9243	4025	34
H(3)	2456	7475	3120	23
H(5)	327(18)	6874(16)	4115(12)	35
H(6)	1231(19)	6145(14)	5695(12)	34
H(26)	3068	4422	4193	29
H(27A)	2789	5171	2706	44

H(27B)	3790	4478	2748	44
H(27C)	4108	5601	2324	44
H(28A)	5277	5500	3437	46
H(28B)	5104	4368	3831	46
H(28C)	4726	4873	4494	46
H(5A)	3861	7263	4203	24
H(5B)	3169	7103	5206	24
H(10D)	2552	365	8937	43
H(10E)	3790	73	9100	43
H(10F)	3685	838	8129	43
H(10G)	2932	1591	10238	48
H(10H)	3298	545	10436	48
H(10I)	2089	829	10202	48
H(11A)	4980	2116	8151	43
H(11B)	5188	1273	9046	43
H(11C)	4768	2242	9070	43
H(113)	4556	2632	5337	27
H(114)	3809	2122	4412	31
H(115)	1845	2003	4540	33
H(116)	541	2404	5591	30
H(102)	252	3618	8070	24
H(11D)	1026	2433	9610	26
H(11E)	-154	2888	9777	26
H(20A)	232	1740	8822	32
H(20B)	176	1689	8837	32
H(12A)	28	622	10373	45
H(12B)	-932	1194	10737	45
H(12C)	-1229	64	9801	53
H(12D)	-2057	-2	10734	53
H(12E)	-2989	1218	10011	51
H(12F)	-2464	1021	9137	51
H(12G)	-1814	2555	9435	36
H(12H)	-1461	2449	8498	36
H(21C)	143	513	10106	33
H(21D)	-433	1058	10706	33
H(22C)	-1609	84	9967	43

H(22D)	-2026	86	10952	43
H(23C)	-2564	1613	10350	53
H(23D)	-2978	1165	9748	53
H(24C)	-1423	1917	8535	42
H(24D)	-1602	2704	8929	42
H(103)	1325	4397	9020	25
H(105)	-220(20)	5204(13)	8857(16)	37
H(106)	237(15)	5456(16)	7205(14)	33
H(126)	2622	7371	7982	38
H(12I)	4197	7246	6914	57
H(12J)	4750	6559	7707	57
H(12K)	4666	7649	7520	57
H(12L)	2385	6417	9541	83
H(12M)	3538	7117	9174	83
H(12N)	3613	6030	9348	83
H(26B)	2791	7346	8018	38
H(27D)	4176	7111	6850	54
H(27E)	4862	6538	7593	54
H(27F)	4730	7641	7322	54
H(28D)	2703	6239	9537	67
H(28E)	3829	6974	9133	67
H(28F)	3929	5923	9200	67
H(10J)	3196	4720	7640	25
H(10K)	2841	4865	6728	25
H(20C)	6047	9300	10639	54
H(20D)	4774	9003	11292	54
H(20E)	4954	9536	10217	54
H(20F)	5772	6804	11342	46
H(20G)	5246	7294	11997	46
H(20H)	6517	7645	11347	46
H(21E)	3828	8237	10138	54
H(21F)	3503	7753	11222	54
H(21G)	4070	7160	10676	54
H(213)	5220	11088	6704	26
H(214)	5971	12675	6168	30
H(215)	7720	13034	6387	32

H(216)	8771	11812	7170	29
H(202)	9046	8254	8372	25
H(21H)	8244	8257	9814	28
H(21I)	7837	7153	10227	28
H(220)	9794	6810	10004	33
H(21J)	8995	7766	11138	44
H(21K)	9141	6652	11458	44
H(21L)	9085	7814	11121	44
H(21M)	9074	6677	11467	44
H(22E)	11126	6912	11100	59
H(22F)	10701	7615	11569	59
H(22G)	12008	8337	9956	81
H(22H)	10968	8915	10204	81
H(22I)	11624	8663	10048	59
H(22J)	12090	7785	9846	59
H(23E)	10846	7598	11457	81
H(23F)	11038	6730	11175	81
H(24I)	10304	8793	9103	50
H(24J)	11143	7994	9056	50
H(24K)	10973	8122	8913	50
H(24L)	10312	8831	9293	50
H(203)	8041	6321	9208	26
H(205)	10116(19)	6928(16)	8090(12)	39
H(206)	9250(20)	7521(18)	6706(15)	46
H(226)	7819	4432	8146	43
H(22K)	6524	4021	9566	76
H(22L)	6081	3446	9085	76
H(22M)	5480	4363	9099	76
H(22N)	7214	5211	6800	76
H(22O)	5911	5103	7367	76
H(22P)	6515	4183	7365	76
H(26C)	7343	4257	8502	39
H(27G)	5999	4098	9825	77
H(27H)	5477	3495	9402	77
H(27I)	5044	4509	9274	77
H(28G)	6939	5018	7083	84

H(28H)	5636	5085	7546	84
H(28I)	6075	4073	7673	84
H(20I)	6396	7078	8295	26
H(20J)	6950	8019	7391	26
H(30A)	8340	2932	1216	41
H(30B)	7163	3035	906	41
H(30C)	7151	2435	1949	41
H(30D)	7877	5313	836	40
H(30E)	7706	4829	195	40
H(30F)	8817	4666	595	40
H(31A)	5728	3505	2425	40
H(31B)	5690	3976	1384	40
H(31C)	6005	4628	1840	40
H(313)	5526	698	4923	26
H(314)	6086	-843	5586	29
H(315)	7969	-1075	5724	30
H(316)	9356	232	5176	28
H(302)	10093	3832	3584	22
H(31D)	9778	4882	1805	26
H(31E)	10975	5005	2023	26
H(320)	10057	3195	2270	26
H(32A)	10546	3726	759	33
H(32B)	11141	4715	617	33
H(32C)	12758	4082	162	39
H(32D)	12219	3008	836	39
H(32E)	13053	4382	1358	38
H(32F)	13442	3326	1604	38
H(32G)	11871	3547	2804	30
H(32H)	11691	2623	2631	30
H(303)	9370	5716	2917	23
H(305)	10770(20)	5939(13)	3411(16)	36
H(306)	9818(14)	4352(13)	4963(15)	35
H(326)	8042	7356	4223	45
H(32I)	7948	7874	2725	113
H(32J)	6989	8341	3211	113
H(32K)	6627	7456	3045	113

H(32L)	6512	6401	5434	94
H(32M)	5715	6539	4755	94
H(32N)	6094	7421	4916	94
H(26D)	7657	7369	4279	45
H(27J)	7396	7682	2793	113
H(27K)	6498	8146	3326	113
H(27L)	6108	7192	3283	113
H(28J)	6432	6105	5525	94
H(28K)	5600	6118	4903	94
H(28L)	5723	7000	5139	94
H(30G)	7215	4742	3943	24
H(30H)	7372	3786	4777	24
H(1W)	8670(70)	6990(40)	5390(50)	108
H(2W)	9460(50)	7770(50)	5130(40)	108

Table 6. Hydrogen bonds for D11023 [Å and °].

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
O(5)-H(5)...O(6)	0.845(16)	2.18(2)	2.6709(15)	117.0(18)
O(5)-H(5)...O(307)#1	0.845(16)	2.284(19)	3.0061(17)	144(2)
O(6)-H(6)...O(106)	0.824(16)	1.929(18)	2.7046(15)	156(2)
O(105)-H(105)...O(205)#1	0.817(17)	2.029(18)	2.8259(17)	165(2)
O(106)-H(106)...O(207)#1	0.834(16)	2.036(18)	2.793(4)	151(2)
O(106)-H(106)...O(07C)#1	0.834(16)	2.06(2)	2.863(10)	161(2)
O(106)-H(106)...O(105)	0.834(16)	2.40(2)	2.8210(15)	111.7(17)
O(205)-H(205)...O(206)	0.829(16)	2.31(2)	2.7410(16)	112.5(19)
O(205)-H(205)...O(107)#2	0.829(16)	2.34(2)	3.0293(18)	140(2)
O(206)-H(206)...O(207)	0.831(17)	2.07(3)	2.572(6)	118(2)
O(206)-H(206)...O(1W)	0.831(17)	2.15(2)	2.849(4)	141(2)
O(206)-H(206)...O(07C)	0.831(17)	2.53(3)	2.931(13)	111(2)
O(305)-H(305)...O(5)#2	0.821(16)	1.931(17)	2.7453(17)	171(2)
O(306)-H(306)...O(305)	0.781(16)	2.40(2)	2.7945(15)	112.4(19)
O(1W)-H(1W)...O(307)	0.90(2)	2.05(3)	2.927(5)	164(8)
O(1W)-H(2W)...O(4)#2	0.89(2)	2.20(6)	2.795(4)	123(6)

Symmetry transformations used to generate equivalent atoms:

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

Absolute configuration of the products from cycloaddition of the phosphorus-substituted olefin: Hydrolysis product (carboxylic acid) of Table 4, entry 1, derived from catalyst (*S*)-**1**.

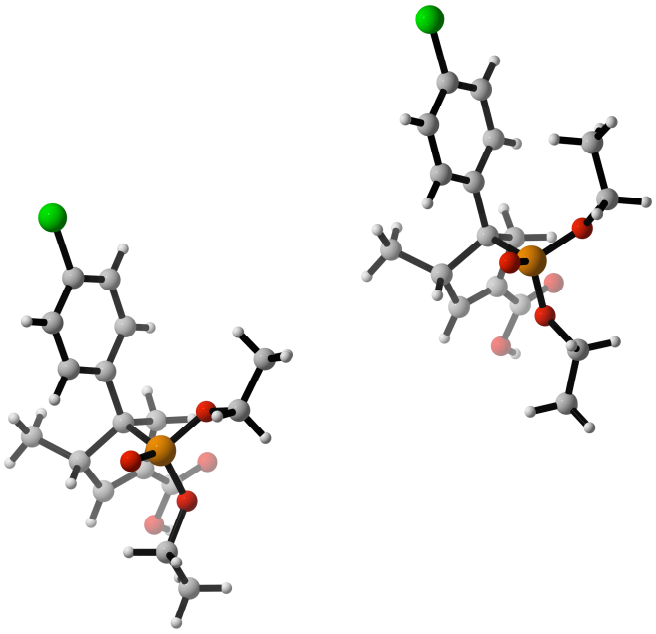


Table 1. Crystal data and structure refinement for D11020.

Identification code	d11020	
Empirical formula	C17 H22 Cl O5 P	
Formula weight	372.77	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 13.1781(3) Å	a= 90°.
	b = 9.1516(2) Å	b= 99.3710(10)°.
	c = 15.7055(3) Å	g = 90°.
Volume	1868.82(7) Å^3	
Z	4	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	2.822 mm^{-1}	
F(000)	784	
Crystal size	0.35 x 0.20 x 0.10 mm^3	

Theta range for data collection	2.85 to 69.31°.
Index ranges	-15<=h<=15, -11<=k<=10, -19<=l<=19
Reflections collected	40092
Independent reflections	6681 [R(int) = 0.0260]
Completeness to theta = 69.31°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7656 and 0.4384
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6681 / 1 / 441
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0266, wR2 = 0.0708
R indices (all data)	R1 = 0.0270, wR2 = 0.0712
Absolute structure parameter	0.010(8)
Largest diff. peak and hole	0.304 and -0.400 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for D11020. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	1590(1)	3175(1)	8900(1)	15(1)
O(1)	1011(1)	1850(1)	9075(1)	20(1)
O(2)	2518(1)	2924(1)	8407(1)	19(1)
C(1)	2443(1)	1825(2)	7717(1)	23(1)
C(2)	3498(2)	1397(3)	7598(1)	39(1)
O(3)	882(1)	4304(1)	8315(1)	19(1)
C(3)	-232(1)	4304(2)	8281(1)	25(1)
C(4)	-635(1)	5733(2)	7897(1)	28(1)
C(5)	2207(1)	4134(2)	9872(1)	16(1)
C(11)	2980(1)	3046(2)	10341(1)	17(1)
C(12)	2631(1)	1790(2)	10710(1)	20(1)
C(13)	3306(1)	749(2)	11111(1)	23(1)
C(14)	4353(1)	966(2)	11145(1)	23(1)
Cl(1)	5212(1)	-342(1)	11651(1)	29(1)
C(15)	4733(1)	2191(2)	10786(1)	22(1)
C(16)	4042(1)	3217(2)	10381(1)	19(1)
C(6)	2671(1)	5599(2)	9610(1)	17(1)
C(7)	1823(1)	6689(2)	9656(1)	17(1)
C(17)	1892(1)	8197(2)	9326(1)	19(1)
O(4)	2588(1)	8602(1)	8965(1)	29(1)
O(5)	1114(1)	9042(1)	9468(1)	25(1)
C(8)	1091(1)	6150(2)	10058(1)	18(1)
C(9)	1333(1)	4627(2)	10393(1)	17(1)
C(10)	1670(1)	4727(2)	11375(1)	24(1)
P(2)	6717(1)	2271(1)	4193(1)	15(1)
O(101)	6250(1)	838(1)	4334(1)	20(1)
O(102)	7566(1)	2201(1)	3598(1)	21(1)
C(101)	7914(1)	852(2)	3232(1)	23(1)
C(102)	8885(1)	305(2)	3774(1)	23(1)
O(103)	5909(1)	3423(1)	3758(1)	20(1)
C(103)	5228(1)	3029(2)	2965(1)	23(1)

C(104)	4277(1)	3950(3)	2900(1)	35(1)
C(105)	7314(1)	3211(2)	5176(1)	16(1)
C(111)	8128(1)	2163(2)	5622(1)	16(1)
C(112)	7836(1)	877(2)	6005(1)	18(1)
C(113)	8562(1)	-101(2)	6403(1)	20(1)
C(114)	9597(1)	204(2)	6427(1)	20(1)
Cl(2)	10518(1)	-998(1)	6954(1)	27(1)
C(115)	9915(1)	1439(2)	6033(1)	20(1)
C(116)	9174(1)	2401(2)	5629(1)	18(1)
C(106)	7749(1)	4712(2)	4934(1)	17(1)
C(107)	6898(1)	5763(2)	5019(1)	18(1)
C(117)	6955(1)	7276(2)	4704(1)	18(1)
O(104)	7655(1)	7694(1)	4354(1)	25(1)
O(105)	6174(1)	8123(1)	4841(1)	25(1)
C(108)	6175(1)	5174(2)	5415(1)	19(1)
C(109)	6431(1)	3630(2)	5706(1)	18(1)
C(110)	6763(1)	3641(2)	6693(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for D11020.

P(1)-O(1)	1.4825(12)
P(1)-O(2)	1.5673(11)
P(1)-O(3)	1.5823(12)
P(1)-C(5)	1.8324(16)
O(2)-C(1)	1.469(2)
C(1)-C(2)	1.485(2)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
O(3)-C(3)	1.4606(19)
C(3)-C(4)	1.500(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(11)	1.525(2)
C(5)-C(6)	1.556(2)
C(5)-C(9)	1.583(2)
C(11)-C(12)	1.399(2)
C(11)-C(16)	1.400(2)
C(12)-C(13)	1.383(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(3)
C(14)-Cl(1)	1.7467(17)
C(15)-C(16)	1.388(2)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(6)-C(7)	1.508(2)
C(6)-H(6A)	0.9900

C(6)-H(6B)	0.9900
C(7)-C(8)	1.331(2)
C(7)-C(17)	1.482(2)
C(17)-O(4)	1.212(2)
C(17)-O(5)	1.332(2)
O(5)-H(5)	0.8400
C(8)-C(9)	1.505(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.537(2)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
P(2)-O(101)	1.4805(13)
P(2)-O(102)	1.5708(11)
P(2)-O(103)	1.5729(12)
P(2)-C(105)	1.8291(16)
O(102)-C(101)	1.467(2)
C(101)-C(102)	1.502(2)
C(101)-H(10D)	0.9900
C(101)-H(10E)	0.9900
C(102)-H(10F)	0.9800
C(102)-H(10G)	0.9800
C(102)-H(10H)	0.9800
O(103)-C(103)	1.4568(19)
C(103)-C(104)	1.500(3)
C(103)-H(10I)	0.9900
C(103)-H(10J)	0.9900
C(104)-H(10K)	0.9800
C(104)-H(10L)	0.9800
C(104)-H(10M)	0.9800
C(105)-C(111)	1.522(2)
C(105)-C(106)	1.559(2)
C(105)-C(109)	1.584(2)
C(111)-C(116)	1.395(2)
C(111)-C(112)	1.404(2)

C(112)-C(113)	1.383(2)
C(112)-H(112)	0.9500
C(113)-C(114)	1.387(2)
C(113)-H(113)	0.9500
C(114)-C(115)	1.385(2)
C(114)-Cl(2)	1.7435(17)
C(115)-C(116)	1.389(2)
C(115)-H(115)	0.9500
C(116)-H(116)	0.9500
C(106)-C(107)	1.499(2)
C(106)-H(10N)	0.9900
C(106)-H(10O)	0.9900
C(107)-C(108)	1.334(2)
C(107)-C(117)	1.476(2)
C(117)-O(104)	1.211(2)
C(117)-O(105)	1.334(2)
O(105)-H(105)	0.8400
C(108)-C(109)	1.506(2)
C(108)-H(108)	0.9500
C(109)-C(110)	1.541(2)
C(109)-H(109)	1.0000
C(110)-H(11A)	0.9800
C(110)-H(11B)	0.9800
C(110)-H(11C)	0.9800

O(1)-P(1)-O(2)	116.06(7)
O(1)-P(1)-O(3)	111.62(6)
O(2)-P(1)-O(3)	104.07(6)
O(1)-P(1)-C(5)	114.15(7)
O(2)-P(1)-C(5)	101.87(6)
O(3)-P(1)-C(5)	108.10(7)
C(1)-O(2)-P(1)	119.97(10)
O(2)-C(1)-C(2)	108.71(14)
O(2)-C(1)-H(1A)	109.9
C(2)-C(1)-H(1A)	109.9
O(2)-C(1)-H(1B)	109.9

C(2)-C(1)-H(1B)	109.9
H(1A)-C(1)-H(1B)	108.3
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(3)-O(3)-P(1)	121.06(10)
O(3)-C(3)-C(4)	107.57(14)
O(3)-C(3)-H(3A)	110.2
C(4)-C(3)-H(3A)	110.2
O(3)-C(3)-H(3B)	110.2
C(4)-C(3)-H(3B)	110.2
H(3A)-C(3)-H(3B)	108.5
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(11)-C(5)-C(6)	115.46(12)
C(11)-C(5)-C(9)	114.94(13)
C(6)-C(5)-C(9)	103.93(13)
C(11)-C(5)-P(1)	105.11(11)
C(6)-C(5)-P(1)	109.41(10)
C(9)-C(5)-P(1)	107.78(10)
C(12)-C(11)-C(16)	117.85(15)
C(12)-C(11)-C(5)	119.83(14)
C(16)-C(11)-C(5)	122.23(15)
C(13)-C(12)-C(11)	121.59(16)
C(13)-C(12)-H(12)	119.2
C(11)-C(12)-H(12)	119.2
C(12)-C(13)-C(14)	118.80(17)
C(12)-C(13)-H(13)	120.6
C(14)-C(13)-H(13)	120.6

C(15)-C(14)-C(13)	121.55(16)
C(15)-C(14)-Cl(1)	119.38(13)
C(13)-C(14)-Cl(1)	119.07(14)
C(14)-C(15)-C(16)	118.79(15)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.6
C(15)-C(16)-C(11)	121.40(16)
C(15)-C(16)-H(16)	119.3
C(11)-C(16)-H(16)	119.3
C(7)-C(6)-C(5)	103.41(12)
C(7)-C(6)-H(6A)	111.1
C(5)-C(6)-H(6A)	111.1
C(7)-C(6)-H(6B)	111.1
C(5)-C(6)-H(6B)	111.1
H(6A)-C(6)-H(6B)	109.0
C(8)-C(7)-C(17)	127.00(15)
C(8)-C(7)-C(6)	112.14(15)
C(17)-C(7)-C(6)	120.73(14)
O(4)-C(17)-O(5)	124.18(16)
O(4)-C(17)-C(7)	122.87(15)
O(5)-C(17)-C(7)	112.95(13)
C(17)-O(5)-H(5)	109.5
C(7)-C(8)-C(9)	112.35(14)
C(7)-C(8)-H(8)	123.8
C(9)-C(8)-H(8)	123.8
C(8)-C(9)-C(10)	107.76(14)
C(8)-C(9)-C(5)	102.39(12)
C(10)-C(9)-C(5)	114.84(12)
C(8)-C(9)-H(9)	110.5
C(10)-C(9)-H(9)	110.5
C(5)-C(9)-H(9)	110.5
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5

H(10B)-C(10)-H(10C)	109.5
O(101)-P(2)-O(102)	114.00(7)
O(101)-P(2)-O(103)	113.01(7)
O(102)-P(2)-O(103)	105.44(6)
O(101)-P(2)-C(105)	114.93(7)
O(102)-P(2)-C(105)	105.70(7)
O(103)-P(2)-C(105)	102.65(7)
C(101)-O(102)-P(2)	124.44(11)
O(102)-C(101)-C(102)	110.50(14)
O(102)-C(101)-H(10D)	109.5
C(102)-C(101)-H(10D)	109.5
O(102)-C(101)-H(10E)	109.5
C(102)-C(101)-H(10E)	109.5
H(10D)-C(101)-H(10E)	108.1
C(101)-C(102)-H(10F)	109.5
C(101)-C(102)-H(10G)	109.5
H(10F)-C(102)-H(10G)	109.5
C(101)-C(102)-H(10H)	109.5
H(10F)-C(102)-H(10H)	109.5
H(10G)-C(102)-H(10H)	109.5
C(103)-O(103)-P(2)	118.98(11)
O(103)-C(103)-C(104)	108.09(14)
O(103)-C(103)-H(10I)	110.1
C(104)-C(103)-H(10I)	110.1
O(103)-C(103)-H(10J)	110.1
C(104)-C(103)-H(10J)	110.1
H(10I)-C(103)-H(10J)	108.4
C(103)-C(104)-H(10K)	109.5
C(103)-C(104)-H(10L)	109.5
H(10K)-C(104)-H(10L)	109.5
C(103)-C(104)-H(10M)	109.5
H(10K)-C(104)-H(10M)	109.5
H(10L)-C(104)-H(10M)	109.5
C(111)-C(105)-C(106)	114.05(12)
C(111)-C(105)-C(109)	115.66(12)
C(106)-C(105)-C(109)	104.18(13)

C(111)-C(105)-P(2)	105.47(11)
C(106)-C(105)-P(2)	109.48(10)
C(109)-C(105)-P(2)	107.83(10)
C(116)-C(111)-C(112)	117.84(15)
C(116)-C(111)-C(105)	121.83(15)
C(112)-C(111)-C(105)	120.25(14)
C(113)-C(112)-C(111)	121.24(15)
C(113)-C(112)-H(112)	119.4
C(111)-C(112)-H(112)	119.4
C(112)-C(113)-C(114)	119.15(16)
C(112)-C(113)-H(113)	120.4
C(114)-C(113)-H(113)	120.4
C(115)-C(114)-C(113)	121.30(15)
C(115)-C(114)-Cl(2)	119.26(13)
C(113)-C(114)-Cl(2)	119.44(14)
C(114)-C(115)-C(116)	118.72(15)
C(114)-C(115)-H(115)	120.6
C(116)-C(115)-H(115)	120.6
C(115)-C(116)-C(111)	121.66(16)
C(115)-C(116)-H(116)	119.2
C(111)-C(116)-H(116)	119.2
C(107)-C(106)-C(105)	103.52(12)
C(107)-C(106)-H(10N)	111.1
C(105)-C(106)-H(10N)	111.1
C(107)-C(106)-H(10O)	111.1
C(105)-C(106)-H(10O)	111.1
H(10N)-C(106)-H(10O)	109.0
C(108)-C(107)-C(117)	127.89(16)
C(108)-C(107)-C(106)	112.55(16)
C(117)-C(107)-C(106)	119.53(14)
O(104)-C(117)-O(105)	123.70(16)
O(104)-C(117)-C(107)	122.13(15)
O(105)-C(117)-C(107)	114.17(14)
C(117)-O(105)-H(105)	109.5
C(107)-C(108)-C(109)	112.29(15)
C(107)-C(108)-H(108)	123.9

C(109)-C(108)-H(108)	123.9
C(108)-C(109)-C(110)	108.20(14)
C(108)-C(109)-C(105)	102.40(13)
C(110)-C(109)-C(105)	114.73(13)
C(108)-C(109)-H(109)	110.4
C(110)-C(109)-H(109)	110.4
C(105)-C(109)-H(109)	110.4
C(109)-C(110)-H(11A)	109.5
C(109)-C(110)-H(11B)	109.5
H(11A)-C(110)-H(11B)	109.5
C(109)-C(110)-H(11C)	109.5
H(11A)-C(110)-H(11C)	109.5
H(11B)-C(110)-H(11C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D11020. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \ldots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	15(1)	12(1)	18(1)	1(1)	4(1)	0(1)
O(1)	18(1)	16(1)	25(1)	2(1)	4(1)	0(1)
O(2)	19(1)	18(1)	21(1)	-4(1)	6(1)	-2(1)
C(1)	25(1)	22(1)	22(1)	-7(1)	6(1)	-4(1)
C(2)	30(1)	41(1)	44(1)	-23(1)	4(1)	8(1)
O(3)	17(1)	19(1)	20(1)	4(1)	3(1)	0(1)
C(3)	17(1)	27(1)	32(1)	6(1)	1(1)	0(1)
C(4)	23(1)	29(1)	31(1)	5(1)	5(1)	7(1)
C(5)	15(1)	16(1)	18(1)	-1(1)	4(1)	-1(1)
C(11)	20(1)	16(1)	16(1)	-1(1)	5(1)	2(1)
C(12)	21(1)	21(1)	21(1)	2(1)	6(1)	2(1)
C(13)	30(1)	20(1)	21(1)	4(1)	8(1)	4(1)
C(14)	27(1)	25(1)	18(1)	4(1)	5(1)	11(1)
Cl(1)	30(1)	31(1)	28(1)	11(1)	9(1)	17(1)
C(15)	20(1)	29(1)	19(1)	1(1)	6(1)	5(1)
C(16)	21(1)	20(1)	17(1)	1(1)	5(1)	2(1)
C(6)	16(1)	13(1)	21(1)	1(1)	4(1)	1(1)
C(7)	17(1)	15(1)	18(1)	-2(1)	2(1)	2(1)
C(17)	19(1)	16(1)	21(1)	0(1)	4(1)	0(1)
O(4)	28(1)	18(1)	44(1)	8(1)	17(1)	2(1)
O(5)	24(1)	13(1)	39(1)	6(1)	12(1)	3(1)
C(8)	18(1)	16(1)	20(1)	-1(1)	3(1)	3(1)
C(9)	16(1)	16(1)	19(1)	0(1)	6(1)	1(1)
C(10)	27(1)	25(1)	19(1)	2(1)	7(1)	6(1)
P(2)	14(1)	12(1)	18(1)	0(1)	3(1)	0(1)
O(101)	18(1)	16(1)	25(1)	0(1)	3(1)	-1(1)
O(102)	23(1)	17(1)	24(1)	-2(1)	10(1)	0(1)
C(101)	26(1)	21(1)	24(1)	-5(1)	8(1)	3(1)
C(102)	25(1)	20(1)	25(1)	0(1)	8(1)	1(1)
O(103)	20(1)	17(1)	20(1)	-1(1)	-1(1)	2(1)
C(103)	25(1)	23(1)	20(1)	-1(1)	-3(1)	2(1)

C(104)	25(1)	45(1)	34(1)	-1(1)	-3(1)	10(1)
C(105)	14(1)	16(1)	18(1)	0(1)	3(1)	-2(1)
C(111)	17(1)	15(1)	16(1)	-1(1)	2(1)	0(1)
C(112)	18(1)	19(1)	19(1)	0(1)	4(1)	-1(1)
C(113)	24(1)	17(1)	19(1)	1(1)	3(1)	-1(1)
C(114)	22(1)	18(1)	19(1)	0(1)	-1(1)	4(1)
Cl(2)	23(1)	20(1)	35(1)	4(1)	-3(1)	5(1)
C(115)	16(1)	20(1)	21(1)	-3(1)	0(1)	-1(1)
C(116)	19(1)	17(1)	19(1)	-1(1)	4(1)	-3(1)
C(106)	17(1)	13(1)	21(1)	0(1)	4(1)	-1(1)
C(107)	19(1)	15(1)	19(1)	-2(1)	2(1)	0(1)
C(117)	19(1)	14(1)	20(1)	-2(1)	2(1)	2(1)
O(104)	27(1)	17(1)	33(1)	3(1)	14(1)	1(1)
O(105)	23(1)	14(1)	41(1)	4(1)	12(1)	3(1)
C(108)	18(1)	18(1)	22(1)	-3(1)	5(1)	1(1)
C(109)	17(1)	17(1)	21(1)	0(1)	6(1)	-1(1)
C(110)	31(1)	28(1)	21(1)	-1(1)	10(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D11020.

	x	y	z	U(eq)
H(1A)	2065	2235	7173	27
H(1B)	2064	958	7875	27
H(2A)	3855	2249	7410	58
H(2B)	3457	628	7160	58
H(2C)	3877	1033	8146	58
H(3A)	-403	4194	8869	30
H(3B)	-546	3482	7922	30
H(4A)	-320	6538	8259	42
H(4B)	-1383	5765	7865	42
H(4C)	-463	5829	7315	42
H(12)	1913	1648	10685	25
H(13)	3057	-98	11358	28
H(15)	5452	2327	10817	27
H(16)	4296	4053	10125	23
H(6A)	3300	5859	10017	20
H(6B)	2838	5542	9019	20
H(5)	1209	9898	9304	37
H(8)	485	6668	10127	22
H(9)	716	3982	10251	20
H(10A)	2305	5299	11502	35
H(10B)	1791	3742	11615	35
H(10C)	1128	5204	11634	35
H(10D)	8039	1039	2637	28
H(10E)	7371	97	3205	28
H(10F)	9406	1078	3833	34
H(10G)	9138	-549	3496	34
H(10H)	8743	30	4346	34
H(10I)	5046	1981	2975	28
H(10J)	5574	3205	2460	28
H(10K)	3924	3736	3389	53

H(10L)	3819	3730	2359	53
H(10M)	4468	4986	2911	53
H(112)	7126	674	5991	22
H(113)	8354	-970	6657	24
H(115)	10625	1624	6040	24
H(116)	9386	3242	5350	22
H(10N)	8384	4967	5335	20
H(10O)	7899	4701	4337	20
H(105)	6253	8967	4651	38
H(108)	5568	5671	5503	23
H(109)	5821	2980	5542	21
H(11A)	7395	4215	6841	39
H(11B)	6888	2637	6901	39
H(11C)	6217	4079	6965	39

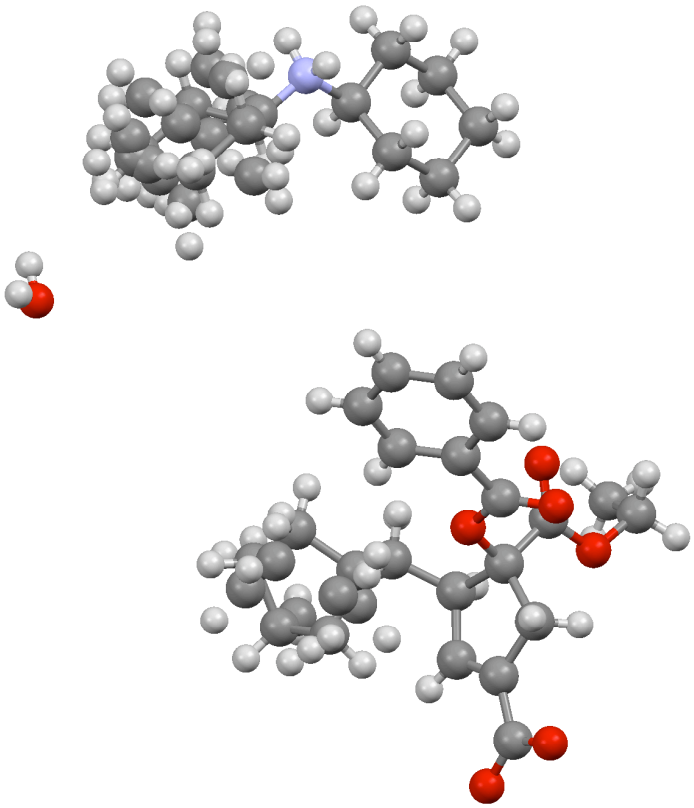
Table 6. Hydrogen bonds for D11020 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(1)#1	0.84	1.83	2.6408(18)	160.9
O(105)-H(105)...O(101)#1	0.84	1.78	2.6158(17)	170.6

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z

Absolute configuration of the products from cycloaddition of the oxygen-substituted olefin: Dicyclohexylamine salt of the hydrolysis product (carboxylic acid) of Table 5, entry 3, derived from catalyst (*R*)-**1**.



The Flack test for this structure is inconclusive. However the method by Spek and Hooft, which is based on Bayesian statistics, results in the following probabilities: The probability P2 of the model to be correct assuming that the sample is KNOWN to be enantiomerically pure is 1.0. The probability P3 of the model to be correct assuming that the structure is either right or wrong or a 50:50 racemic twin is 1.0. The probability of the model to be a 50:50 racemic twin is 0.8E-18. The inverted model gives rise to opposite results in the Bayesian statistics, further improving the confidence in the absolute configuration as determined by X-ray diffraction.

Table 1. Crystal data and structure refinement for D11026.

Identification code	d11026
Empirical formula	C34 H51 N O7
Formula weight	585.76
Temperature	100(2) K

Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.5202(3) Å	a= 90°.
	b = 10.1753(3) Å	b= 94.524(2)°.
	c = 16.8674(5) Å	g = 90°.
Volume	1628.87(9) $Å^3$	
Z	2	
Density (calculated)	1.194 Mg/m^3	
Absorption coefficient	0.662 mm^{-1}	
F(000)	636	
Crystal size	0.45 x 0.15 x 0.07 mm^3	
Theta range for data collection	2.63 to 69.22°.	
Index ranges	-11<=h<=9, -12<=k<=12, -20<=l<=20	
Reflections collected	32466	
Independent reflections	5887 [R(int) = 0.0428]	
Completeness to theta = 69.22°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9551 and 0.7549	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5887 / 714 / 549	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1396	
R indices (all data)	R1 = 0.0555, wR2 = 0.1448	
Absolute structure parameter	-0.1(2)	
Largest diff. peak and hole	0.239 and -0.186 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for D11026. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3930(3)	734(3)	2570(2)	47(1)
C(6)	5454(3)	1181(3)	2680(2)	48(1)
O(1)	6232(2)	951(2)	3260(1)	61(1)
O(2)	5785(2)	1912(2)	2072(1)	59(1)
C(7)	7175(4)	2508(4)	2129(2)	75(1)
C(8)	7191(5)	3740(4)	2616(3)	90(1)
O(3)	3754(2)	-335(2)	3116(1)	47(1)
O(4)	5259(2)	-1581(2)	2469(1)	62(1)
C(10)	4555(3)	-1418(3)	3024(2)	49(1)
C(11)	4442(3)	-2375(3)	3677(2)	47(1)
C(12)	3611(3)	-2158(2)	4307(2)	49(1)
C(13)	3589(3)	-3062(3)	4914(2)	55(1)
C(14)	4385(3)	-4201(3)	4898(2)	60(1)
C(15)	5190(3)	-4430(3)	4266(2)	62(1)
C(16)	5227(3)	-3527(3)	3658(2)	55(1)
C(2)	2936(3)	1887(3)	2819(2)	47(1)
C(17)	2432(3)	1776(3)	3652(2)	58(1)
C(18)	1929(7)	3055(5)	3975(3)	52(1)
C(19)	1644(7)	2959(5)	4858(3)	58(1)
C(20)	645(8)	4074(8)	5007(4)	67(2)
C(21)	71(11)	4541(9)	4206(4)	91(3)
C(22)	532(6)	3527(6)	3610(3)	63(2)
C(18A)	1182(10)	2796(8)	3852(5)	53(2)
C(19A)	752(15)	2744(11)	4708(6)	85(3)
C(20A)	90(17)	4074(13)	4825(7)	82(3)
C(21A)	594(13)	4979(10)	4209(8)	68(3)
C(22A)	1615(10)	4176(8)	3750(5)	66(2)
C(3)	1812(3)	1909(3)	2142(2)	48(1)
C(4)	2056(3)	1113(2)	1551(2)	45(1)
C(23)	1178(3)	931(2)	782(2)	47(1)
O(5)	1537(2)	9(2)	352(1)	52(1)

O(6)	140(2)	1676(2)	622(1)	65(1)
C(5)	3387(3)	365(3)	1712(2)	56(1)
N(1)	9018(2)	1361(3)	9071(1)	52(1)
C(31)	9492(3)	2414(3)	8539(2)	50(1)
C(32)	11045(3)	2721(4)	8750(2)	64(1)
C(33)	11554(3)	3784(4)	8215(2)	73(1)
C(34)	11295(3)	3418(4)	7344(2)	65(1)
C(35)	9760(3)	3101(3)	7134(2)	66(1)
C(36)	9242(3)	2029(3)	7674(2)	56(1)
C(41)	7408(7)	1284(8)	9054(5)	41(2)
C(42)	6809(5)	1889(5)	9771(3)	39(1)
C(43)	5212(6)	1720(6)	9741(4)	50(1)
C(44)	4761(10)	313(10)	9606(6)	61(2)
C(45)	5400(7)	-269(8)	8898(5)	74(2)
C(46)	6985(6)	-134(6)	8944(4)	60(2)
C(41A)	7516(10)	764(10)	9036(8)	50(2)
C(42A)	6588(10)	1846(11)	9324(9)	64(2)
C(43A)	5062(11)	1379(13)	9314(11)	80(3)
C(44A)	4986(17)	104(15)	9808(11)	81(3)
C(45A)	5830(12)	-915(11)	9426(7)	78(2)
C(46A)	7386(11)	-484(10)	9503(7)	66(2)
C(41B)	7542(12)	1500(16)	9256(8)	46(3)
C(42B)	7449(11)	382(13)	9846(7)	53(2)
C(43B)	5952(12)	417(16)	10107(7)	62(3)
C(44B)	4872(19)	300(20)	9417(10)	62(3)
C(45B)	5056(11)	1380(14)	8824(8)	53(3)
C(46B)	6539(10)	1353(12)	8524(6)	47(2)
O(1W)	610(2)	-887(2)	8894(1)	55(1)

Table 3. Bond lengths [Å] and angles [°] for D11026.

C(1)-O(3)	1.444(3)
C(1)-C(6)	1.518(4)
C(1)-C(5)	1.543(4)
C(1)-C(2)	1.585(4)
C(6)-O(1)	1.202(3)
C(6)-O(2)	1.326(3)
O(2)-C(7)	1.451(4)
C(7)-C(8)	1.498(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
O(3)-C(10)	1.356(3)
O(4)-C(10)	1.205(3)
C(10)-C(11)	1.480(4)
C(11)-C(16)	1.391(4)
C(11)-C(12)	1.392(4)
C(12)-C(13)	1.378(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.381(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.379(4)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(2)-C(3)	1.502(4)
C(2)-C(17)	1.525(4)
C(2)-H(2)	1.0000
C(17)-C(18)	1.503(6)
C(17)-C(18A)	1.634(8)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(17)-H(17C)	0.9900
C(17)-H(17D)	0.9900
C(18)-C(22)	1.500(7)
C(18)-C(19)	1.539(6)
C(18)-H(18)	1.0000
C(19)-C(20)	1.514(8)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.494(9)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.530(8)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(18A)-C(22A)	1.477(11)
C(18A)-C(19A)	1.533(11)
C(18A)-H(18A)	1.0000
C(19A)-C(20A)	1.512(13)
C(19A)-H(19C)	0.9900
C(19A)-H(19D)	0.9900
C(20A)-C(21A)	1.497(13)
C(20A)-H(20C)	0.9900
C(20A)-H(20D)	0.9900
C(21A)-C(22A)	1.527(12)
C(21A)-H(21C)	0.9900
C(21A)-H(21D)	0.9900
C(22A)-H(22C)	0.9900
C(22A)-H(22D)	0.9900
C(3)-C(4)	1.319(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.485(4)
C(4)-C(23)	1.498(3)
C(23)-O(5)	1.250(3)
C(23)-O(6)	1.258(3)

C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
N(1)-C(41B)	1.470(12)
N(1)-C(31)	1.491(4)
N(1)-C(41)	1.532(7)
N(1)-C(41A)	1.551(9)
N(1)-H(1A)	0.858(19)
N(1)-H(1B)	0.888(18)
C(31)-C(36)	1.512(4)
C(31)-C(32)	1.526(4)
C(31)-H(31)	1.0000
C(32)-C(33)	1.513(5)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.517(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.511(4)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.528(4)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(41)-C(46)	1.505(9)
C(41)-C(42)	1.509(8)
C(41)-H(41)	1.0000
C(42)-C(43)	1.527(7)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.507(10)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.504(10)
C(44)-H(44A)	0.9900

C(44)-H(44B)	0.9900
C(45)-C(46)	1.512(8)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(41A)-C(46A)	1.504(11)
C(41A)-C(42A)	1.515(11)
C(41A)-H(41A)	1.0000
C(42A)-C(43A)	1.527(11)
C(42A)-H(42C)	0.9900
C(42A)-H(42D)	0.9900
C(43A)-C(44A)	1.546(13)
C(43A)-H(43C)	0.9900
C(43A)-H(43D)	0.9900
C(44A)-C(45A)	1.489(13)
C(44A)-H(44C)	0.9900
C(44A)-H(44D)	0.9900
C(45A)-C(46A)	1.540(11)
C(45A)-H(45C)	0.9900
C(45A)-H(45D)	0.9900
C(46A)-H(46C)	0.9900
C(46A)-H(46D)	0.9900
C(41B)-C(46B)	1.508(12)
C(41B)-C(42B)	1.519(13)
C(41B)-H(41B)	1.0000
C(42B)-C(43B)	1.524(12)
C(42B)-H(42E)	0.9900
C(42B)-H(42F)	0.9900
C(43B)-C(44B)	1.497(14)
C(43B)-H(43E)	0.9900
C(43B)-H(43F)	0.9900
C(44B)-C(45B)	1.508(14)
C(44B)-H(44E)	0.9900
C(44B)-H(44F)	0.9900
C(45B)-C(46B)	1.538(12)

C(45B)-H(45E)	0.9900
C(45B)-H(45F)	0.9900
C(46B)-H(46E)	0.9900
C(46B)-H(46F)	0.9900
O(1W)-H(1W1)	0.837(19)
O(1W)-H(1W2)	0.844(19)

O(3)-C(1)-C(6)	107.8(2)
O(3)-C(1)-C(5)	111.6(2)
C(6)-C(1)-C(5)	115.7(2)
O(3)-C(1)-C(2)	106.65(19)
C(6)-C(1)-C(2)	109.3(2)
C(5)-C(1)-C(2)	105.4(2)
O(1)-C(6)-O(2)	124.7(3)
O(1)-C(6)-C(1)	124.3(2)
O(2)-C(6)-C(1)	110.9(2)
C(6)-O(2)-C(7)	117.0(3)
O(2)-C(7)-C(8)	110.8(3)
O(2)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
O(2)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-O(3)-C(1)	116.4(2)
O(4)-C(10)-O(3)	123.6(2)
O(4)-C(10)-C(11)	124.4(2)
O(3)-C(10)-C(11)	112.0(2)
C(16)-C(11)-C(12)	119.3(3)
C(16)-C(11)-C(10)	117.8(2)
C(12)-C(11)-C(10)	122.9(2)

C(13)-C(12)-C(11)	120.3(2)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	120.2(3)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	119.6(3)
C(15)-C(14)-H(14)	120.2
C(13)-C(14)-H(14)	120.2
C(16)-C(15)-C(14)	120.6(3)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(15)-C(16)-C(11)	119.9(3)
C(15)-C(16)-H(16)	120.0
C(11)-C(16)-H(16)	120.0
C(3)-C(2)-C(17)	116.4(2)
C(3)-C(2)-C(1)	102.4(2)
C(17)-C(2)-C(1)	115.3(2)
C(3)-C(2)-H(2)	107.4
C(17)-C(2)-H(2)	107.4
C(1)-C(2)-H(2)	107.4
C(18)-C(17)-C(2)	113.7(3)
C(2)-C(17)-C(18A)	115.5(3)
C(18)-C(17)-H(17A)	108.8
C(2)-C(17)-H(17A)	108.8
C(18A)-C(17)-H(17A)	82.5
C(18)-C(17)-H(17B)	108.8
C(2)-C(17)-H(17B)	108.8
C(18A)-C(17)-H(17B)	128.2
H(17A)-C(17)-H(17B)	107.7
C(18)-C(17)-H(17C)	83.5
C(2)-C(17)-H(17C)	108.4
C(18A)-C(17)-H(17C)	108.4
H(17A)-C(17)-H(17C)	131.0
C(18)-C(17)-H(17D)	130.2
C(2)-C(17)-H(17D)	108.4

C(18A)-C(17)-H(17D)	108.4
H(17B)-C(17)-H(17D)	80.4
H(17C)-C(17)-H(17D)	107.5
C(22)-C(18)-C(17)	115.3(4)
C(22)-C(18)-C(19)	101.5(4)
C(17)-C(18)-C(19)	112.4(4)
C(22)-C(18)-H(18)	109.1
C(17)-C(18)-H(18)	109.1
C(19)-C(18)-H(18)	109.1
C(20)-C(19)-C(18)	105.9(4)
C(20)-C(19)-H(19A)	110.6
C(18)-C(19)-H(19A)	110.6
C(20)-C(19)-H(19B)	110.6
C(18)-C(19)-H(19B)	110.6
H(19A)-C(19)-H(19B)	108.7
C(21)-C(20)-C(19)	106.2(5)
C(21)-C(20)-H(20A)	110.5
C(19)-C(20)-H(20A)	110.5
C(21)-C(20)-H(20B)	110.5
C(19)-C(20)-H(20B)	110.5
H(20A)-C(20)-H(20B)	108.7
C(20)-C(21)-C(22)	106.0(5)
C(20)-C(21)-H(21A)	110.5
C(22)-C(21)-H(21A)	110.5
C(20)-C(21)-H(21B)	110.5
C(22)-C(21)-H(21B)	110.5
H(21A)-C(21)-H(21B)	108.7
C(18)-C(22)-C(21)	103.8(5)
C(18)-C(22)-H(22A)	111.0
C(21)-C(22)-H(22A)	111.0
C(18)-C(22)-H(22B)	111.0
C(21)-C(22)-H(22B)	111.0
H(22A)-C(22)-H(22B)	109.0
C(22A)-C(18A)-C(19A)	103.9(7)
C(22A)-C(18A)-C(17)	111.4(7)
C(19A)-C(18A)-C(17)	115.1(6)

C(22A)-C(18A)-H(18A)	108.7
C(19A)-C(18A)-H(18A)	108.7
C(17)-C(18A)-H(18A)	108.7
C(20A)-C(19A)-C(18A)	103.7(7)
C(20A)-C(19A)-H(19C)	111.0
C(18A)-C(19A)-H(19C)	111.0
C(20A)-C(19A)-H(19D)	111.0
C(18A)-C(19A)-H(19D)	111.0
H(19C)-C(19A)-H(19D)	109.0
C(21A)-C(20A)-C(19A)	107.5(9)
C(21A)-C(20A)-H(20C)	110.2
C(19A)-C(20A)-H(20C)	110.2
C(21A)-C(20A)-H(20D)	110.2
C(19A)-C(20A)-H(20D)	110.2
H(20C)-C(20A)-H(20D)	108.5
C(20A)-C(21A)-C(22A)	106.0(8)
C(20A)-C(21A)-H(21C)	110.5
C(22A)-C(21A)-H(21C)	110.5
C(20A)-C(21A)-H(21D)	110.5
C(22A)-C(21A)-H(21D)	110.5
H(21C)-C(21A)-H(21D)	108.7
C(18A)-C(22A)-C(21A)	104.8(7)
C(18A)-C(22A)-H(22C)	110.8
C(21A)-C(22A)-H(22C)	110.8
C(18A)-C(22A)-H(22D)	110.8
C(21A)-C(22A)-H(22D)	110.8
H(22C)-C(22A)-H(22D)	108.9
C(4)-C(3)-C(2)	114.0(2)
C(4)-C(3)-H(3)	123.0
C(2)-C(3)-H(3)	123.0
C(3)-C(4)-C(5)	112.0(2)
C(3)-C(4)-C(23)	127.6(2)
C(5)-C(4)-C(23)	120.3(2)
O(5)-C(23)-O(6)	125.0(2)
O(5)-C(23)-C(4)	115.8(2)
O(6)-C(23)-C(4)	119.1(2)

C(4)-C(5)-C(1)	105.4(2)
C(4)-C(5)-H(5A)	110.7
C(1)-C(5)-H(5A)	110.7
C(4)-C(5)-H(5B)	110.7
C(1)-C(5)-H(5B)	110.7
H(5A)-C(5)-H(5B)	108.8
C(41B)-N(1)-C(31)	113.5(6)
C(41B)-N(1)-C(41)	15.8(6)
C(31)-N(1)-C(41)	112.0(4)
C(31)-N(1)-C(41A)	125.5(5)
C(41B)-N(1)-H(1A)	123(2)
C(31)-N(1)-H(1A)	108(2)
C(41)-N(1)-H(1A)	111(2)
C(41A)-N(1)-H(1A)	92(2)
C(41B)-N(1)-H(1B)	92(2)
C(31)-N(1)-H(1B)	114(2)
C(41)-N(1)-H(1B)	106(2)
C(41A)-N(1)-H(1B)	109(2)
H(1A)-N(1)-H(1B)	105(3)
N(1)-C(31)-C(36)	111.3(2)
N(1)-C(31)-C(32)	109.9(2)
C(36)-C(31)-C(32)	110.8(2)
N(1)-C(31)-H(31)	108.3
C(36)-C(31)-H(31)	108.3
C(32)-C(31)-H(31)	108.3
C(33)-C(32)-C(31)	111.0(3)
C(33)-C(32)-H(32A)	109.4
C(31)-C(32)-H(32A)	109.4
C(33)-C(32)-H(32B)	109.4
C(31)-C(32)-H(32B)	109.4
H(32A)-C(32)-H(32B)	108.0
C(32)-C(33)-C(34)	111.5(3)
C(32)-C(33)-H(33A)	109.3
C(34)-C(33)-H(33A)	109.3
C(32)-C(33)-H(33B)	109.3
C(34)-C(33)-H(33B)	109.3

H(33A)-C(33)-H(33B)	108.0
C(35)-C(34)-C(33)	111.1(3)
C(35)-C(34)-H(34A)	109.4
C(33)-C(34)-H(34A)	109.4
C(35)-C(34)-H(34B)	109.4
C(33)-C(34)-H(34B)	109.4
H(34A)-C(34)-H(34B)	108.0
C(34)-C(35)-C(36)	111.4(3)
C(34)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35A)	109.4
C(34)-C(35)-H(35B)	109.4
C(36)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	108.0
C(31)-C(36)-C(35)	110.9(3)
C(31)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	108.0
C(46)-C(41)-C(42)	112.1(6)
C(46)-C(41)-N(1)	108.0(5)
C(42)-C(41)-N(1)	113.8(5)
C(46)-C(41)-H(41)	107.6
C(42)-C(41)-H(41)	107.6
N(1)-C(41)-H(41)	107.6
C(41)-C(42)-C(43)	111.5(5)
C(41)-C(42)-H(42A)	109.3
C(43)-C(42)-H(42A)	109.3
C(41)-C(42)-H(42B)	109.3
C(43)-C(42)-H(42B)	109.3
H(42A)-C(42)-H(42B)	108.0
C(44)-C(43)-C(42)	112.5(5)
C(44)-C(43)-H(43A)	109.1
C(42)-C(43)-H(43A)	109.1
C(44)-C(43)-H(43B)	109.1
C(42)-C(43)-H(43B)	109.1

H(43A)-C(43)-H(43B)	107.8
C(45)-C(44)-C(43)	111.5(7)
C(45)-C(44)-H(44A)	109.3
C(43)-C(44)-H(44A)	109.3
C(45)-C(44)-H(44B)	109.3
C(43)-C(44)-H(44B)	109.3
H(44A)-C(44)-H(44B)	108.0
C(44)-C(45)-C(46)	112.8(6)
C(44)-C(45)-H(45A)	109.0
C(46)-C(45)-H(45A)	109.0
C(44)-C(45)-H(45B)	109.0
C(46)-C(45)-H(45B)	109.0
H(45A)-C(45)-H(45B)	107.8
C(41)-C(46)-C(45)	110.5(5)
C(41)-C(46)-H(46A)	109.6
C(45)-C(46)-H(46A)	109.6
C(41)-C(46)-H(46B)	109.6
C(45)-C(46)-H(46B)	109.6
H(46A)-C(46)-H(46B)	108.1
C(46A)-C(41A)-C(42A)	111.8(9)
C(46A)-C(41A)-N(1)	115.1(8)
C(42A)-C(41A)-N(1)	105.2(7)
C(46A)-C(41A)-H(41A)	108.2
C(42A)-C(41A)-H(41A)	108.2
N(1)-C(41A)-H(41A)	108.2
C(41A)-C(42A)-C(43A)	110.4(9)
C(41A)-C(42A)-H(42C)	109.6
C(43A)-C(42A)-H(42C)	109.6
C(41A)-C(42A)-H(42D)	109.6
C(43A)-C(42A)-H(42D)	109.6
H(42C)-C(42A)-H(42D)	108.1
C(42A)-C(43A)-C(44A)	109.9(11)
C(42A)-C(43A)-H(43C)	109.7
C(44A)-C(43A)-H(43C)	109.7
C(42A)-C(43A)-H(43D)	109.7
C(44A)-C(43A)-H(43D)	109.7

H(43C)-C(43A)-H(43D)	108.2
C(45A)-C(44A)-C(43A)	107.6(11)
C(45A)-C(44A)-H(44C)	110.2
C(43A)-C(44A)-H(44C)	110.2
C(45A)-C(44A)-H(44D)	110.2
C(43A)-C(44A)-H(44D)	110.2
H(44C)-C(44A)-H(44D)	108.5
C(44A)-C(45A)-C(46A)	108.3(10)
C(44A)-C(45A)-H(45C)	110.0
C(46A)-C(45A)-H(45C)	110.0
C(44A)-C(45A)-H(45D)	110.0
C(46A)-C(45A)-H(45D)	110.0
H(45C)-C(45A)-H(45D)	108.4
C(41A)-C(46A)-C(45A)	108.4(9)
C(41A)-C(46A)-H(46C)	110.0
C(45A)-C(46A)-H(46C)	110.0
C(41A)-C(46A)-H(46D)	110.0
C(45A)-C(46A)-H(46D)	110.0
H(46C)-C(46A)-H(46D)	108.4
N(1)-C(41B)-C(46B)	111.8(10)
N(1)-C(41B)-C(42B)	100.0(9)
C(46B)-C(41B)-C(42B)	113.3(11)
N(1)-C(41B)-H(41B)	110.5
C(46B)-C(41B)-H(41B)	110.5
C(42B)-C(41B)-H(41B)	110.5
C(41B)-C(42B)-C(43B)	106.0(9)
C(41B)-C(42B)-H(42E)	110.5
C(43B)-C(42B)-H(42E)	110.5
C(41B)-C(42B)-H(42F)	110.5
C(43B)-C(42B)-H(42F)	110.5
H(42E)-C(42B)-H(42F)	108.7
C(44B)-C(43B)-C(42B)	111.9(11)
C(44B)-C(43B)-H(43E)	109.2
C(42B)-C(43B)-H(43E)	109.2
C(44B)-C(43B)-H(43F)	109.2
C(42B)-C(43B)-H(43F)	109.2

H(43E)-C(43B)-H(43F)	107.9
C(43B)-C(44B)-C(45B)	110.3(13)
C(43B)-C(44B)-H(44E)	109.6
C(45B)-C(44B)-H(44E)	109.6
C(43B)-C(44B)-H(44F)	109.6
C(45B)-C(44B)-H(44F)	109.6
H(44E)-C(44B)-H(44F)	108.1
C(44B)-C(45B)-C(46B)	111.2(11)
C(44B)-C(45B)-H(45E)	109.4
C(46B)-C(45B)-H(45E)	109.4
C(44B)-C(45B)-H(45F)	109.4
C(46B)-C(45B)-H(45F)	109.4
H(45E)-C(45B)-H(45F)	108.0
C(41B)-C(46B)-C(45B)	105.5(9)
C(41B)-C(46B)-H(46E)	110.6
C(45B)-C(46B)-H(46E)	110.6
C(41B)-C(46B)-H(46F)	110.6
C(45B)-C(46B)-H(46F)	110.6
H(46E)-C(46B)-H(46F)	108.8
H(1W1)-O(1W)-H(1W2)	97(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D11026. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(1)	42(1)	50(1)	4(1)	1(1)	2(1)
C(6)	48(1)	46(1)	50(1)	-1(1)	9(1)	-2(1)
O(1)	48(1)	69(1)	64(1)	8(1)	-4(1)	-6(1)
O(2)	72(1)	53(1)	54(1)	-1(1)	16(1)	-12(1)
C(7)	85(2)	66(2)	80(2)	-16(2)	41(2)	-32(2)
C(8)	121(3)	71(2)	86(2)	-25(2)	43(2)	-36(2)
O(3)	38(1)	39(1)	64(1)	4(1)	5(1)	1(1)
O(4)	57(1)	62(1)	68(1)	8(1)	8(1)	18(1)
C(10)	35(1)	49(1)	61(2)	1(1)	-1(1)	2(1)
C(11)	37(1)	43(1)	59(1)	-1(1)	-6(1)	-2(1)
C(12)	41(1)	40(1)	64(2)	-1(1)	-5(1)	3(1)
C(13)	54(2)	51(2)	60(2)	-1(1)	0(1)	-2(1)
C(14)	69(2)	46(1)	62(2)	4(1)	-6(1)	3(1)
C(15)	68(2)	44(2)	73(2)	1(1)	-3(1)	13(1)
C(16)	54(2)	46(1)	64(2)	-2(1)	-3(1)	8(1)
C(2)	51(1)	35(1)	54(1)	5(1)	-1(1)	-1(1)
C(17)	70(2)	49(2)	53(1)	7(1)	-3(1)	9(1)
C(18)	63(3)	48(3)	44(2)	0(2)	6(2)	4(2)
C(19)	74(3)	56(3)	44(2)	3(2)	6(2)	0(2)
C(20)	75(4)	79(3)	48(3)	-5(2)	14(2)	7(3)
C(21)	117(6)	96(5)	58(3)	-12(4)	3(4)	51(4)
C(22)	77(3)	65(3)	45(2)	-2(2)	2(2)	23(3)
C(18A)	47(4)	53(4)	58(4)	7(3)	0(3)	15(4)
C(19A)	101(7)	84(5)	72(5)	22(4)	24(5)	27(5)
C(20A)	109(8)	82(5)	59(6)	3(5)	26(5)	23(6)
C(21A)	80(6)	60(4)	67(5)	-13(4)	16(4)	2(4)
C(22A)	65(5)	61(4)	75(4)	-7(3)	18(3)	-1(3)
C(3)	53(1)	39(1)	53(1)	6(1)	2(1)	8(1)
C(4)	51(1)	32(1)	51(1)	6(1)	0(1)	0(1)
C(23)	54(1)	33(1)	53(1)	3(1)	-1(1)	1(1)
O(5)	53(1)	40(1)	63(1)	-9(1)	-7(1)	2(1)

O(6)	79(1)	55(1)	58(1)	-4(1)	-16(1)	25(1)
C(5)	54(2)	52(2)	59(2)	-7(1)	-4(1)	10(1)
N(1)	50(1)	60(1)	47(1)	-5(1)	6(1)	6(1)
C(31)	41(1)	48(1)	62(2)	-4(1)	7(1)	6(1)
C(32)	43(2)	88(2)	62(2)	-14(2)	8(1)	-3(2)
C(33)	50(2)	88(2)	84(2)	-17(2)	17(2)	-14(2)
C(34)	56(2)	66(2)	75(2)	3(2)	17(1)	-1(1)
C(35)	63(2)	64(2)	70(2)	15(2)	1(1)	-8(1)
C(36)	59(2)	52(2)	56(2)	6(1)	-2(1)	-2(1)
C(41)	44(3)	44(3)	36(3)	-6(3)	8(2)	4(2)
C(42)	44(2)	32(2)	41(3)	-6(2)	10(2)	-4(2)
C(43)	44(2)	55(3)	52(3)	-6(2)	11(2)	0(2)
C(44)	42(3)	71(4)	70(5)	3(4)	2(3)	-10(3)
C(45)	58(3)	67(4)	98(5)	-34(3)	-1(3)	-12(3)
C(46)	56(3)	50(3)	75(4)	-22(3)	13(3)	-5(3)
C(41A)	58(4)	40(5)	53(5)	-8(4)	16(4)	-16(4)
C(42A)	52(4)	56(4)	83(6)	-6(5)	11(5)	-7(3)
C(43A)	55(4)	91(5)	97(7)	-6(6)	22(6)	-20(4)
C(44A)	60(5)	105(6)	80(7)	-1(5)	7(5)	-39(4)
C(45A)	85(5)	71(4)	79(6)	9(4)	8(4)	-47(4)
C(46A)	76(5)	51(4)	72(6)	5(4)	18(5)	-20(4)
C(41B)	49(5)	39(6)	49(6)	-3(5)	1(4)	6(5)
C(42B)	56(4)	49(5)	55(5)	2(4)	9(4)	5(5)
C(43B)	63(5)	72(7)	54(5)	1(5)	16(4)	4(5)
C(44B)	55(5)	63(6)	67(6)	-3(5)	10(4)	-6(5)
C(45B)	40(4)	57(6)	61(6)	-4(5)	2(4)	-5(5)
C(46B)	42(5)	42(5)	56(5)	-3(4)	-1(4)	-2(4)
O(1W)	67(1)	47(1)	52(1)	-5(1)	12(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D11026.

	x	y	z	U(eq)
H(7A)	7449	2716	1589	90
H(7B)	7871	1878	2376	90
H(8A)	6412	4310	2417	136
H(8B)	8088	4200	2576	136
H(8C)	7085	3515	3173	136
H(12)	3056	-1383	4318	59
H(13)	3027	-2905	5345	66
H(14)	4377	-4820	5319	72
H(15)	5724	-5217	4250	74
H(16)	5787	-3691	3227	66
H(2)	3481	2724	2797	56
H(17A)	1655	1129	3643	69
H(17B)	3215	1437	4017	69
H(17C)	3249	1920	4043	69
H(17D)	2093	868	3727	69
H(18)	2656	3748	3909	62
H(19A)	1210	2102	4971	69
H(19B)	2532	3050	5201	69
H(20A)	-126	3763	5320	80
H(20B)	1153	4793	5303	80
H(21A)	453	5419	4091	109
H(21B)	-970	4599	4182	109
H(22A)	-152	2794	3547	75
H(22B)	629	3934	3084	75
H(18A)	332	2616	3481	63
H(19C)	67	2028	4774	102
H(19D)	1584	2610	5090	102
H(20C)	-951	4003	4764	98
H(20D)	372	4412	5364	98
H(21C)	1078	5750	4463	82

H(21D)	-207	5292	3848	82
H(22C)	1539	4423	3180	79
H(22D)	2599	4313	3970	79
H(3)	997	2449	2139	58
H(5A)	4082	616	1332	67
H(5B)	3211	-592	1667	67
H(1A)	9370(30)	630(20)	8926(19)	63
H(1B)	9330(30)	1460(30)	9578(12)	63
H(31)	8933	3225	8628	60
H(32A)	11177	3013	9311	77
H(32B)	11611	1915	8694	77
H(33A)	12575	3929	8344	88
H(33B)	11059	4616	8314	88
H(34A)	11580	4157	7011	78
H(34B)	11878	2646	7230	78
H(35A)	9634	2806	6573	79
H(35B)	9188	3905	7186	79
H(36A)	8222	1880	7542	67
H(36B)	9743	1198	7581	67
H(41)	7013	1778	8574	50
H(42A)	7043	2837	9794	46
H(42B)	7246	1470	10260	46
H(43A)	4873	2032	10248	60
H(43B)	4768	2272	9308	60
H(44A)	5052	-212	10085	73
H(44B)	3721	273	9520	73
H(45A)	4992	171	8409	89
H(45B)	5149	-1213	8858	89
H(46A)	7409	-660	9395	72
H(46B)	7345	-476	8449	72
H(41A)	7207	576	8467	59
H(42C)	6640	2626	8976	76
H(42D)	6930	2105	9871	76
H(43C)	4686	1213	8759	96
H(43D)	4479	2069	9540	96
H(44C)	5374	259	10362	98

H(44D)	3996	-187	9817	98
H(45C)	5496	-1011	8859	94
H(45D)	5727	-1774	9692	94
H(46C)	7702	-333	10069	79
H(46D)	7983	-1179	9294	79
H(41B)	7394	2364	9520	55
H(42E)	8143	506	10309	64
H(42F)	7637	-471	9592	64
H(43E)	5828	-312	10484	75
H(43F)	5805	1254	10388	75
H(44E)	3916	346	9607	74
H(44F)	4970	-567	9156	74
H(45E)	4899	2240	9077	64
H(45F)	4344	1280	8368	64
H(46E)	6705	511	8252	57
H(46F)	6659	2083	8148	57
H(1W1)	300(40)	-1610(30)	9030(20)	82
H(1W2)	1120(40)	-740(40)	9317(16)	82

Table 6. Hydrogen bonds for D11026 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1W)#1	0.858(19)	1.95(2)	2.774(3)	161(3)
N(1)-H(1B)...O(6)#2	0.888(18)	1.879(19)	2.765(3)	175(3)
O(1W)-H(1W1)...O(6)#3	0.837(19)	1.89(2)	2.723(3)	172(4)
O(1W)-H(1W2)...O(5)#4	0.844(19)	1.92(3)	2.705(3)	154(4)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x+1,y,z+1 #3 -x,y-1/2,-z+1

#4 x,y,z+1

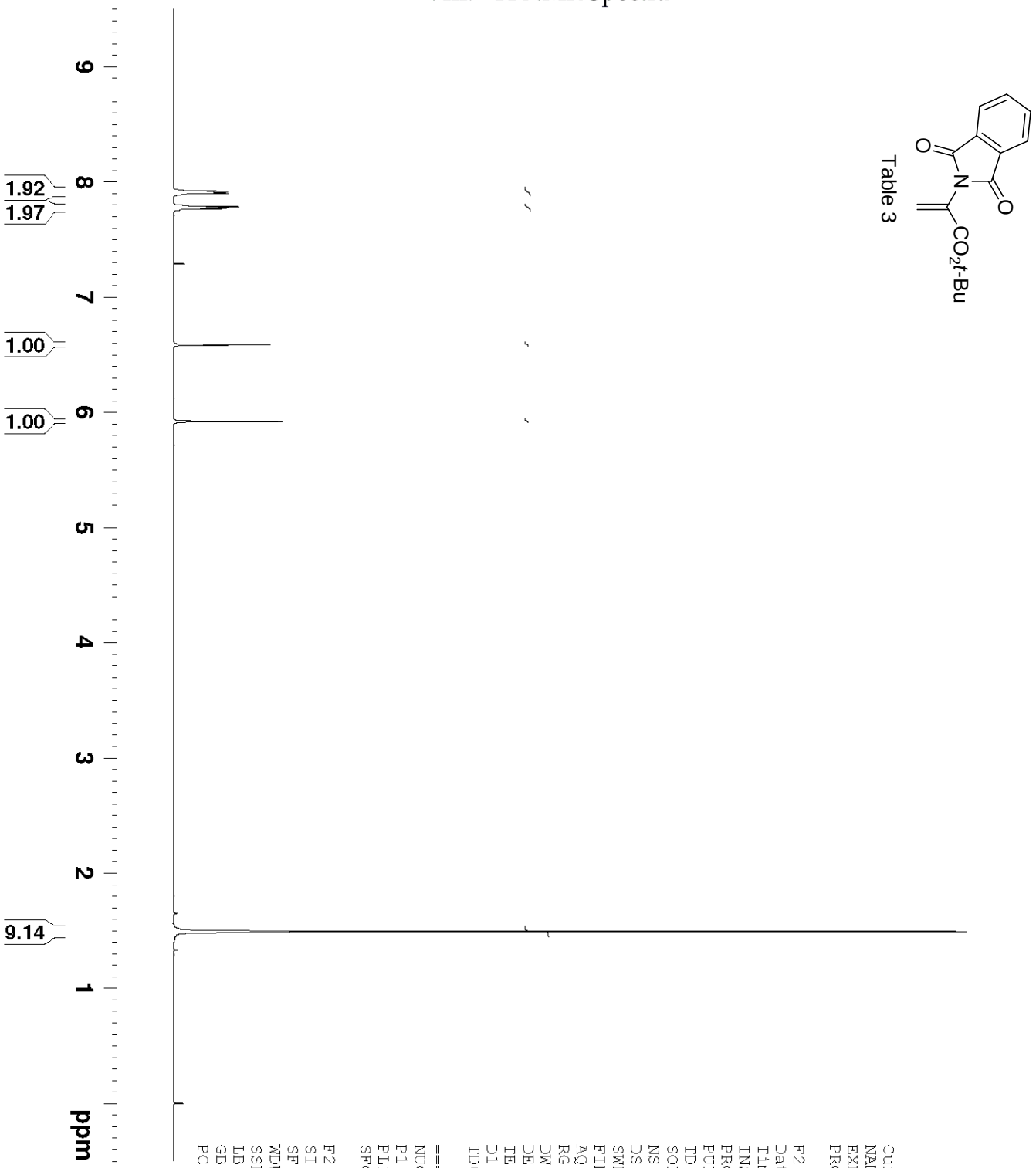


Table 3
O
N
O
O
CO2t-Bu
1.92
1.97
1.00
1.00
9.14
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME YF1019-A
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110301
Time_ 18.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 40.3
DW 60.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.07 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1299970 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

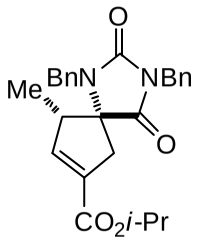
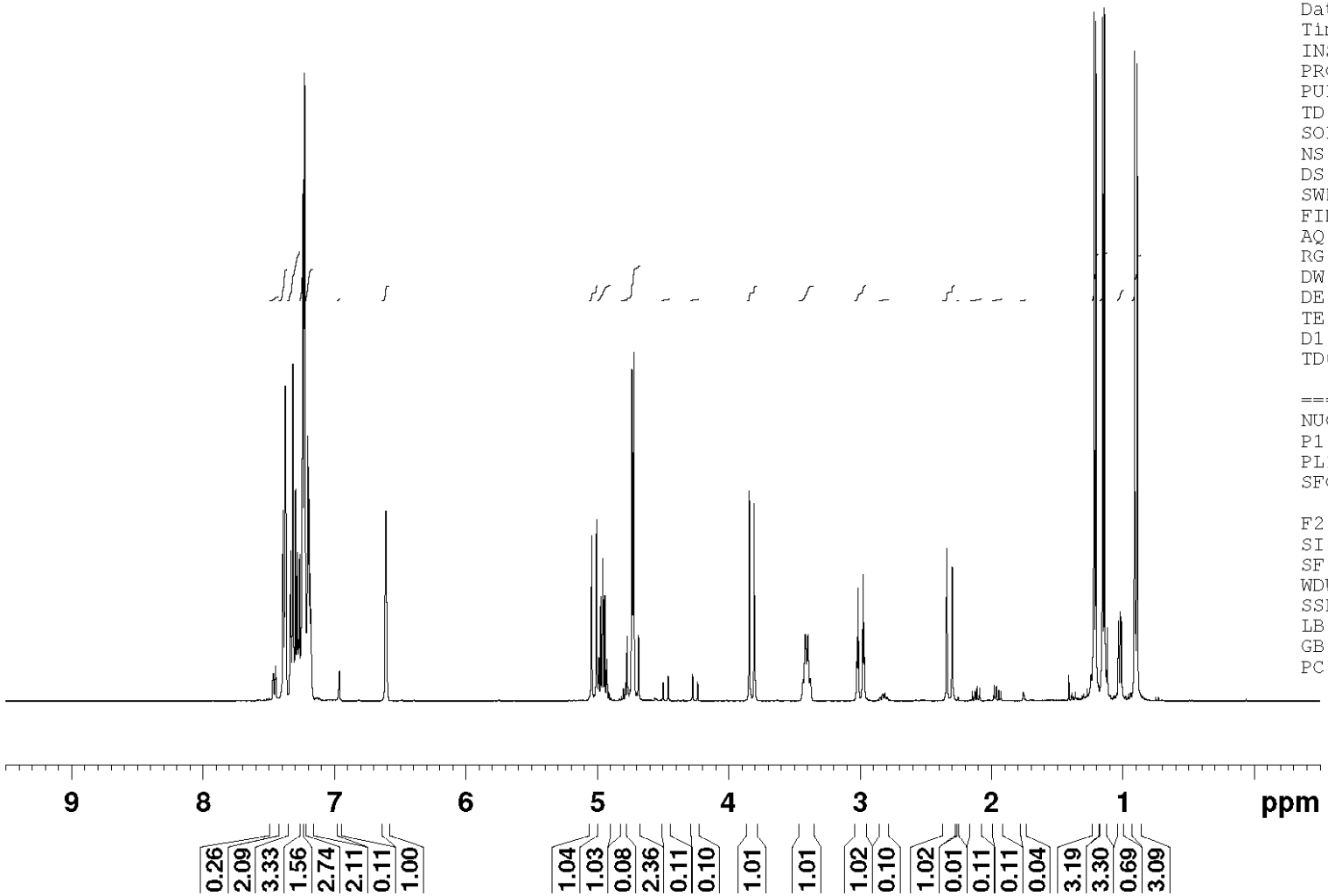


Table 2, entry 1




```
Current Data Parameters
NAME            YF1048-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110201
Time               19.35
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  35.9
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300170 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00
```

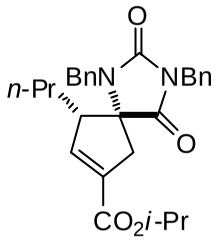
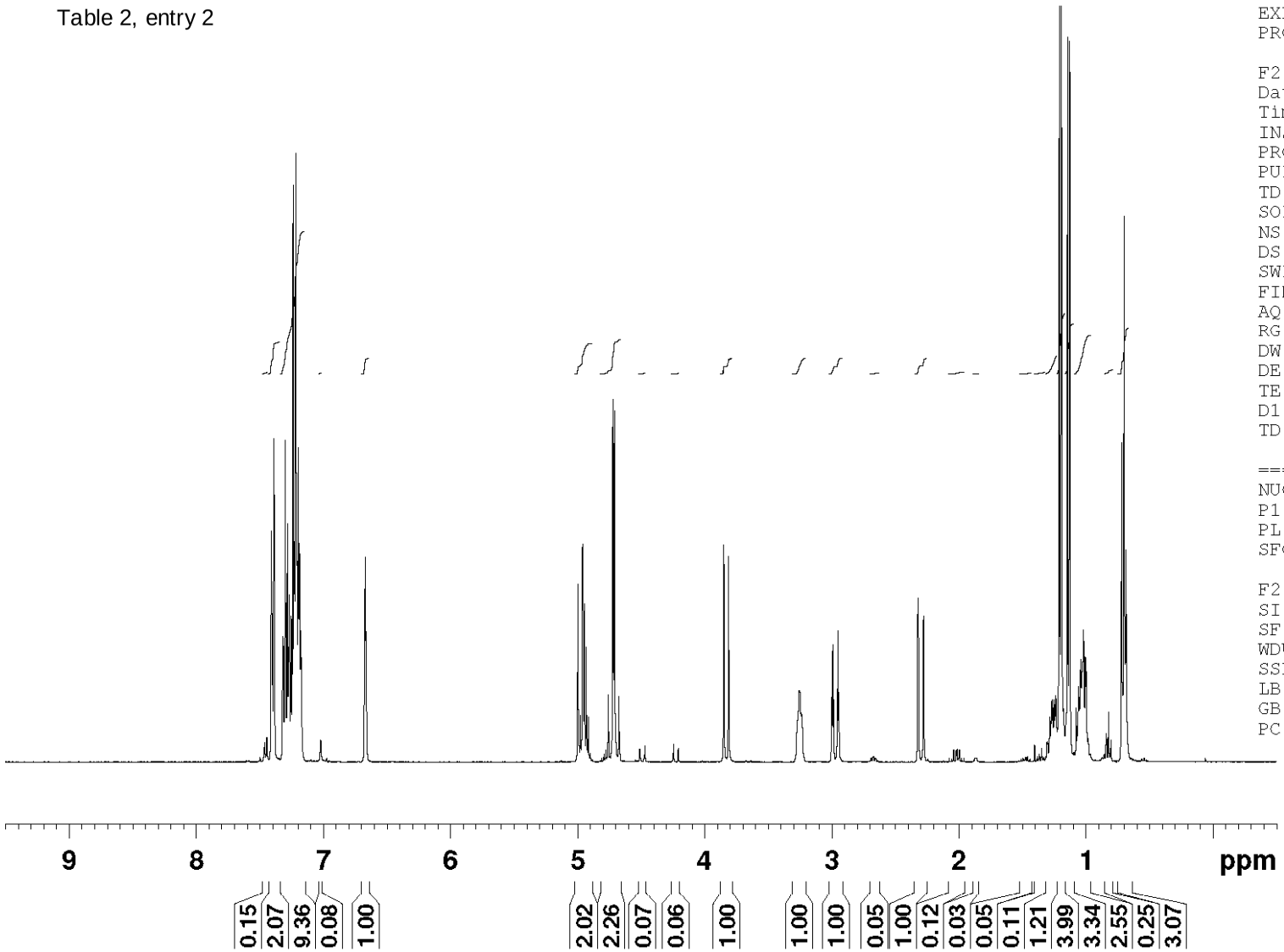


Table 2, entry 2




```
Current Data Parameters
NAME                  YF1049-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110201
Time                     19.46
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        22.6
DW                      60.400 usec
DE                       6.00 usec
TE                      296.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1                       0.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1300169 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
```

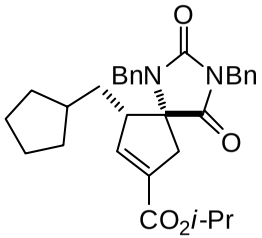
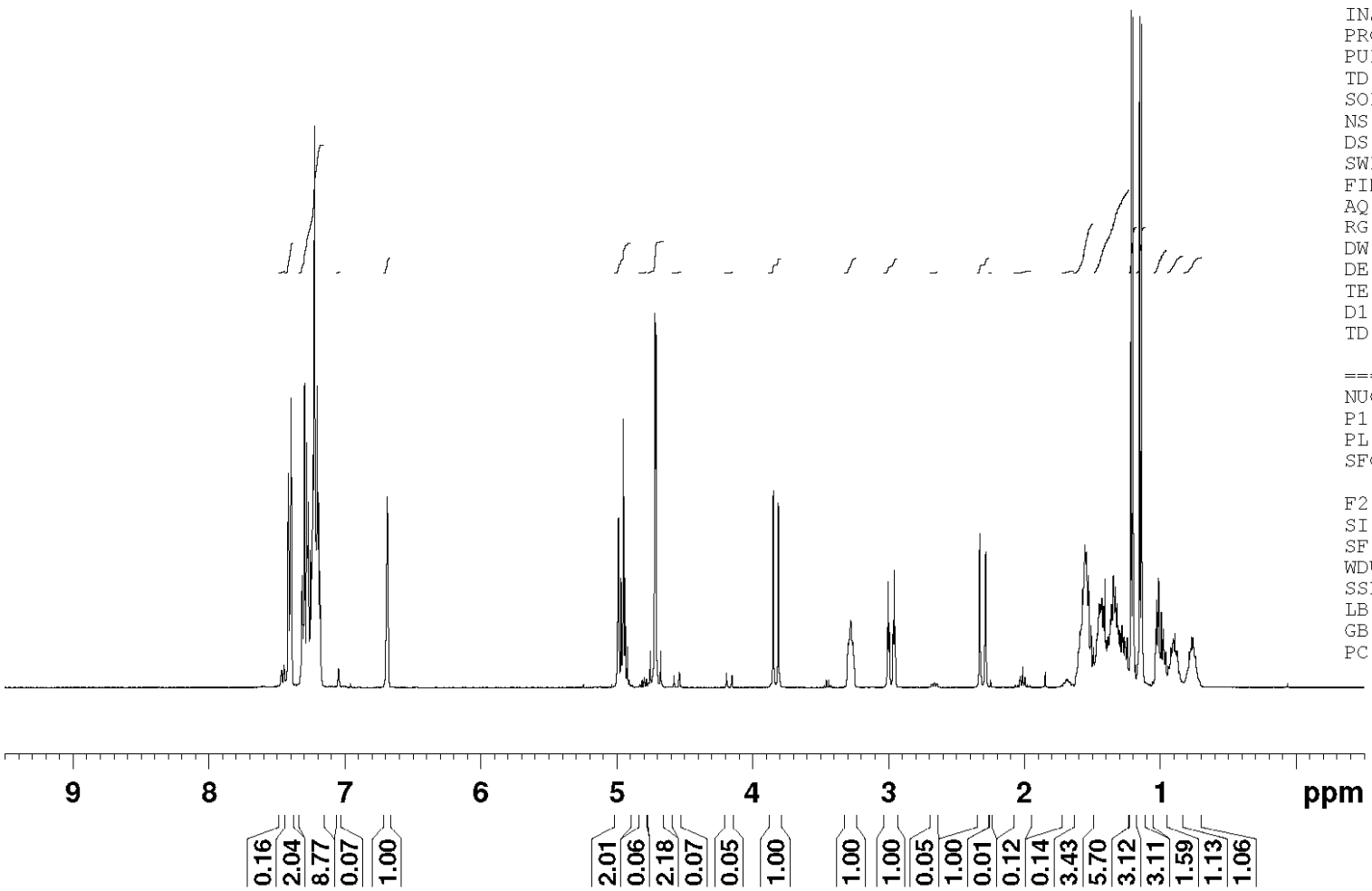


Table 2, entry 3




```
Current Data Parameters
NAME                  YF1051-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110201
Time                     19.54
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                        22.6
DW                     60.400 usec
DE                      6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1300152 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.40
```

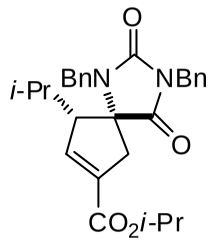
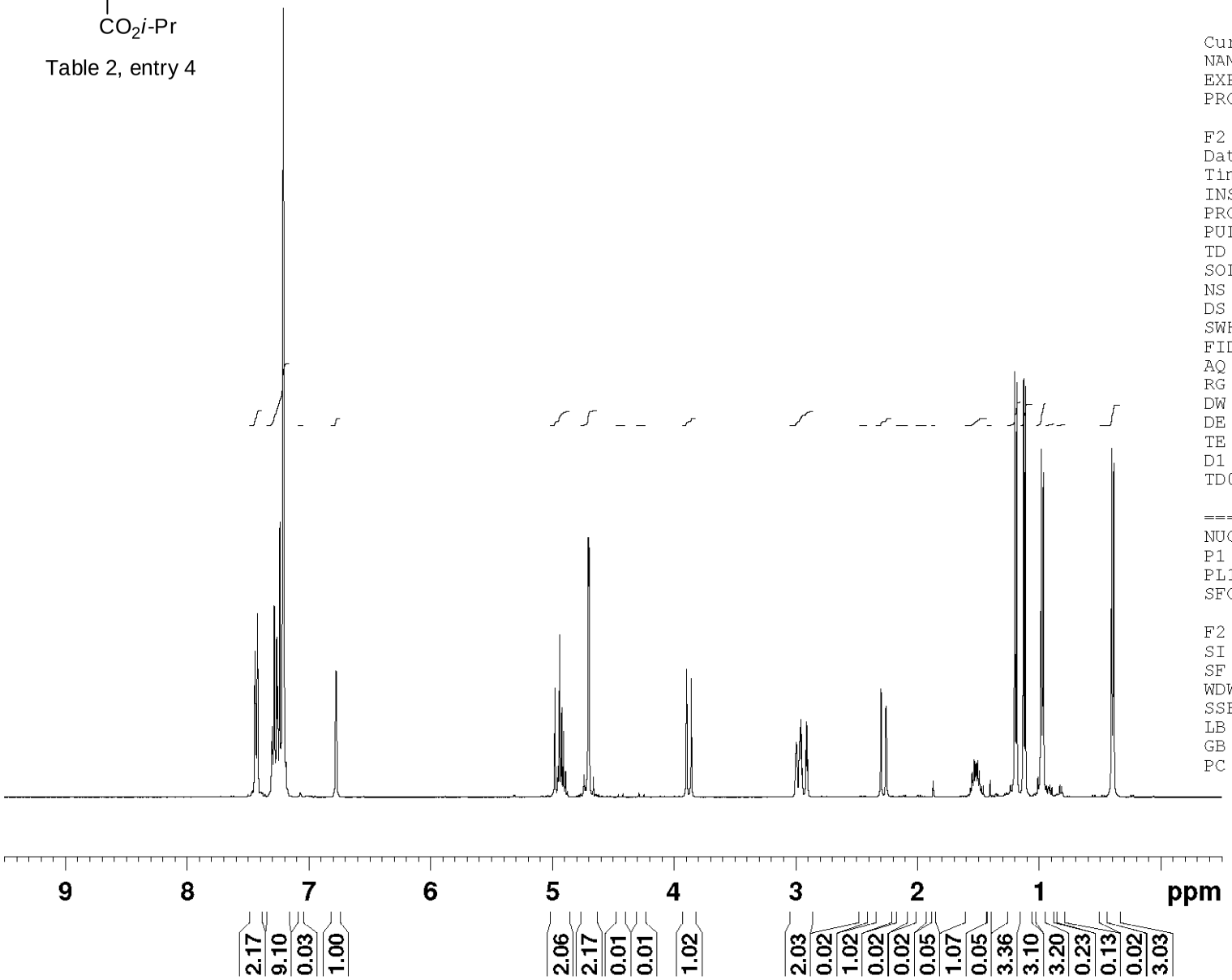


Table 2, entry 4




```
Current Data Parameters
NAME            YF1050-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110202
Time               13.05
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  20.2
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300168 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00
```

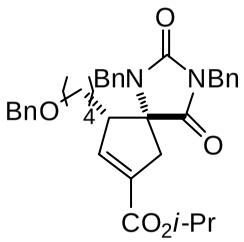
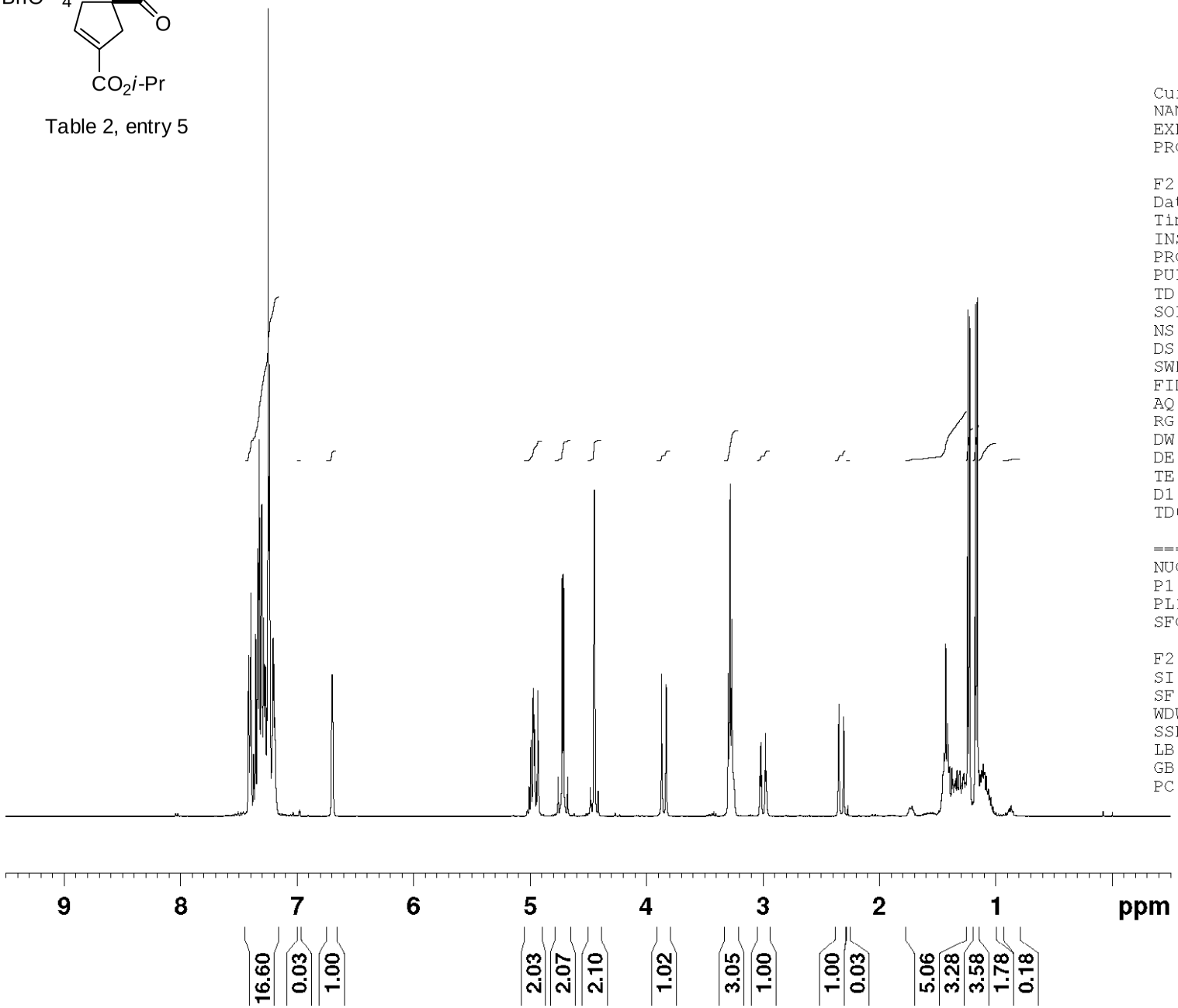


Table 2, entry 5




```
Current Data Parameters
NAME            YF1137-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110311
Time               17.23
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  35.9
DW                 60.400 usec
DE                  6.00 usec
TE                 296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300134 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

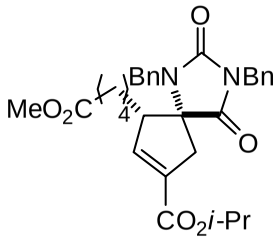
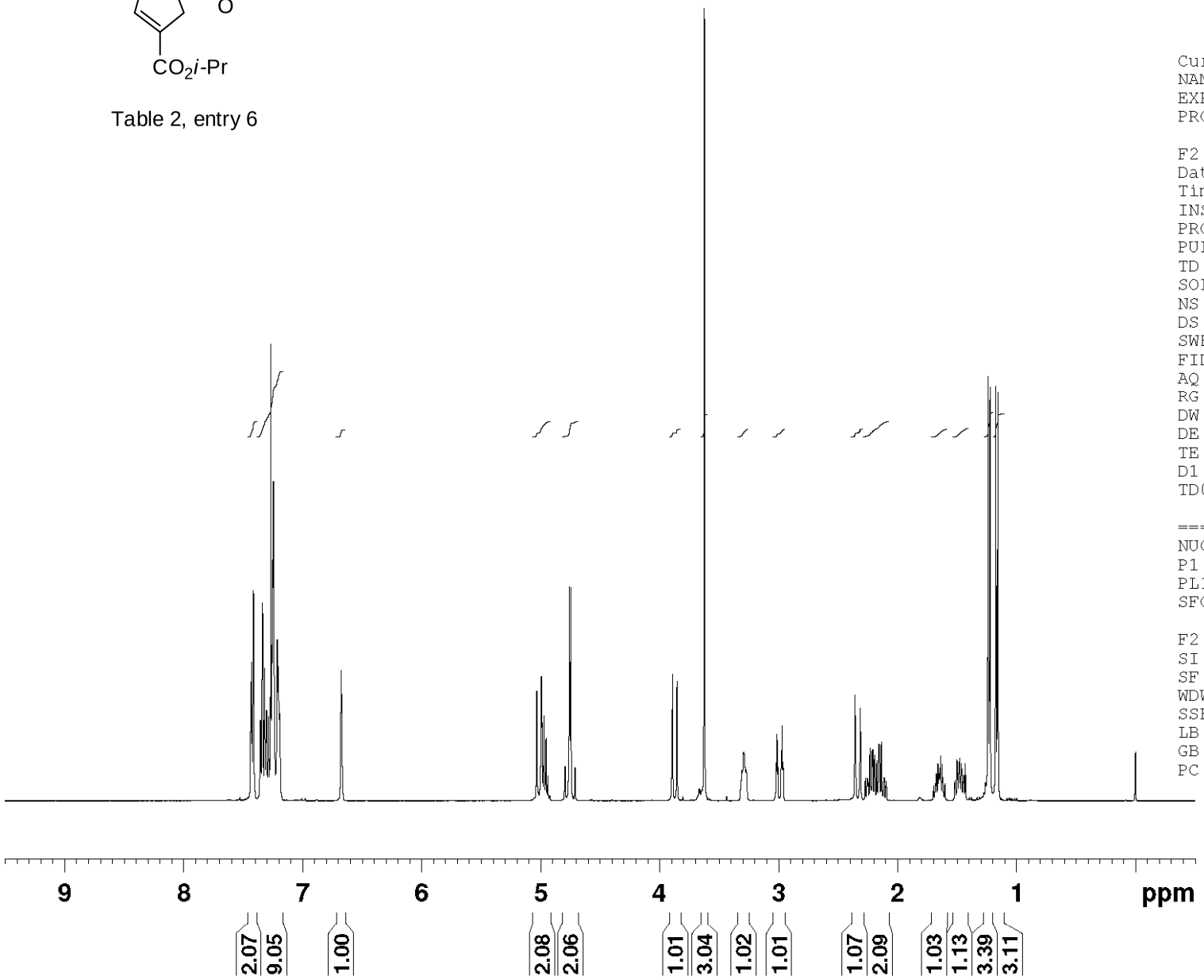


Table 2, entry 6




```
Current Data Parameters
NAME                  YF1054-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110202
Time                     18.09
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       65536
SOLVENT
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        35.9
DW                      60.400 usec
DE                       6.00 usec
TE                      296.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1                       0.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1300052 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.00
```

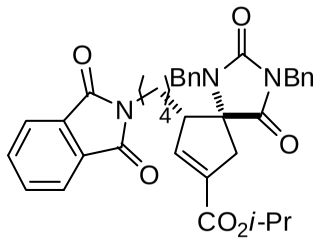
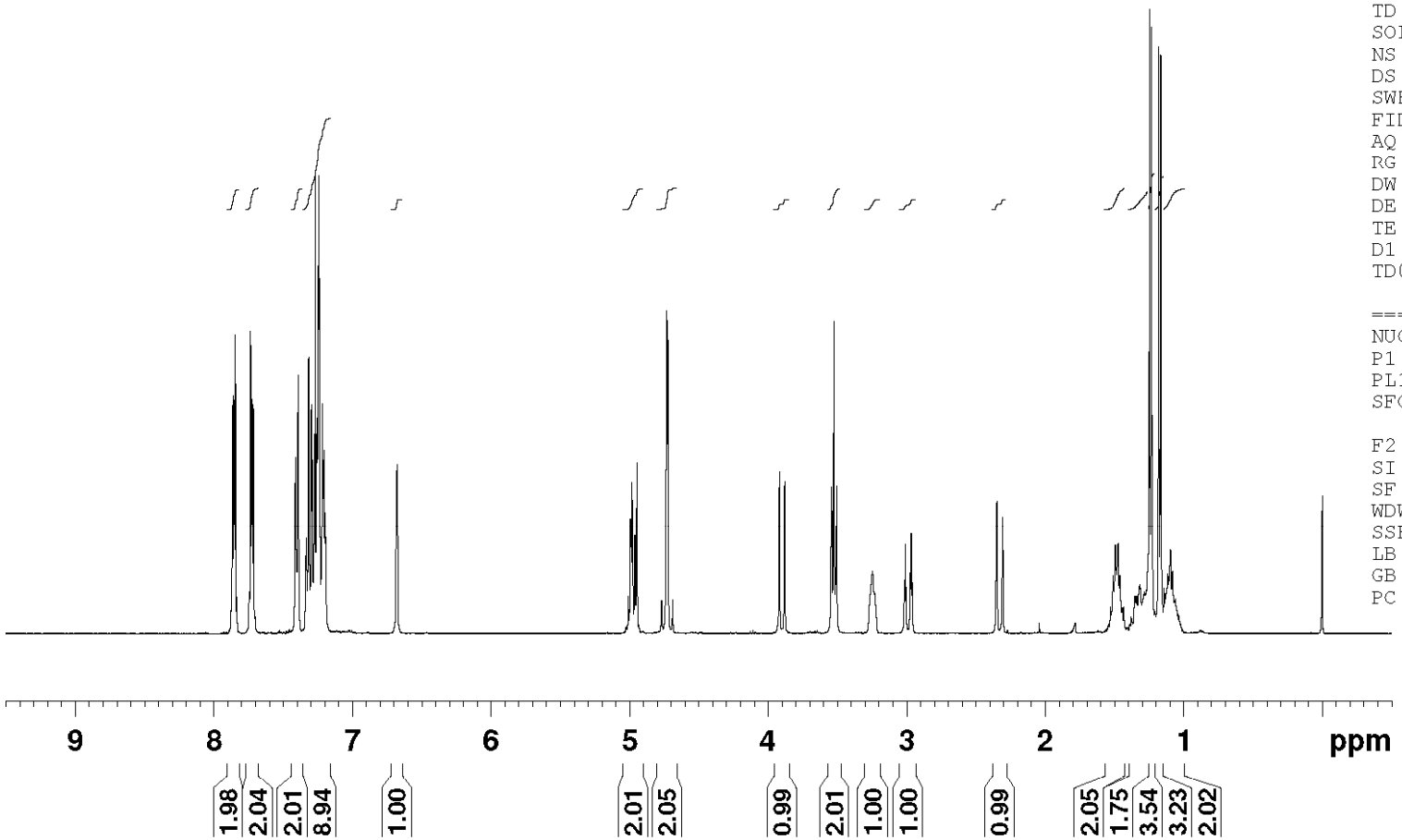


Table 2, entry 7




```
Current Data Parameters
NAME                  YF1052-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110205
Time                     17.48
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                        40.3
DW                     60.400 usec
DE                      6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1300050 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.40
```

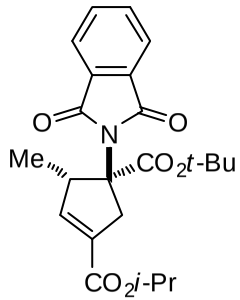
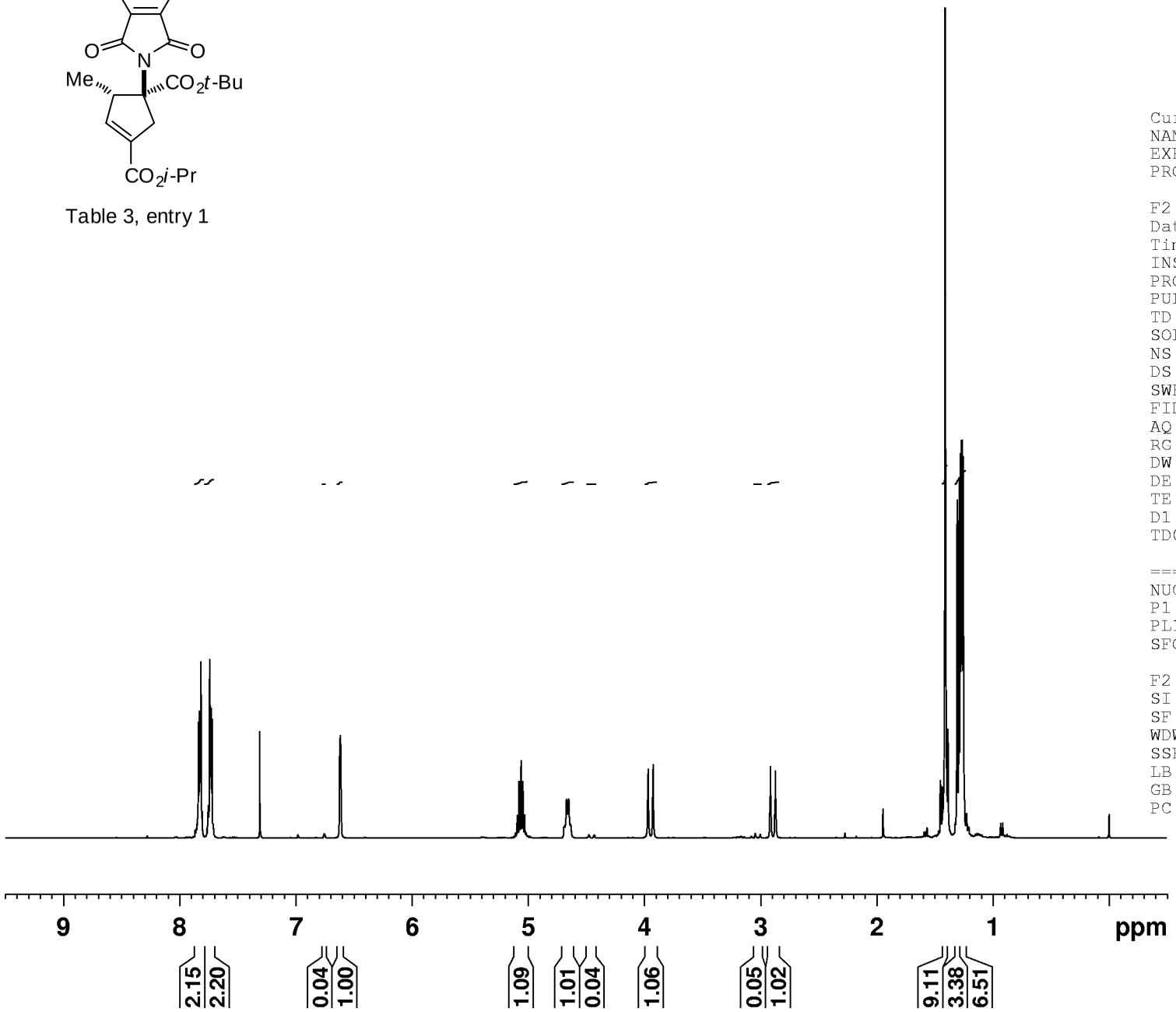


Table 3, entry 1




```
Current Data Parameters
NAME                  YF1082-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110222
Time                     19.50
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                        28.5
DW                    60.400 usec
DE                     6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1                       0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF               400.1299885 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00
```

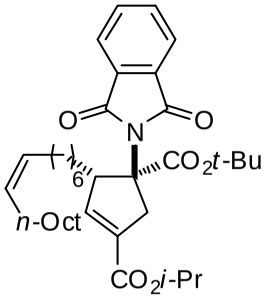
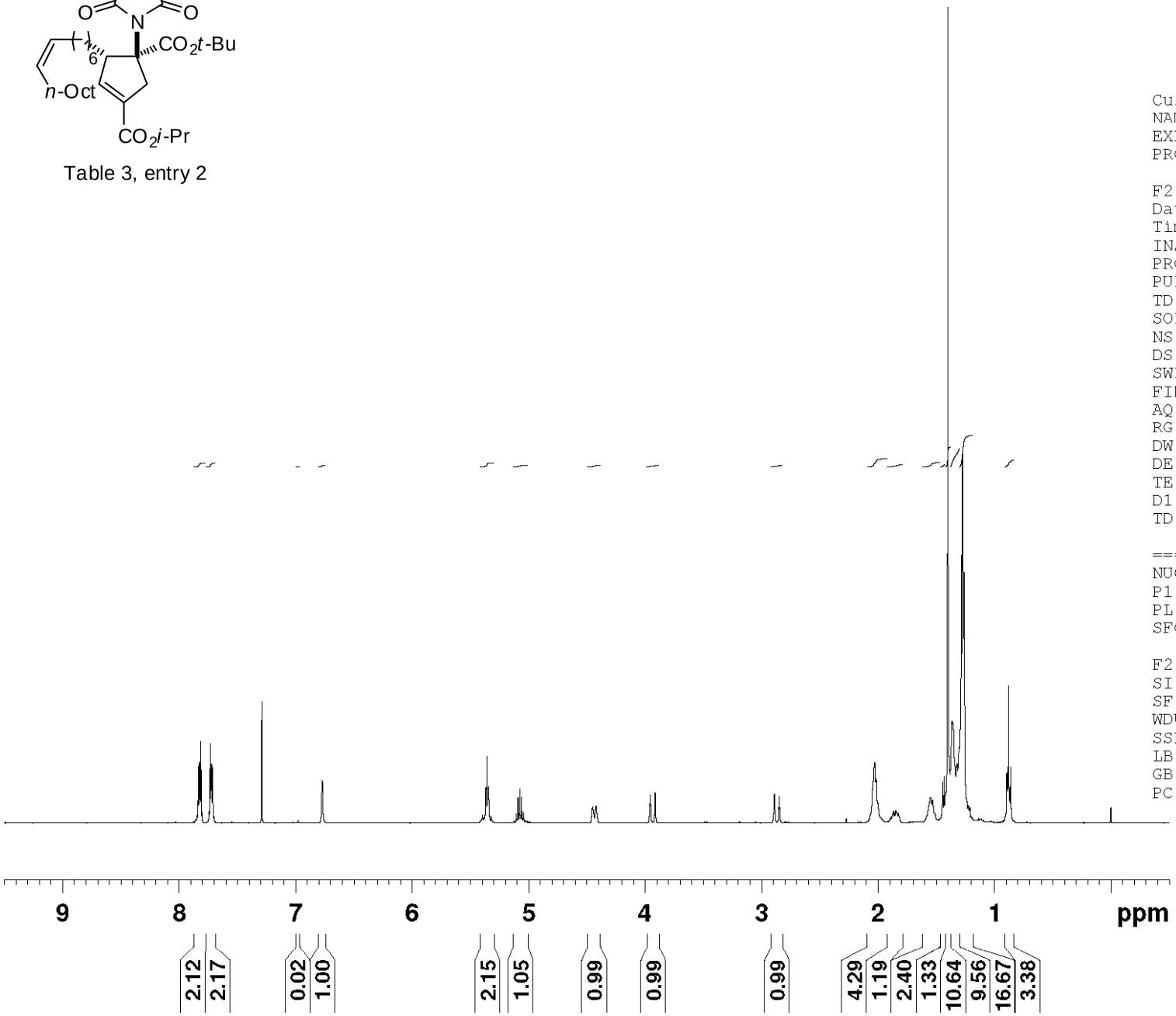


Table 3, entry 2




```
Current Data Parameters
NAME          YF1100-2-B
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110219
Time               18.01
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  20.2
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1299968 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.40
```

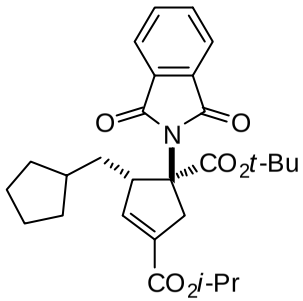
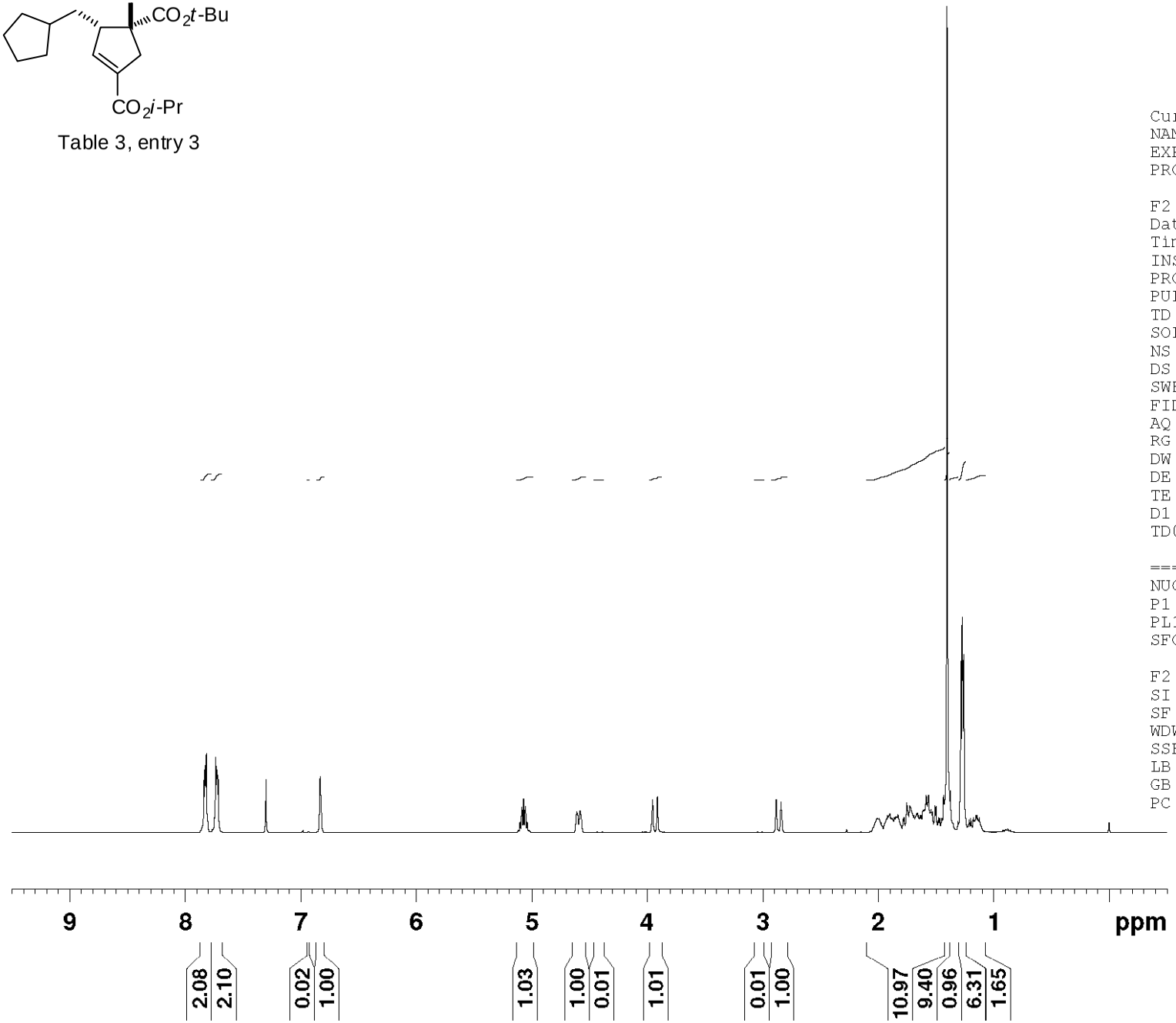
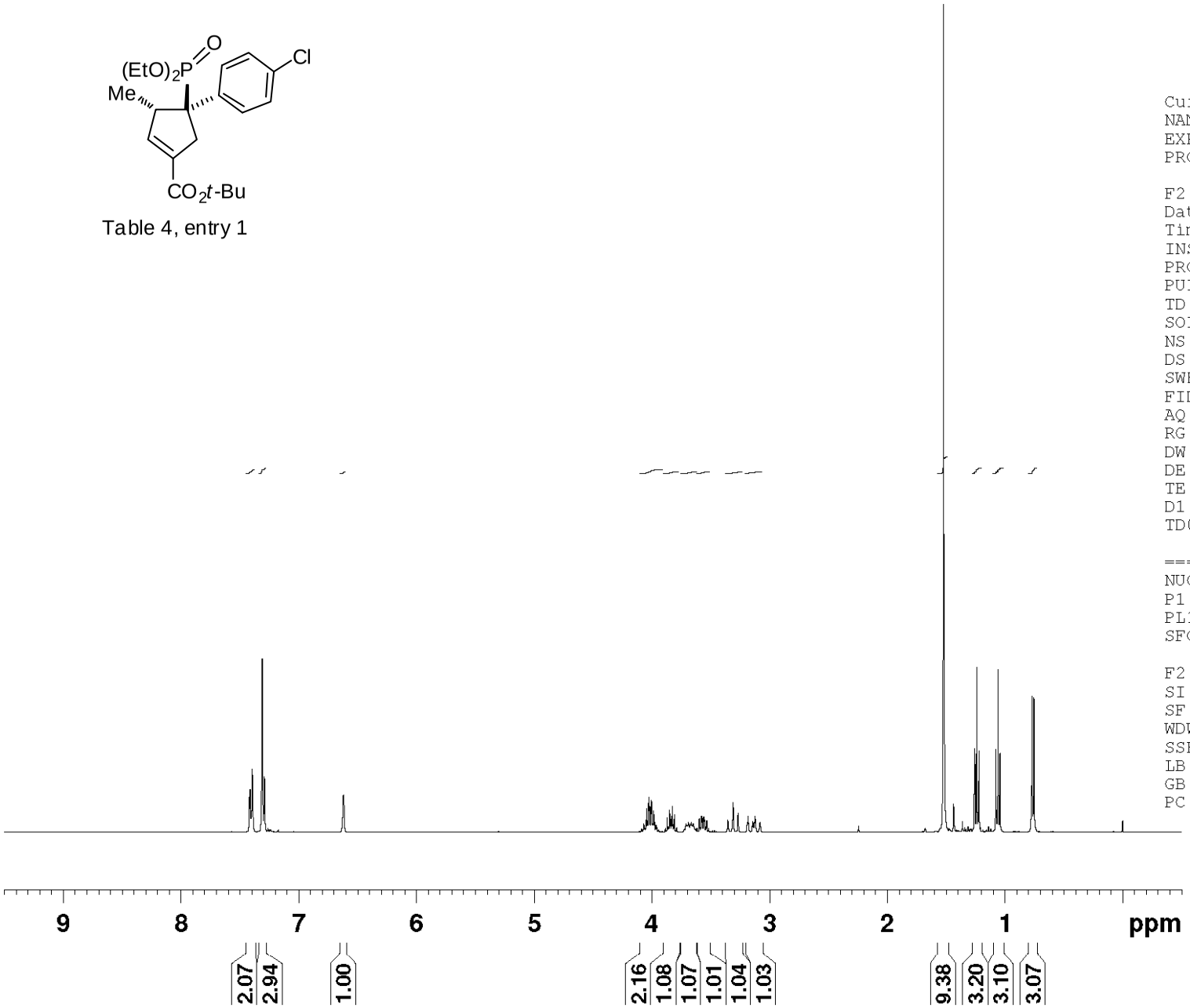


Table 3, entry 3




```
Current Data Parameters
NAME          YF1056-2-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110218
Time               19.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  22.6
DW                60.400 usec
DE                 6.00 usec
TE                295.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1299919 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

Table 4, entry 1




```
Current Data Parameters
NAME            YF1064-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110214
Time               19.40
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  28.5
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1299892 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

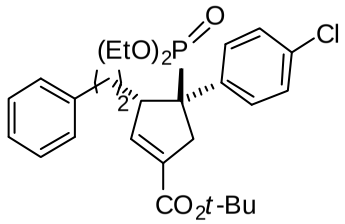
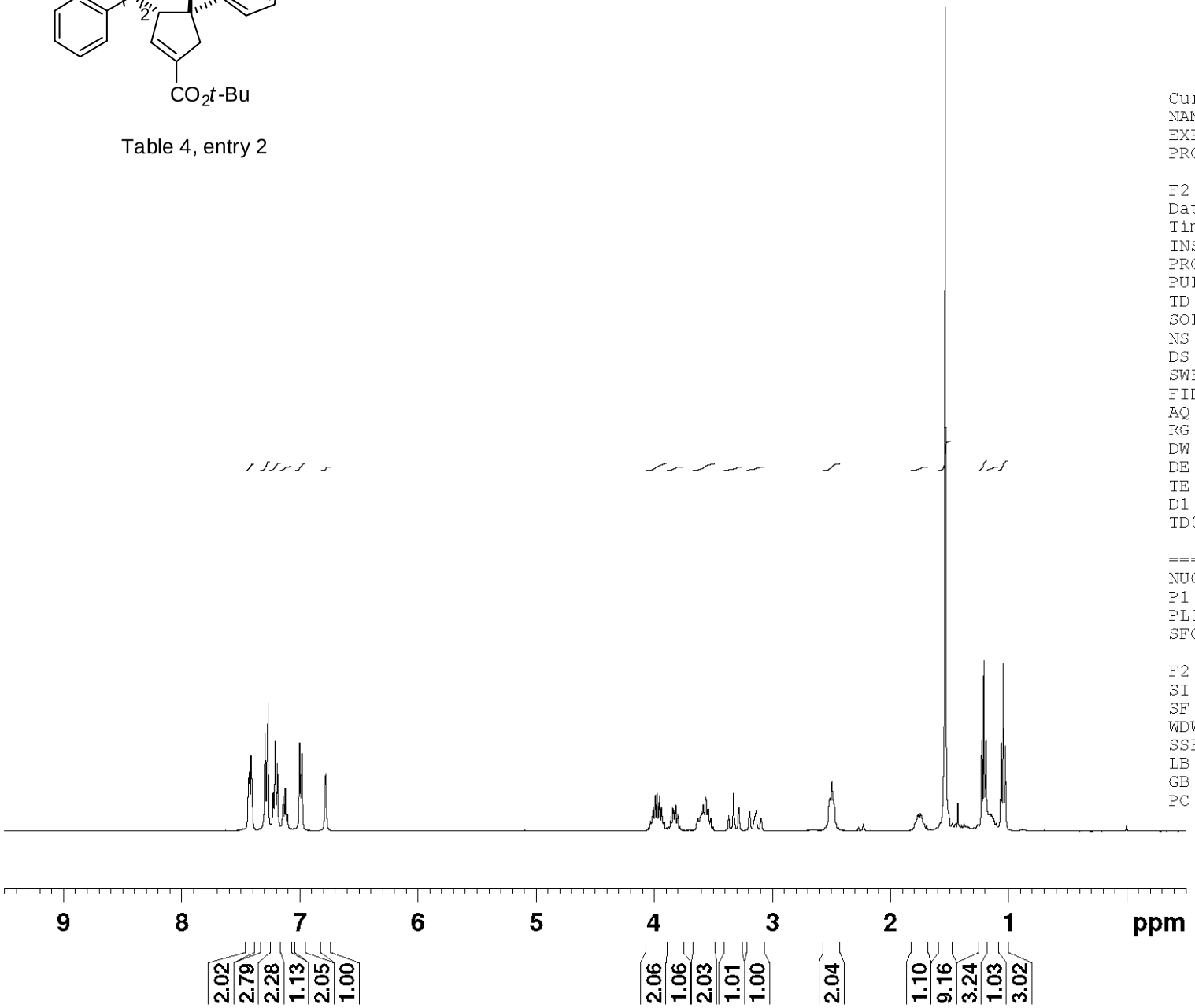


Table 4, entry 2




```
Current Data Parameters
NAME                  YF1066-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110207
Time                     19.08
INSTRUM                  spect
PROBHD   5 mm BBO BB-1H
PULPROG                   zg30
TD                       65536
SOLVENT
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        20.2
DW                      60.400 usec
DE                       6.00 usec
TE                       296.2 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1                       0.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1300060 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```

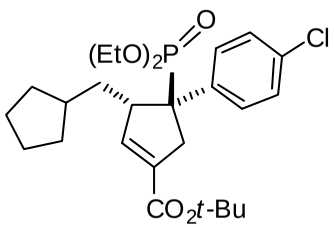
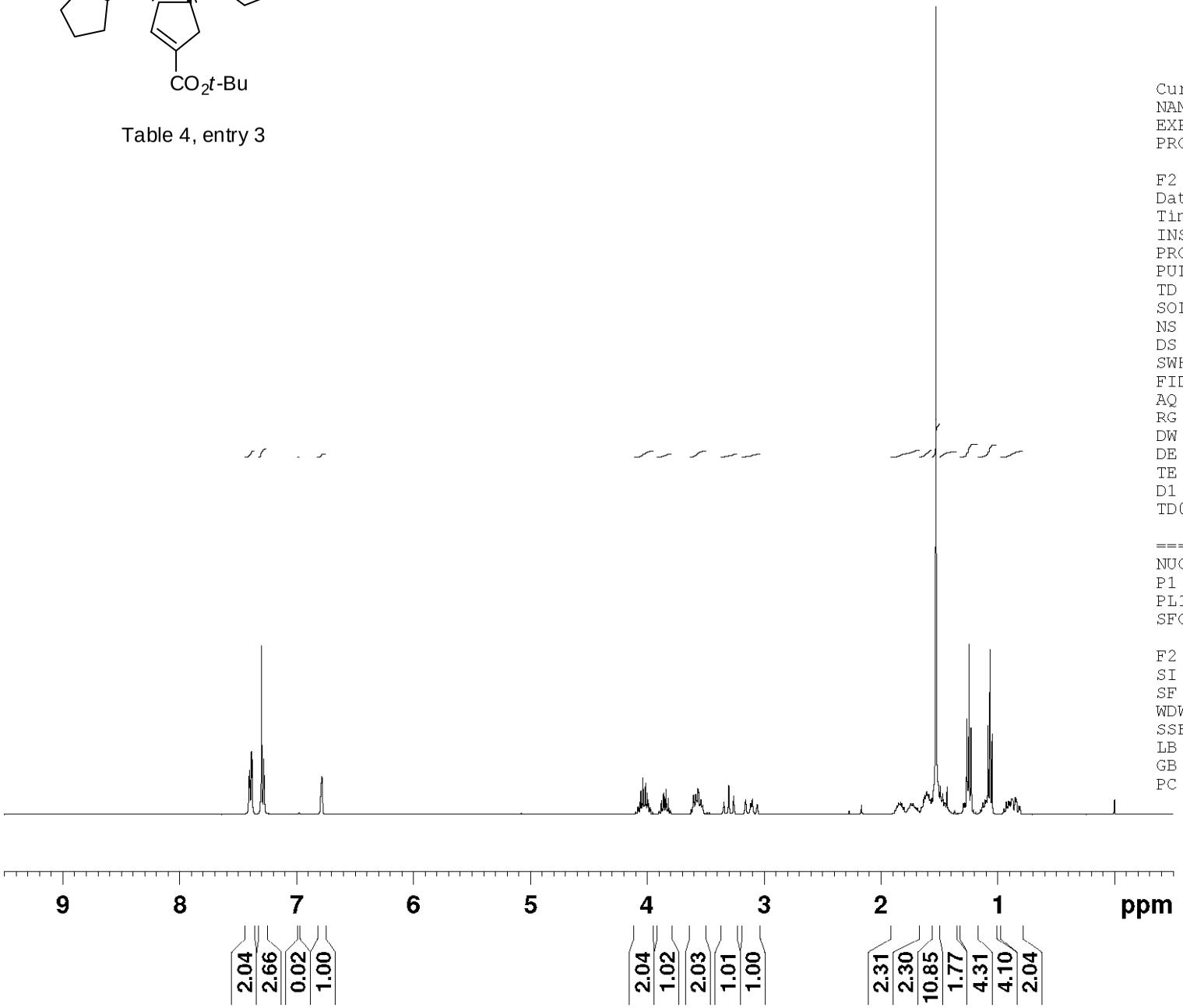


Table 4, entry 3




```
Current Data Parameters
NAME            YF1065-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110205
Time               17.40
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  25.4
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1299928 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

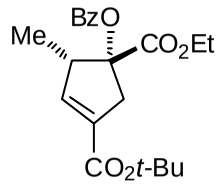
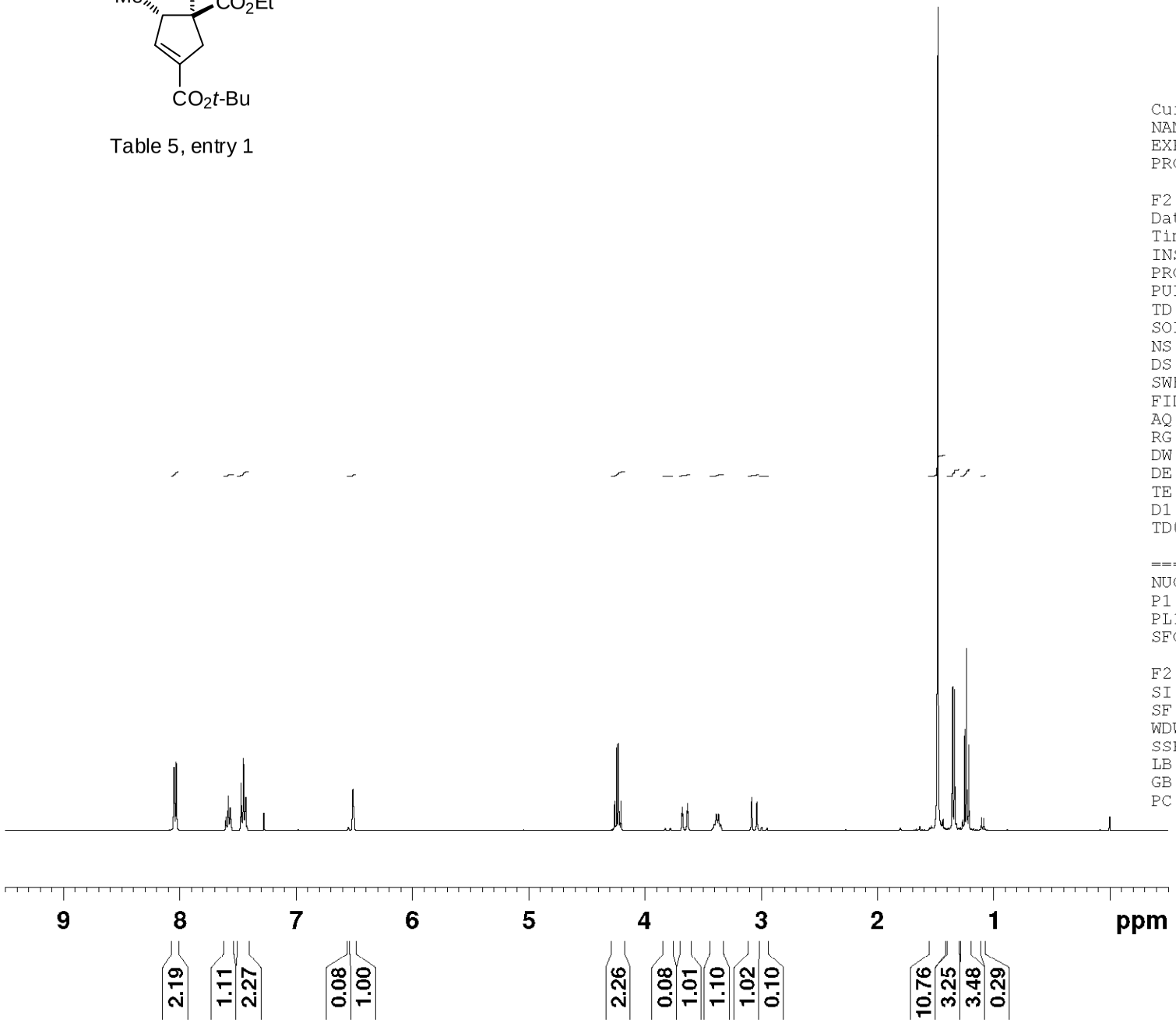


Table 5, entry 1




```
Current Data Parameters
NAME            YF1058-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110203
Time               19.05
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                    32
DW                60.400 usec
DE                 6.00 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300021 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00
```

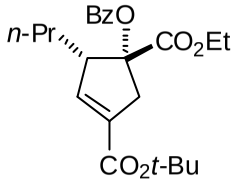
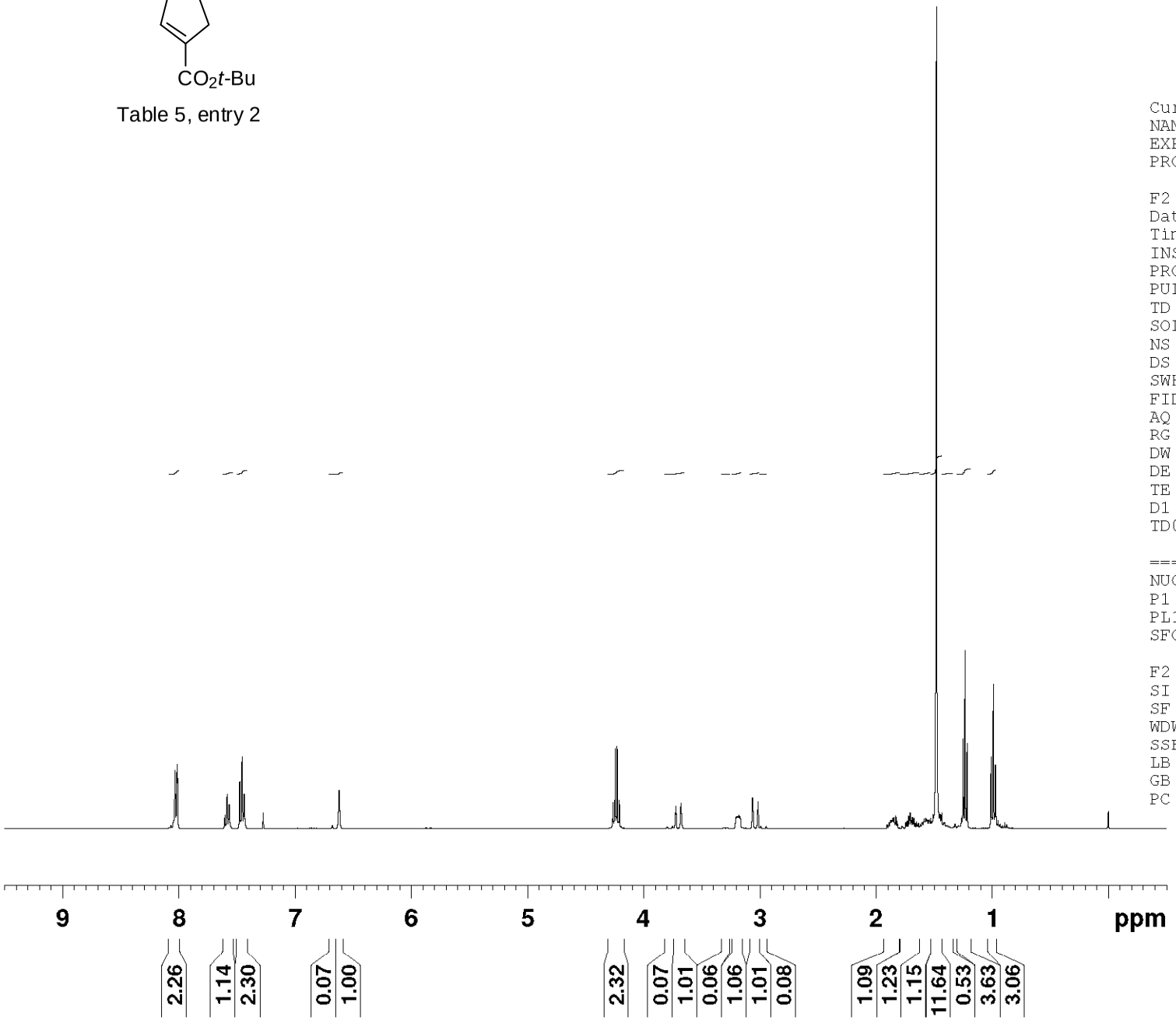


Table 5, entry 2




```
Current Data Parameters
NAME                  YF1059-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110203
Time                     19.13
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                        28.5
DW                    60.400 usec
DE                     6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1300032 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.40
```

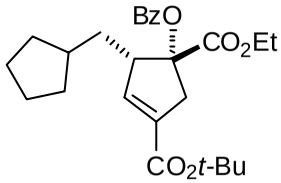
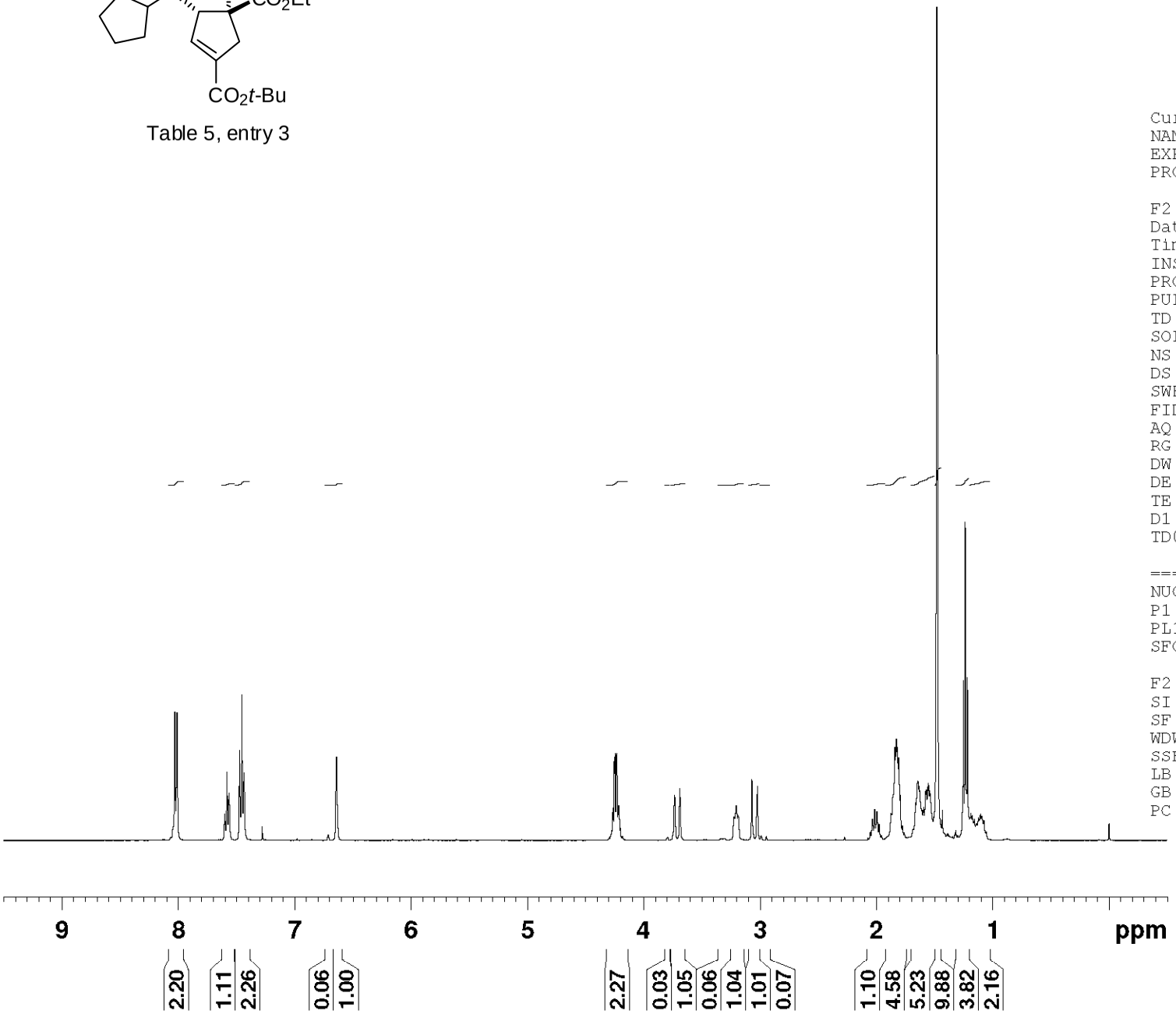


Table 5, entry 3




```
Current Data Parameters
NAME            YF1120-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110304
Time               20.13
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                  25.4
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.07 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300019 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

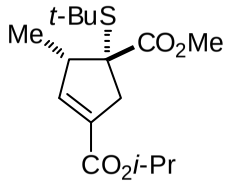
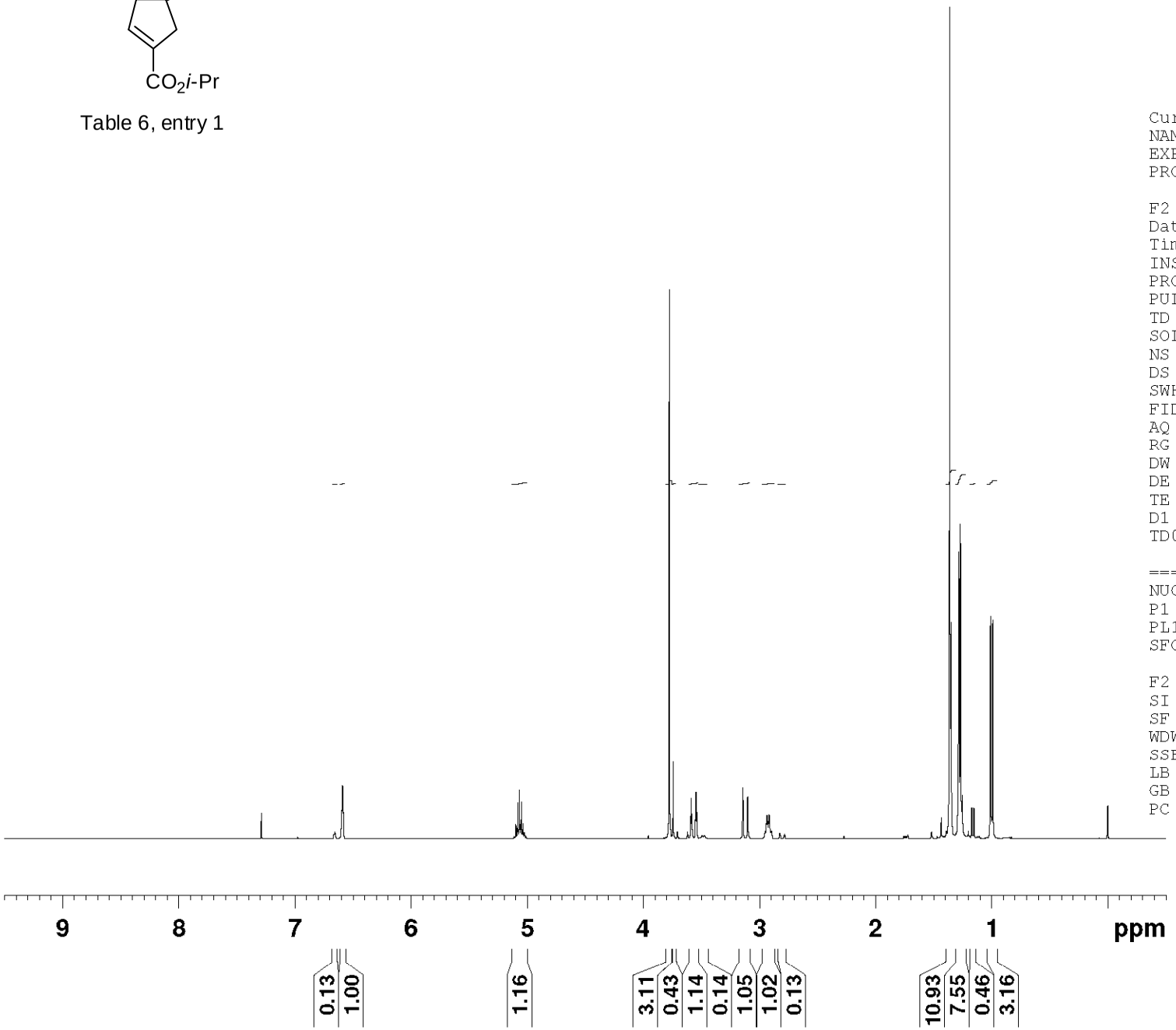


Table 6, entry 1




```
Current Data Parameters
NAME                  YF1095-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20110301
Time                    20.24
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           8
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                        40.3
DW                    60.400 usec
DE                     6.00 usec
TE                     300.0 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF               400.1299974 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.40
```

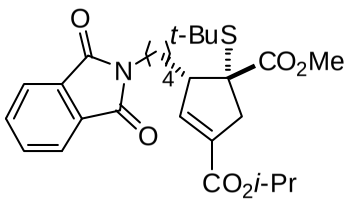
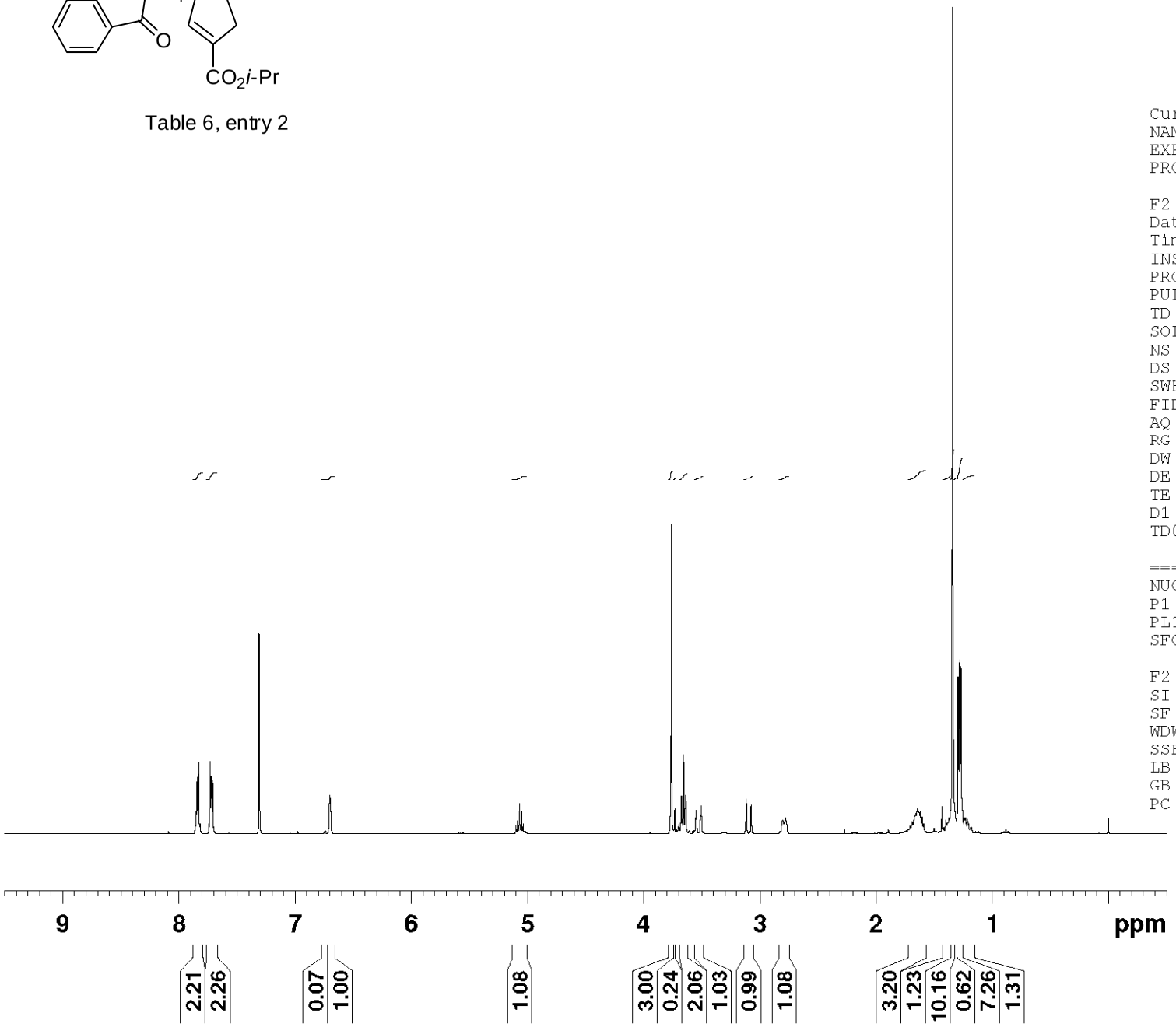


Table 6, entry 2




```
Current Data Parameters
NAME                  YF1103-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110223
Time                     21.05
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                          32
DW                     60.400 usec
DE                      6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF               400.1299891 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                       1.00
```

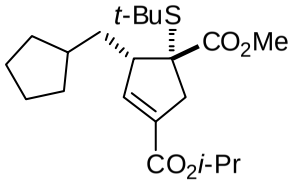
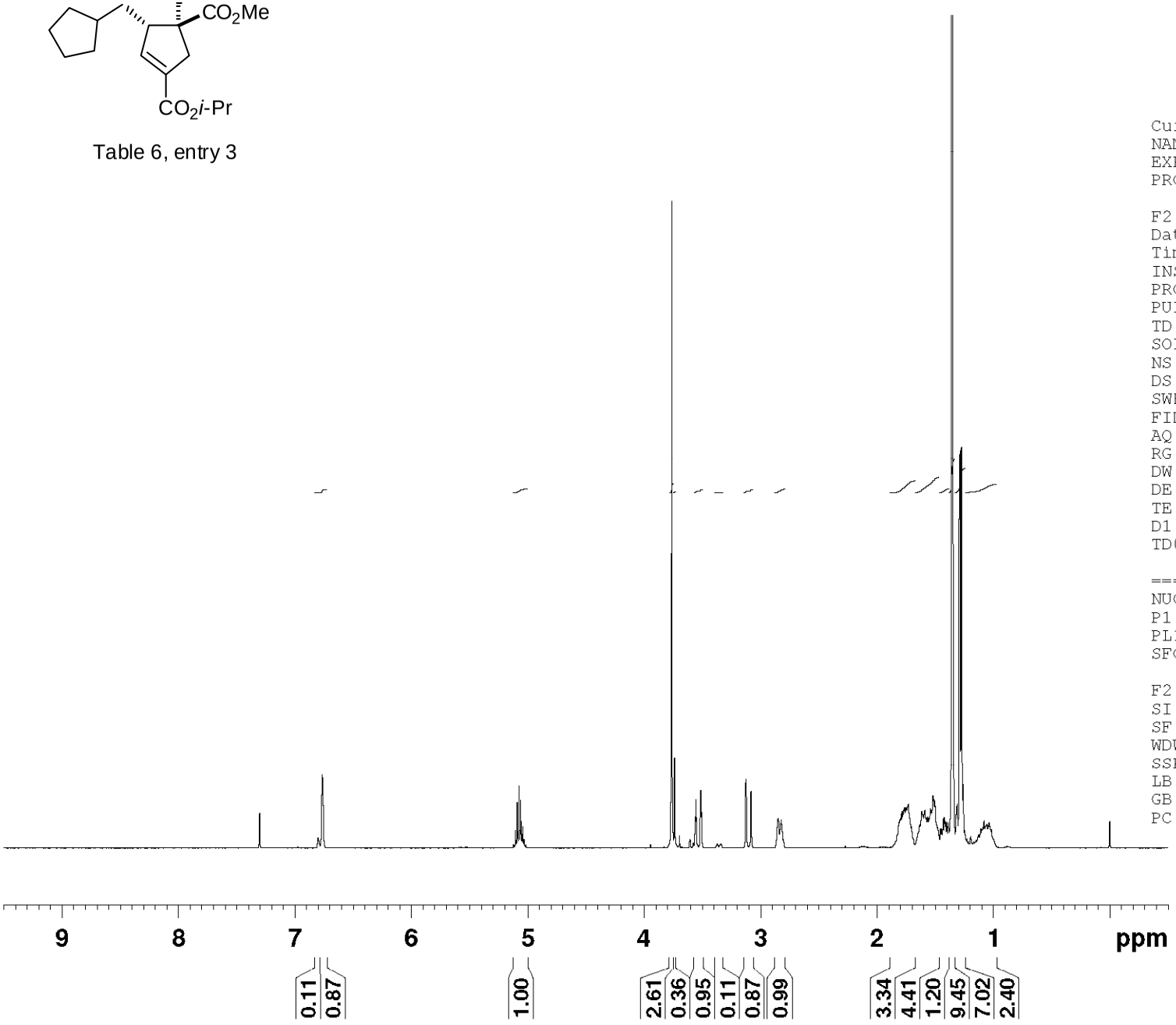
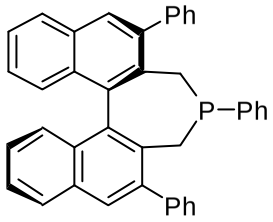


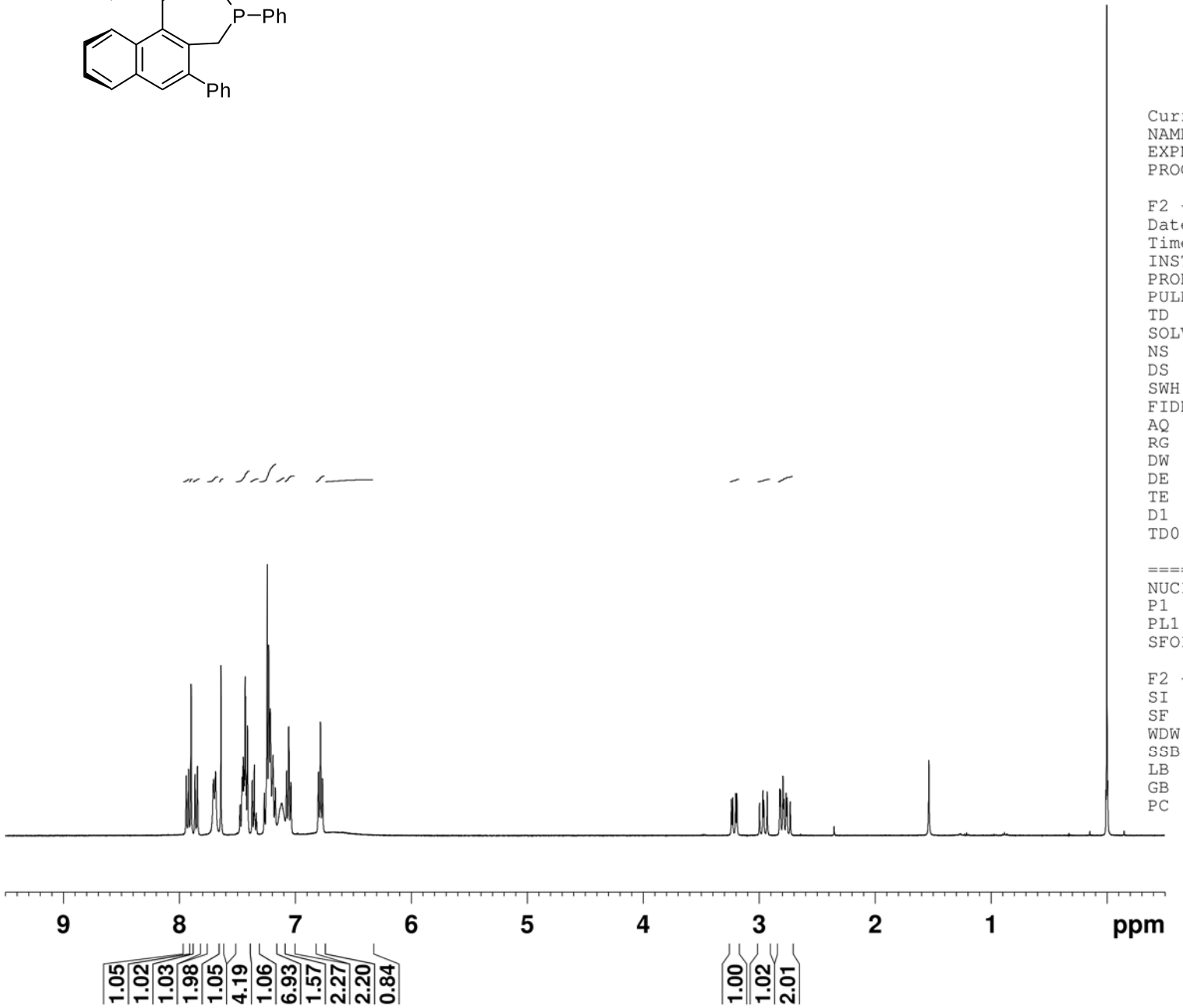
Table 6, entry 3

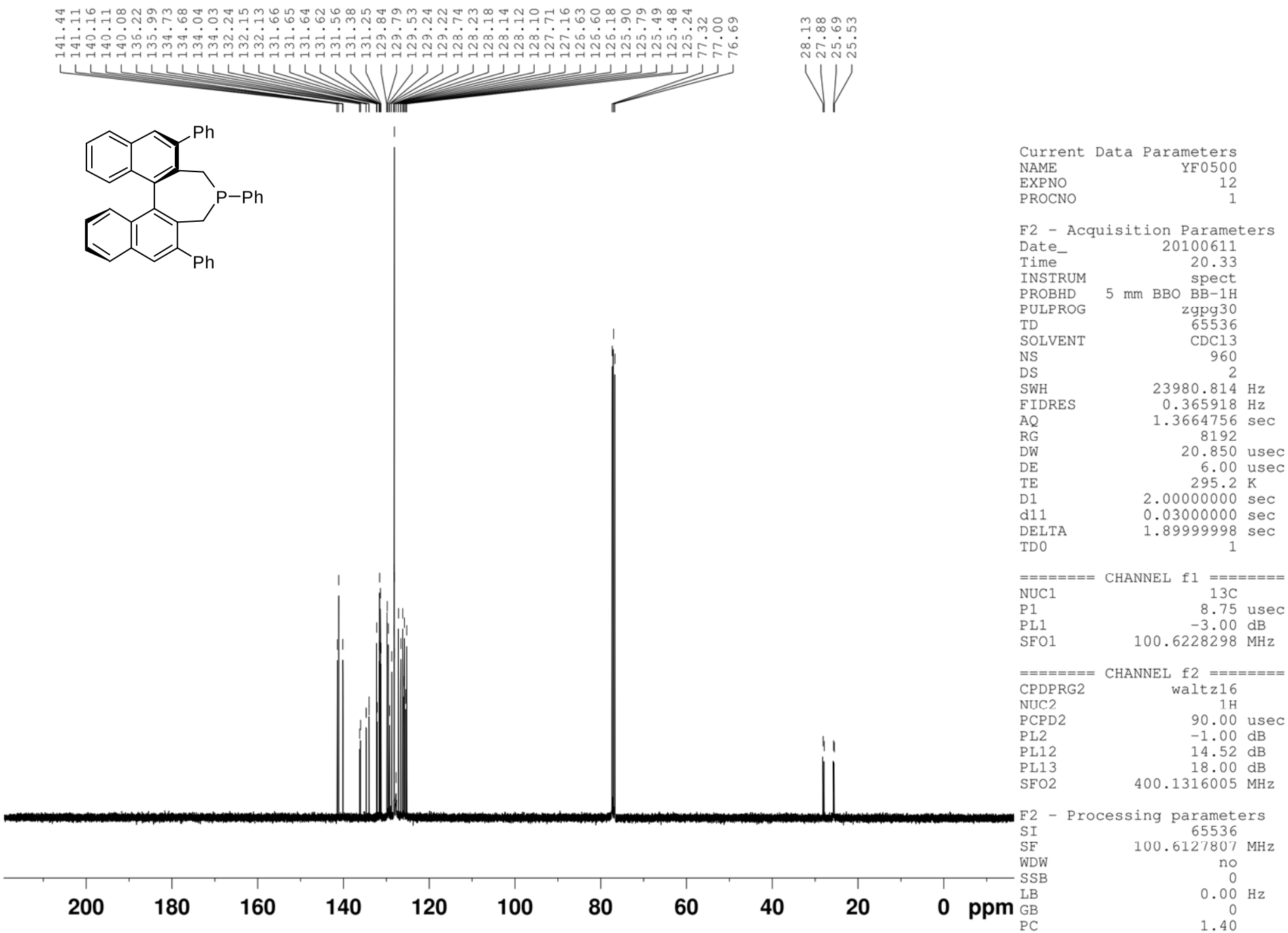



```
Current Data Parameters
NAME                  YF1118-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110303
Time                     18.57
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                           4
DS                           2
SWH                 8278.146 Hz
FIDRES               0.126314 Hz
AQ                  3.9584243 sec
RG                        25.4
DW                     60.400 usec
DE                      6.00 usec
TE                     296.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF               400.1299913 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00
```

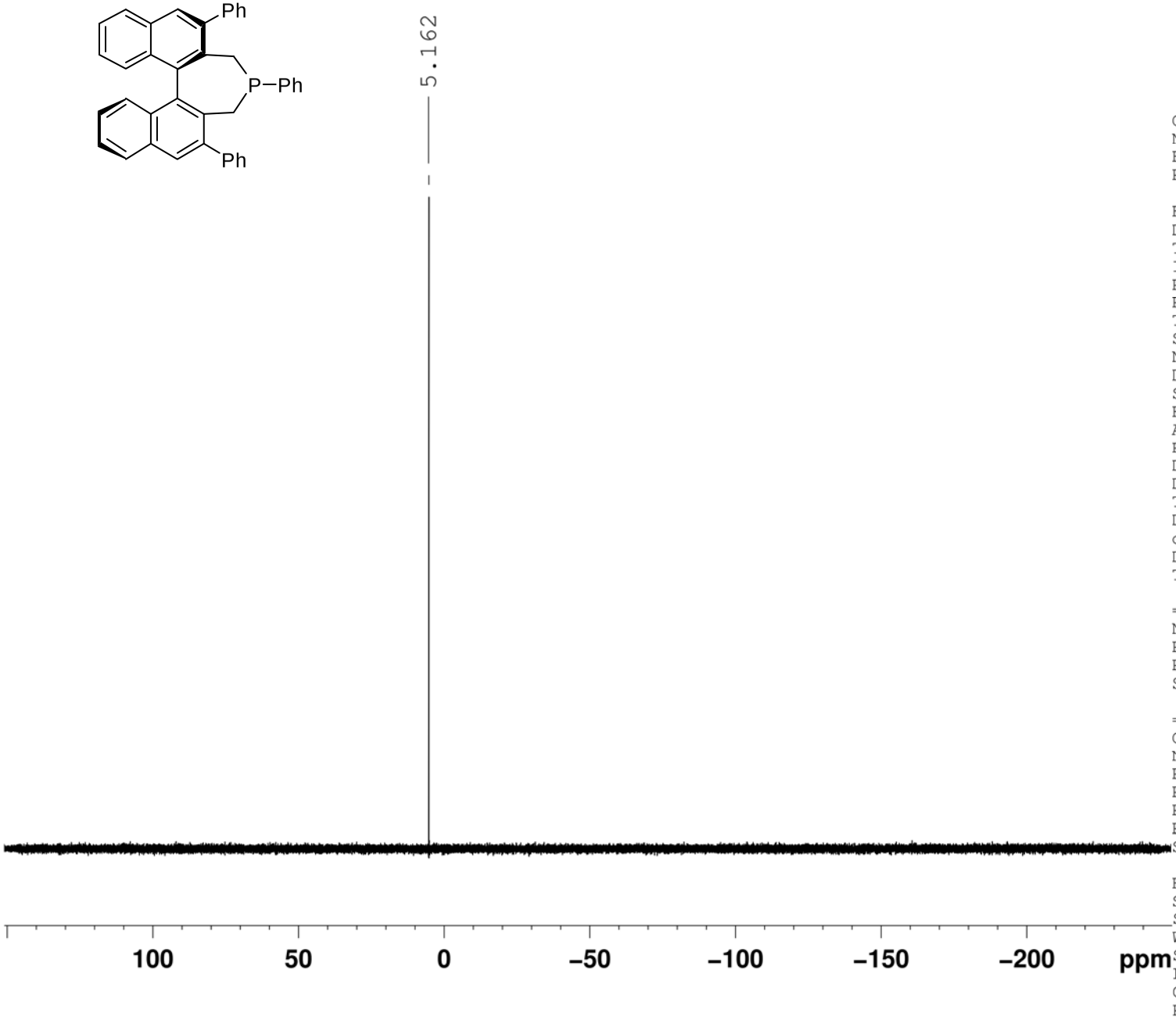



```
Current Data Parameters
NAME              YF0500
EXPNO                103
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100619
Time               13.29
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   256
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300168 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

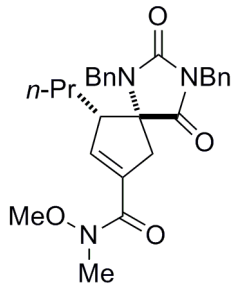




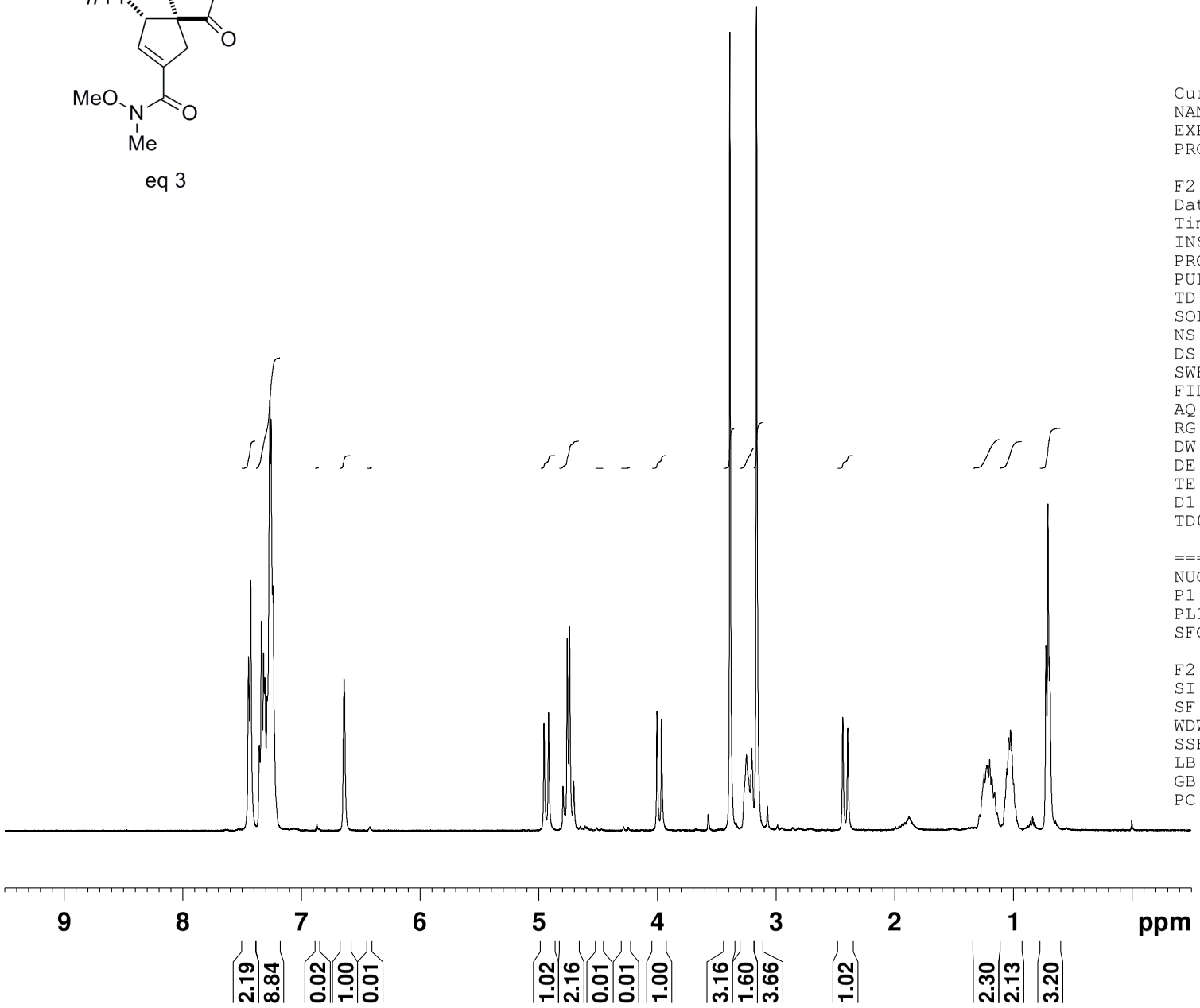

```
Current Data Parameters
NAME                 YF0500
EXPNO                    12
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100611
Time                  20.33
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      960
DS                        2
SWH              23980.814 Hz
FIDRES            0.365918 Hz
AQ                1.3664756 sec
RG                     8192
DW                   20.850 usec
DE                    6.00 usec
TE                   295.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                     8.75 usec
PL1                   -3.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -1.00 dB
PL12                 14.52 dB
PL13                 18.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    65536
SF             100.6127807 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.40
```




```
Current Data Parameters
NAME                 YF0500
EXPNO                   101
PROCNO                    1

F2 - Acquisition Parameters
Date_             20100619
Time                 13.20
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        4
SWH              64935.066 Hz
FIDRES            0.990830 Hz
AQ                0.5046772 sec
RG                    22800
DW                  7.700 usec
DE                  6.00 usec
TE                  294.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                  31P
P1                  9.25 usec
PL1                 3.00 dB
SFO1         161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316000 MHz

F2 - Processing parameters
SI                    65536
SF           161.9755004 MHz
WDW                      no
SSB                       0
LB                  0.00 Hz
GB                        0
PC                     1.40
```

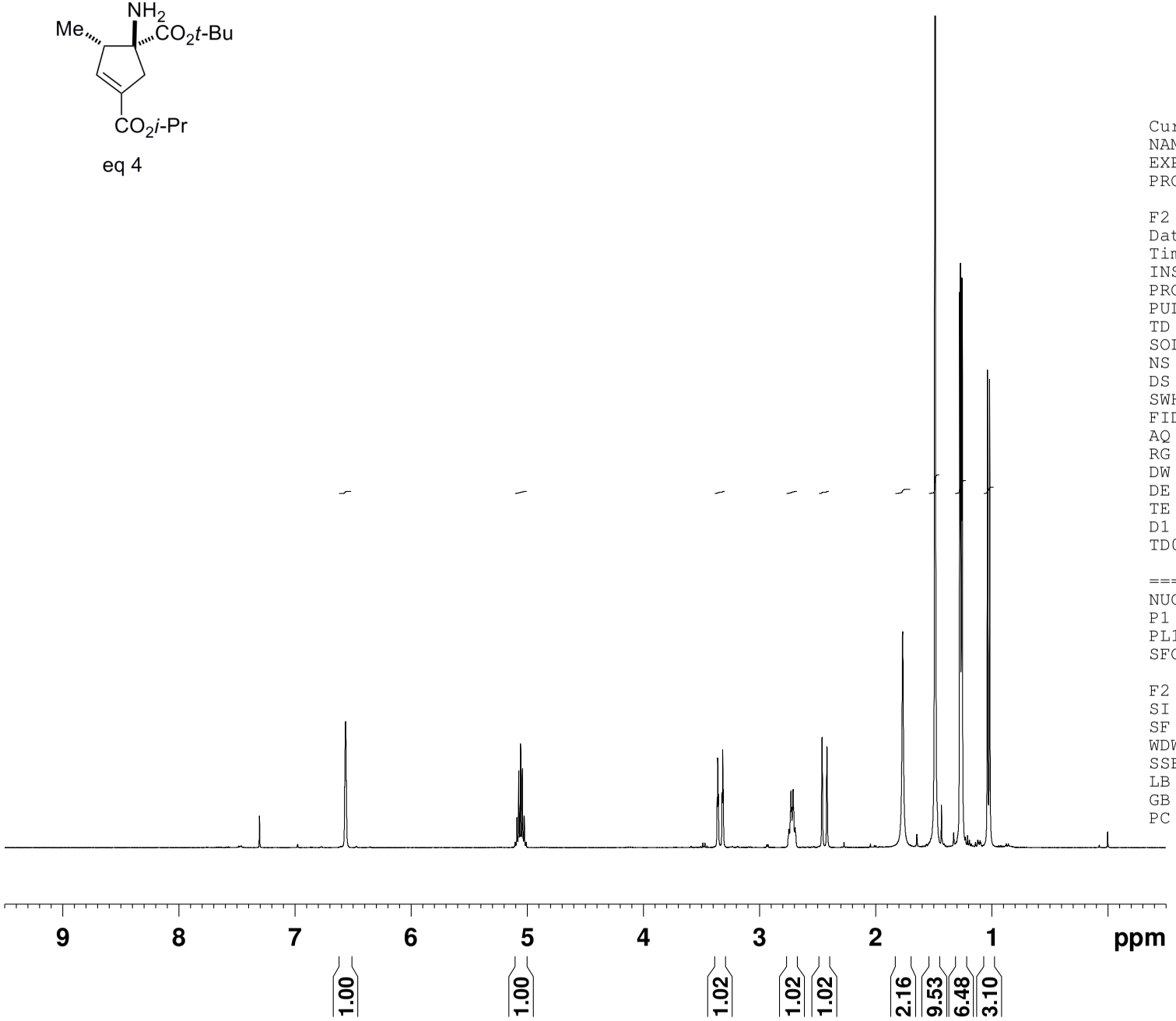


eq 3

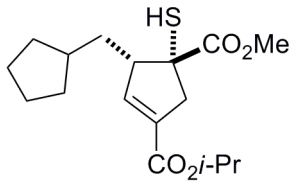



```
Current Data Parameters
NAME            YF1225-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110427
Time               18.39
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ             3.9584243 sec
RG                 143.7
DW                60.400 usec
DE                 6.00 usec
TE                683.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300058 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

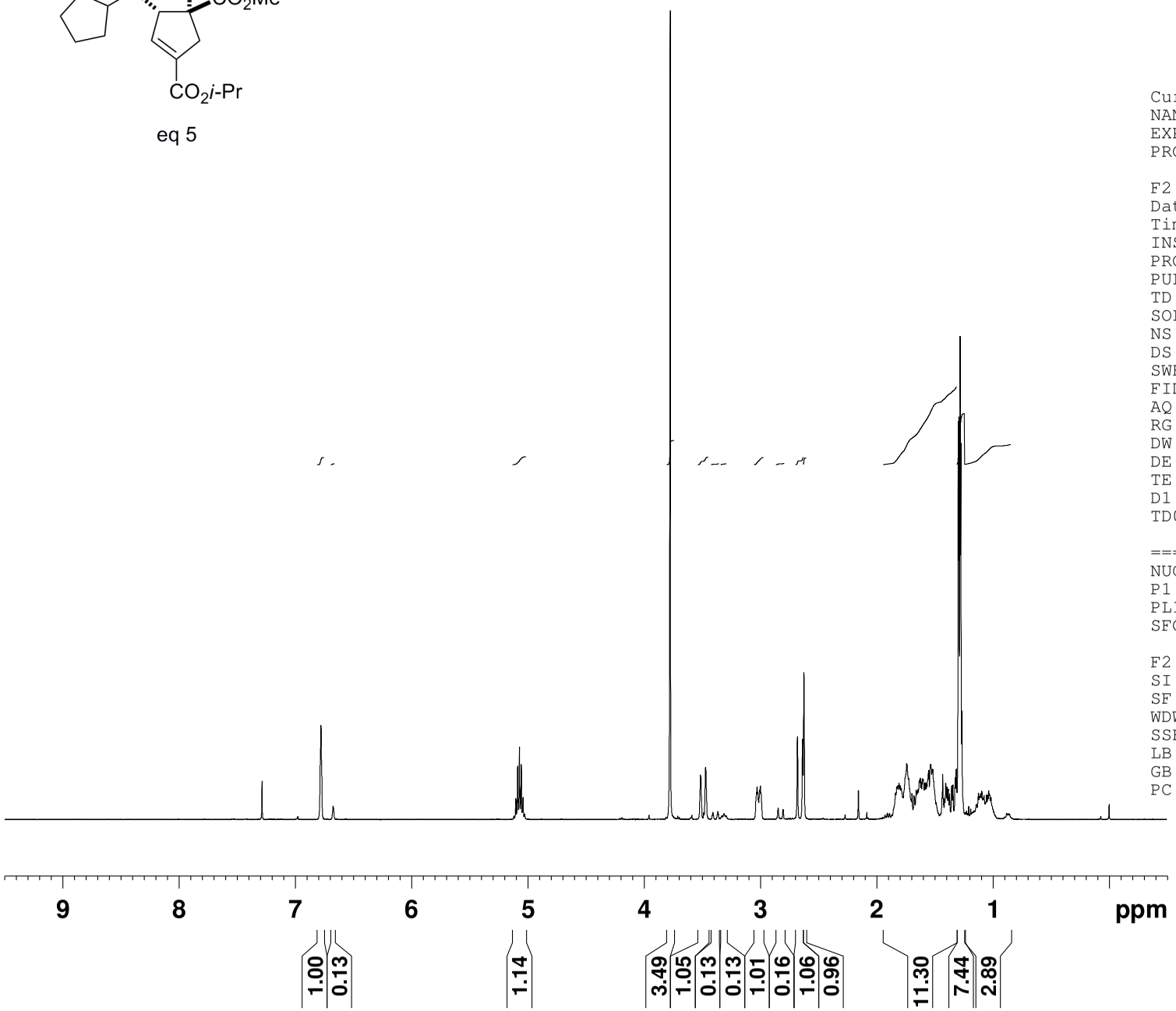
eq 4



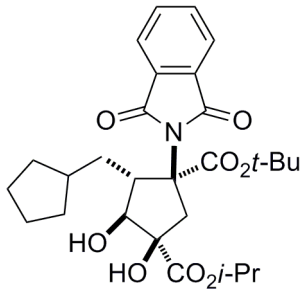

```
Current Data Parameters
NAME                  YF1212-3
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110422
Time                      8.06
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                  8278.146 Hz
FIDRES               0.126314 Hz
AQ                   3.9584243 sec
RG                          32
DW                     60.400 usec
DE                      6.00 usec
TE                     297.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF               400.1299903 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00
```



eq 5

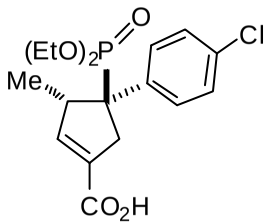


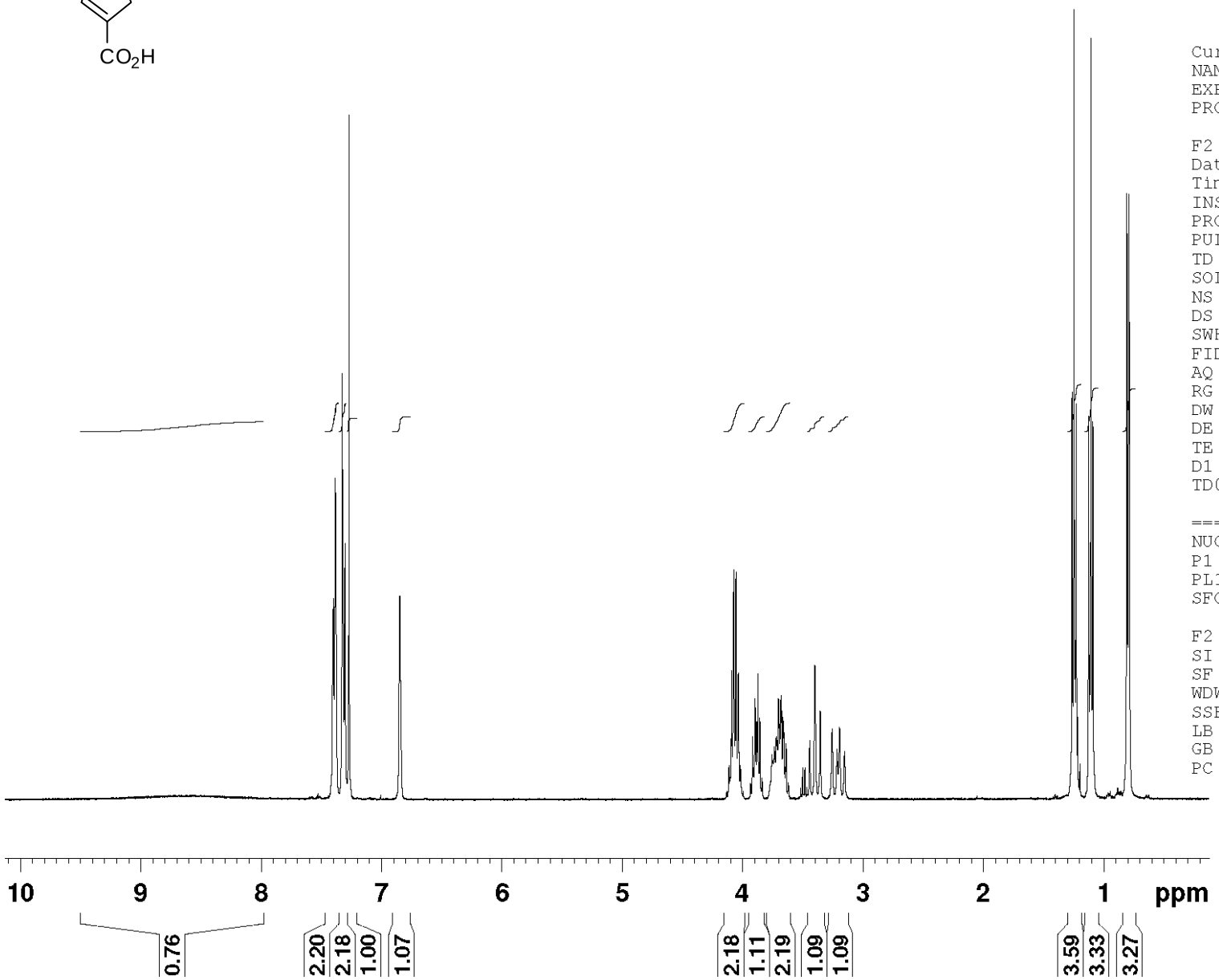

```
Current Data Parameters
NAME                  YF1221-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110423
Time                     16.30
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        90.5
DW                       60.400 usec
DE                        6.00 usec
TE                       683.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1299989 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```



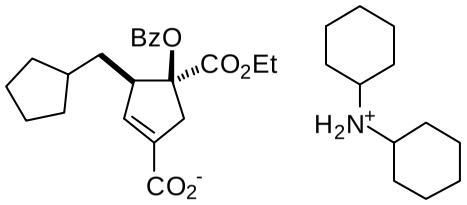
eq 6

```
Current Data Parameters
NAME                  YF1195-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110411
Time                     17.29
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        40.3
DW                      60.400 usec
DE                       6.00 usec
TE                       683.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1299969 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```

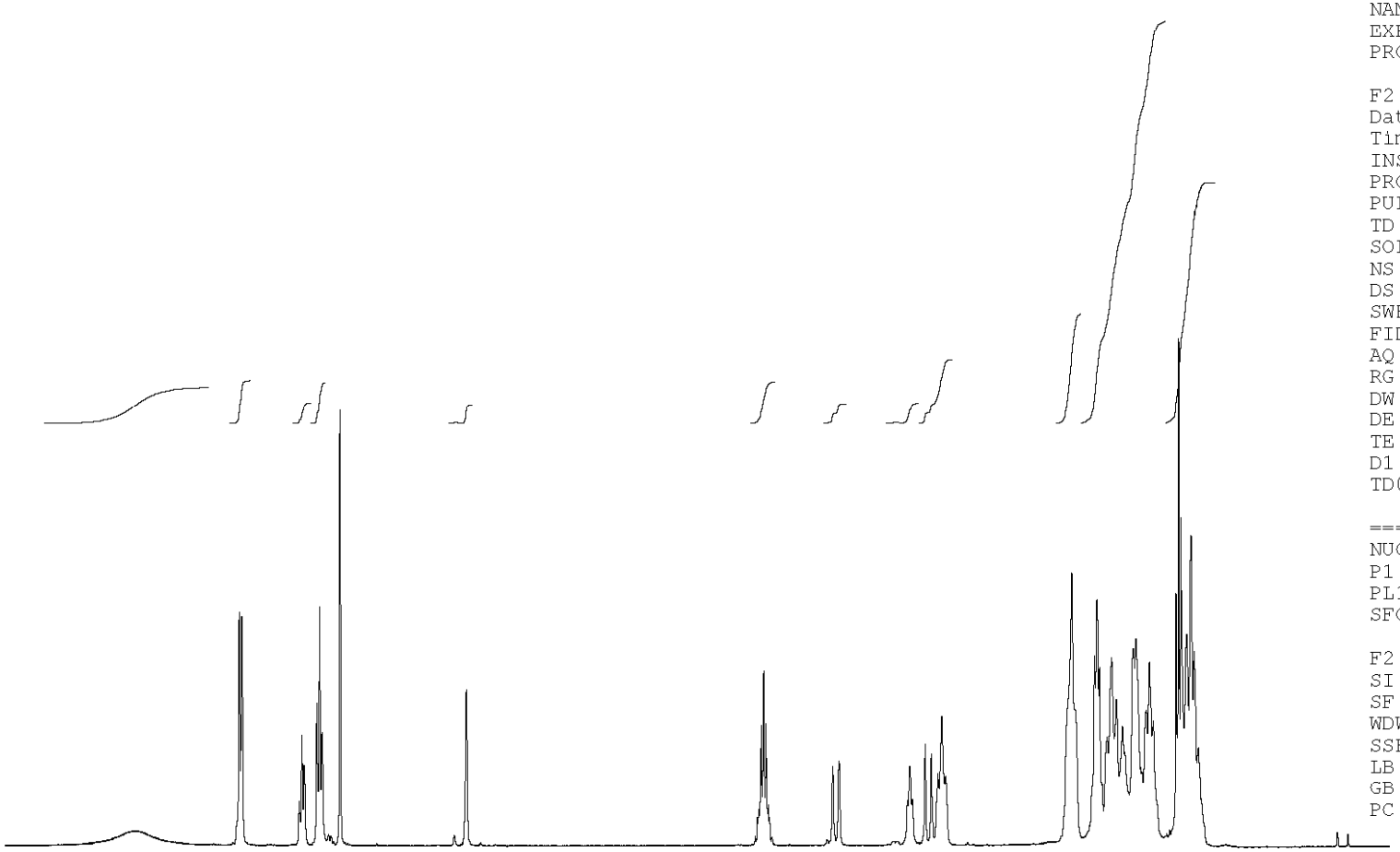


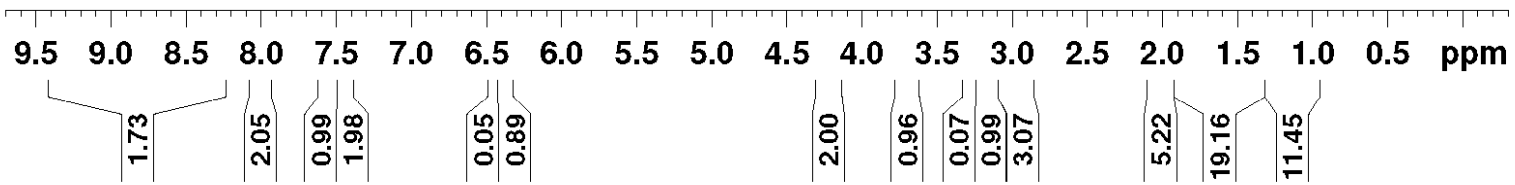



```
Current Data Parameters
NAME                  YF1247
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20110504
Time                  19.37
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9584243 sec
RG                     812.7
DW                    60.400 usec
DE                     6.00 usec
TE                    683.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.00 usec
PL1                     0.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF             400.1300060 MHz
WDW                         no
SSB                          0
LB                      0.00 Hz
GB                           0
PC                      1.00
```

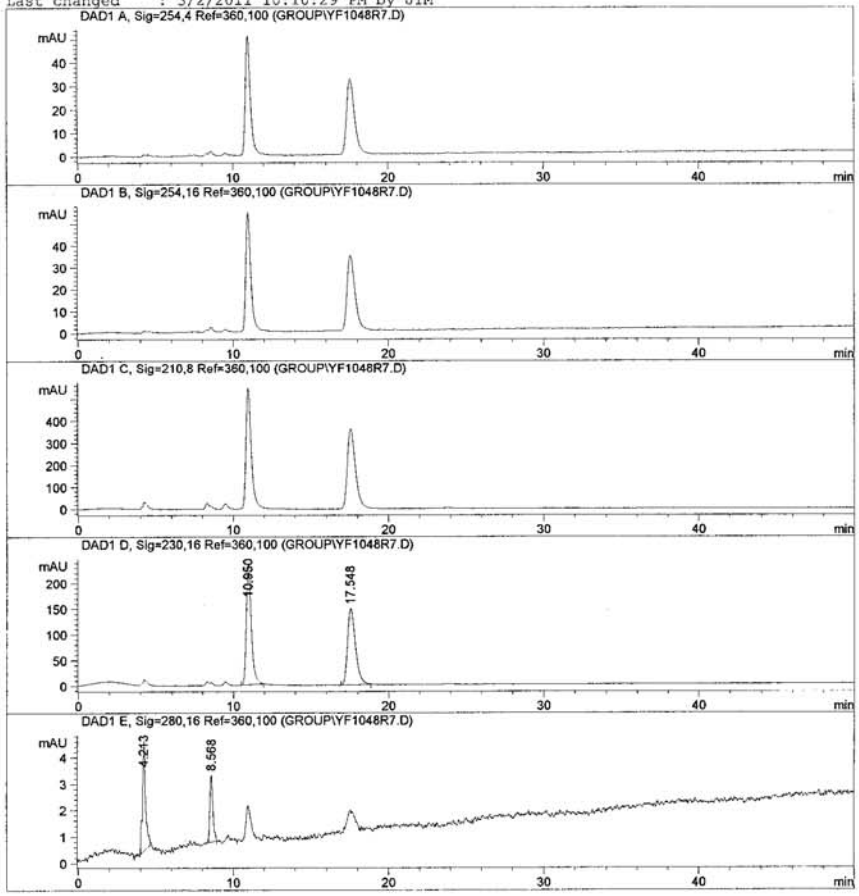



```
Current Data Parameters
NAME                  YF1228-5
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110507
Time                     14.05
INSTRUM                  spect
PROBHD   5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT
NS                           4
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                          32
DW                       60.400 usec
DE                        6.00 usec
TE                       299.2 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1                       0.00 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                 400.1300009 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```





```
Injection Date  : 3/3/2011 2:35:36 AM          Seq. Line :  10
Sample Name     : YF1048 RAC                    Location : Vial 56
Acq. Operator   : JTM                           Inj :  1
Acq. Instrument : Instrument 1                  Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3050.M
Last changed    : 3/2/2011 10:09:34 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100


Signal 2: DAD1 B, Sig=254,16 Ref=360,100


Signal 3: DAD1 C, Sig=210,8 Ref=360,100


Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.950 PB    0.3411 5293.27539  234.67831  50.3783
   2  17.548 BB    0.5333 5213.78613  148.60362  49.6217

Totals :                  1.05071e4   383.28194

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.213 PB    0.1953   57.50676   4.15948  62.5202
   2   8.568 BB    0.1963   34.47427   2.54110  37.4798

Totals :                    91.98103   6.70058

 Results obtained with enhanced integrator!
```

*** End of Report ***

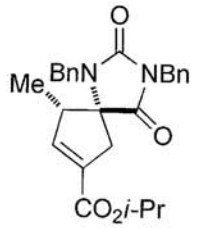
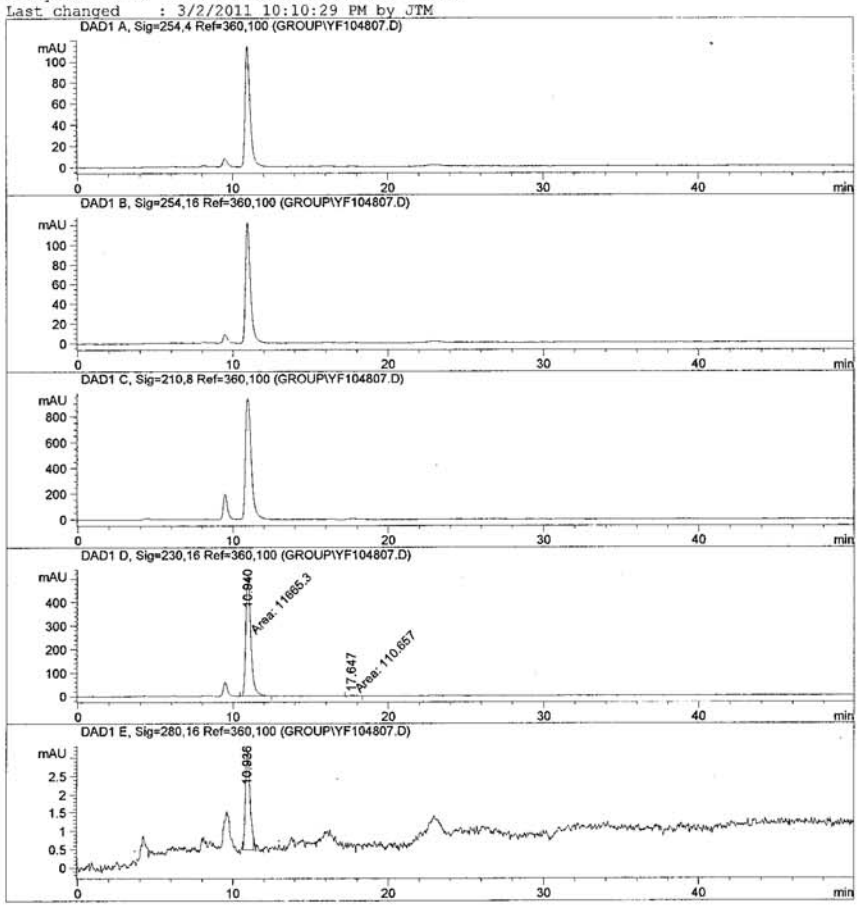


Table 2, entry 1

racemic sample

```
Injection Date  : 3/3/2011 3:26:51 AM          Seq. Line :  11
Sample Name     : YF1048 S-cat                  Location : Vial 57
Acq. Operator   : JTM                             Inj :  1
Acq. Instrument : Instrument 1                Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3050.M
Last changed    : 3/2/2011 10:09:34 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.940 MM    0.3770 1.16653e4   515.71472  99.0603
   2  17.647 MM    0.6190  110.65682    2.97947   0.9397

Totals :                  1.17759e4   518.69419

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.936 BB    0.2591   56.46589    2.68731 100.0000

Totals :                    56.46589    2.68731

 Results obtained with enhanced integrator!

                *** End of Report ***
```

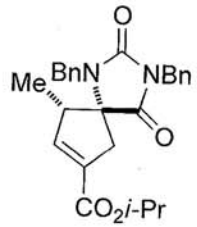
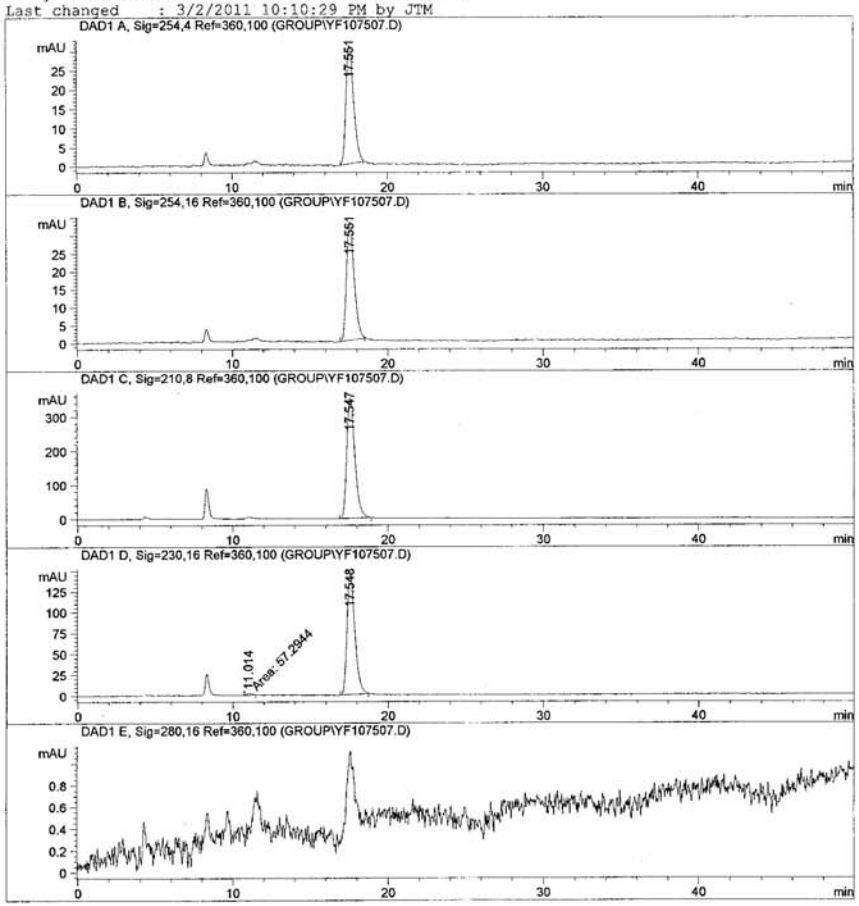


Table 2, entry 1

with (*S*)-catalyst

Injection Date : 3/3/2011 4:18:06 AM Seq. Line : 12
Sample Name : YF1075 R-cat Location : Vial 58
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IC-3050.M
Last changed : 3/2/2011 10:09:34 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed : 3/2/2011 10:10:29 PM by JTM



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.551	BB	0.4886	1050.73804	30.91210	100.0000
Totals :				1050.73804	30.91210	

Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.551	BB	0.4913	1131.36682	33.05995	100.0000
Totals :				1131.36682	33.05995	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.547	BB	0.5472	1.26251e4	353.08881	100.0000
Totals :				1.26251e4	353.08881	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.014	MM	0.4460	57.29445	2.14089	1.1258
2	17.548	PB	0.5333	5031.85107	144.12061	98.8742
Totals :				5089.14552	146.26150	

Results obtained with enhanced integrator!

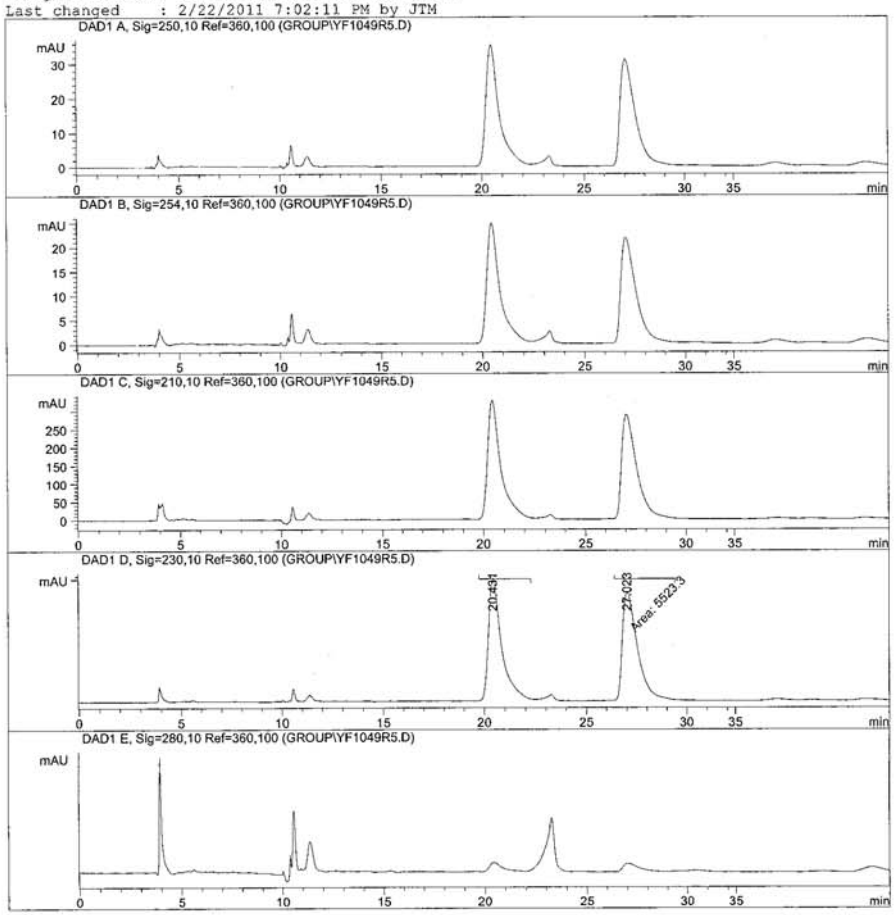
Signal 5: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 2, entry 1

with (*R*)-catalyst

```
Injection Date  : 2/22/2011 8:01:01 PM          Seq. Line :   3
Sample Name     : YF1049 RAC                     Location : Vial 7
Acq. Operator   : YL                                Inj :   1
Acq. Instrument : Instrument 1                Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-40.M
Last changed    : 2/18/2007 7:39:36 PM by GROUP
Analysis Method : C:\HPCHEM\1\METHODS\OJ-AD20.M
Last changed    : 2/22/2011 7:02:11 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  20.431 BB    0.6563 5441.49072  122.02242  49.6269
   2  27.023 MM    0.8579 5523.30078  107.30299  50.3731

Totals :                  1.09648e4   229.32542

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100
```

*** End of Report ***

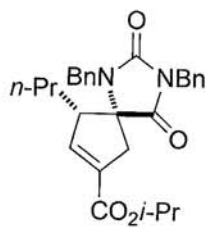
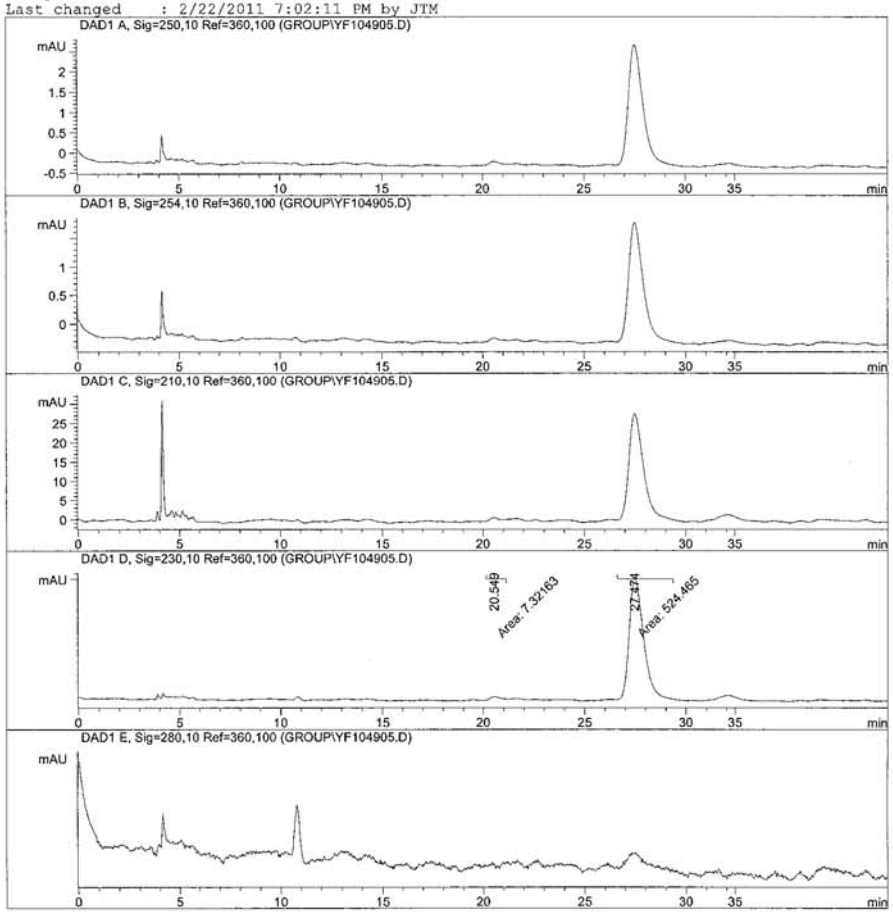


Table 2, entry 2

racemic sample

```
Injection Date  : 2/22/2011 8:42:15 PM          Seq. Line :   4
Sample Name     : YF1049 S-cat                  Location : Vial 8
Acq. Operator   : YL                               Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-40.M
Last changed    : 2/18/2007 7:39:36 PM by GROUP
Analysis Method : C:\HPCHEM\1\METHODS\OJ-AD20.M
Last changed    : 2/22/2011 7:02:11 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.549	MM	0.4435	7.32163	2.75120e-1	1.3768
2	27.474	MM	0.8419	524.46497	10.38302	98.6232
Totals :				531.78660	10.65814	

```
 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100
```

*** End of Report ***

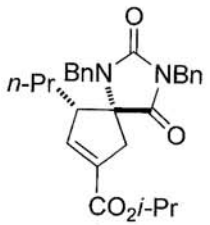
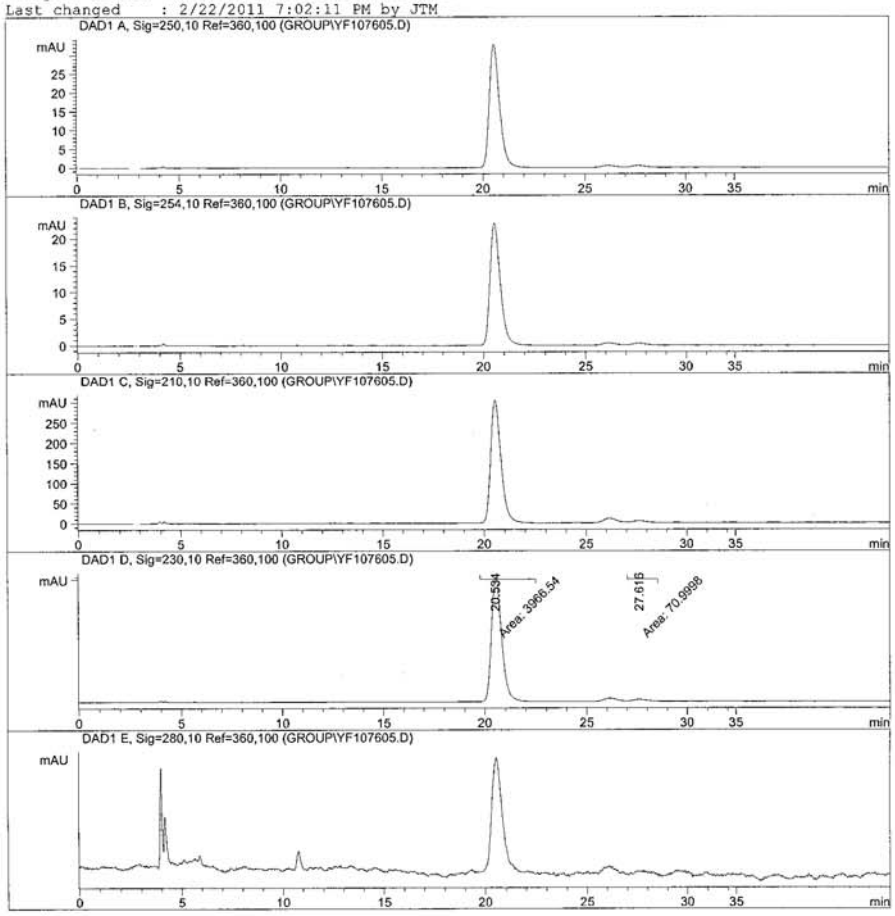


Table 2, entry 2

with (*S*)-catalyst

```
Injection Date  : 2/22/2011 9:23:28 PM          Seq. Line :   5
Sample Name     : YF1076 R-cat                  Location : Vial 9
Acq. Operator   : YL                               Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-40.M
Last changed    : 2/18/2007 7:39:36 PM by GROUP
Analysis Method : C:\HPCHEM\1\METHODS\OJ-AD20.M
Last changed    : 2/22/2011 7:02:11 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.534	MM	0.5828	3966.53564	113.43987	98.2415
2	27.616	MM	0.7389	70.99984	1.60149	1.7585
Totals :				4037.53548	115.04136	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

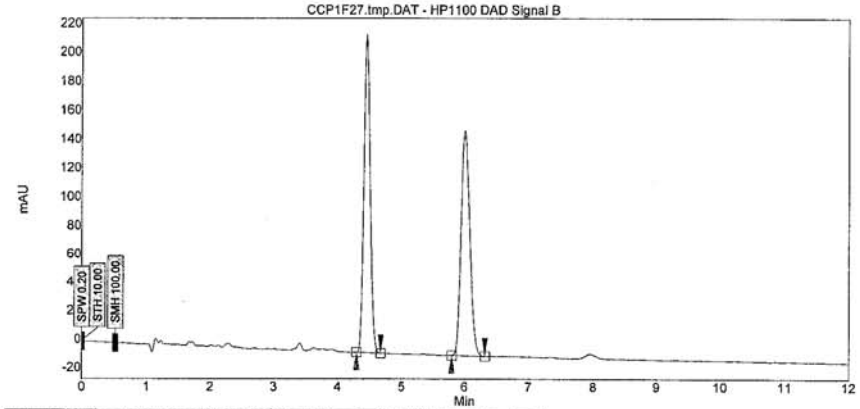
*** End of Report ***

in-Pr R-cat

Table 2, entry 2

with (*R*)-catalyst

yf1151-r-5 Vial 61 Method: IC 20.0% MeOH



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.30	4.45	4.67	0.00	50.01	221.3	24.8	50.013
2	UNKNOWN	5.80	6.01	6.32	0.00	49.99	157.3	24.8	49.987
Total						100.00	378.6	49.6	100.000

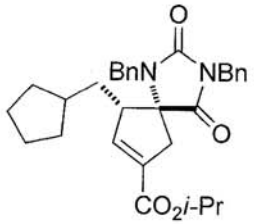
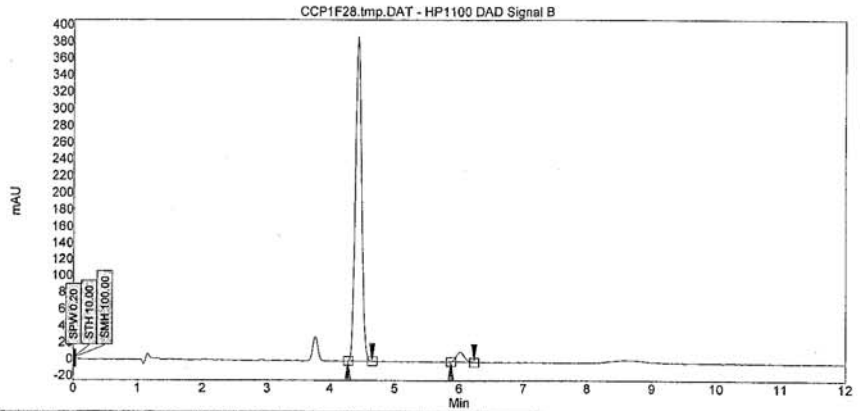


Table 2, entry 3

racemic sample

yf1151-5 Vial 62 Method: IC 20.0% MeOH



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.28	4.43	4.66	0.00	96.05	388.2	44.1	96.054
2	UNKNOWN	5.87	6.02	6.23	0.00	3.95	12.0	1.8	3.946
Total						100.00	400.2	46.0	100.000

92

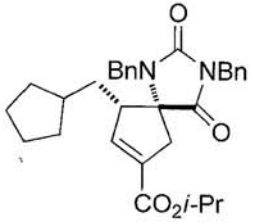
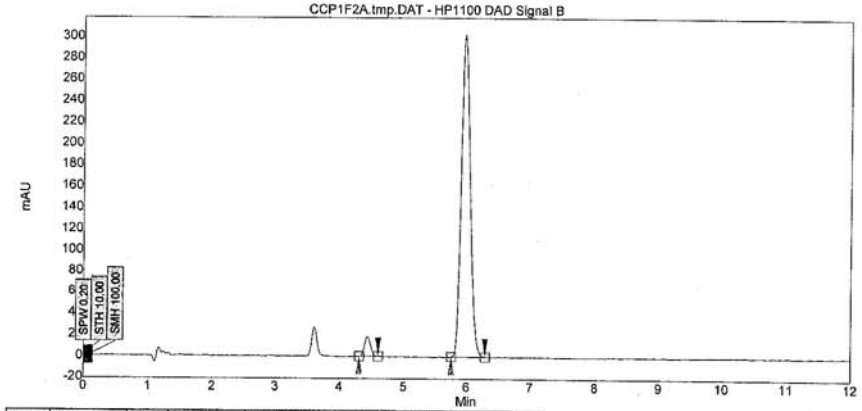


Table 2, entry 3

with (*S*)-catalyst

yf1178-5 Vial 83 Method: IC 20.0% MeOH



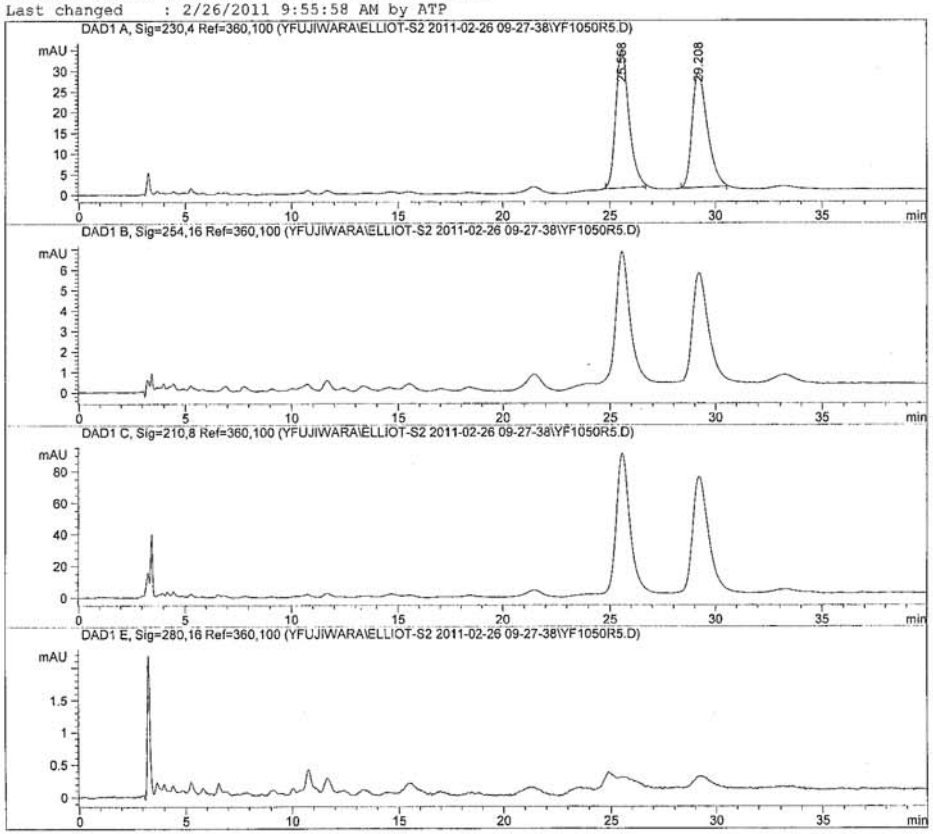
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.31	4.44	4.61	0.00	3.85	18.1	2.0	3.845
2	UNKNOWN	5.76	5.97	6.30	0.00	96.15	302.1	49.4	96.155
Total						100.00	320.2	51.4	100.000

Table 2, entry 3

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1050R5.D
ample Name: YF1050 RAC

Acq. Operator : ATP Seq. Line : 15
Acq. Instrument : Instrument 1 Location : Vial 13
Injection Date : 2/26/2011 5:37:01 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H03-40.M
Last changed : 2/26/2011 9:29:04 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 9:55:58 AM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1050R5.D
Sample Name: YF1050 RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.568	BB	0.6491	1459.88733	33.58491	50.4819
2	29.208	BB	0.7678	1432.01428	27.85373	49.5181
Totals :				2891.90161	61.43864	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

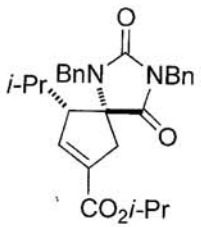
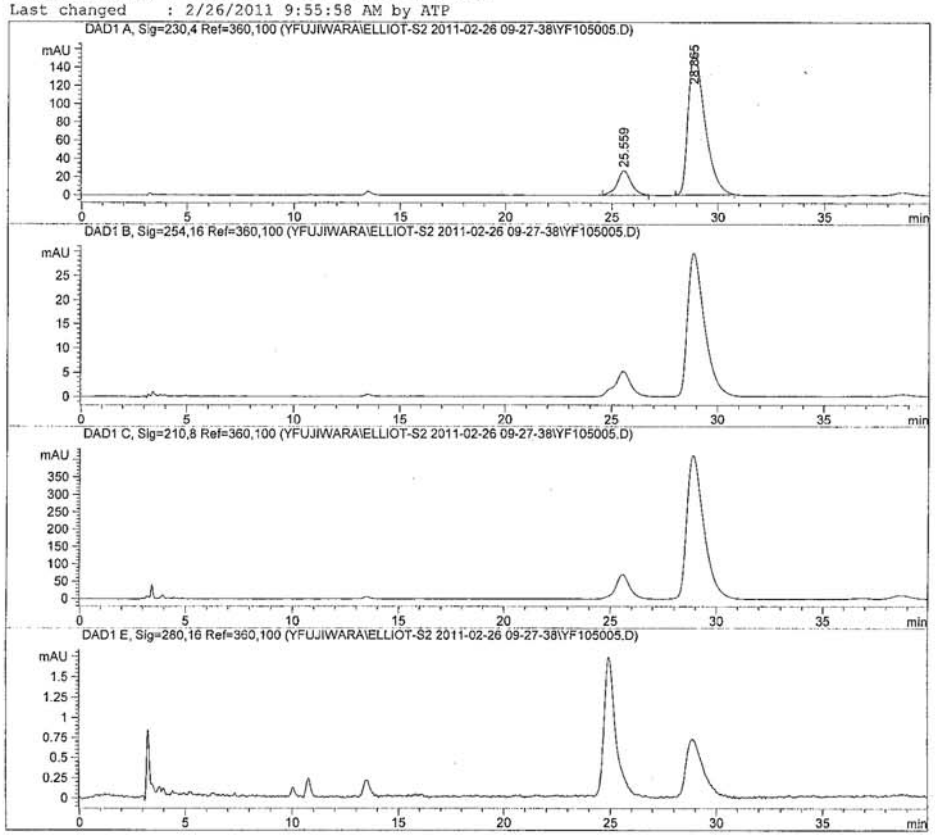


Table 2, entry 4

racemic sample

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF105005.D
ample Name: YF1050 S

Acq. Operator : ATP Seq. Line : 16
Acq. Instrument : Instrument 1 Location : Vial 14
Injection Date : 2/26/2011 6:18:17 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H03-40.M
Last changed : 2/26/2011 9:29:04 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 9:55:58 AM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF105005.D
Sample Name: YF1050 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: . : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.559	BB	0.6715	1229.21667	26.78090	12.5102
2	28.865	BB	0.8207	8596.53125	157.03171	87.4898
Totals :				9825.74792	183.81261	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

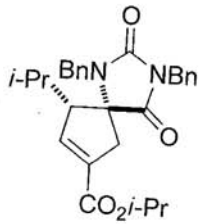
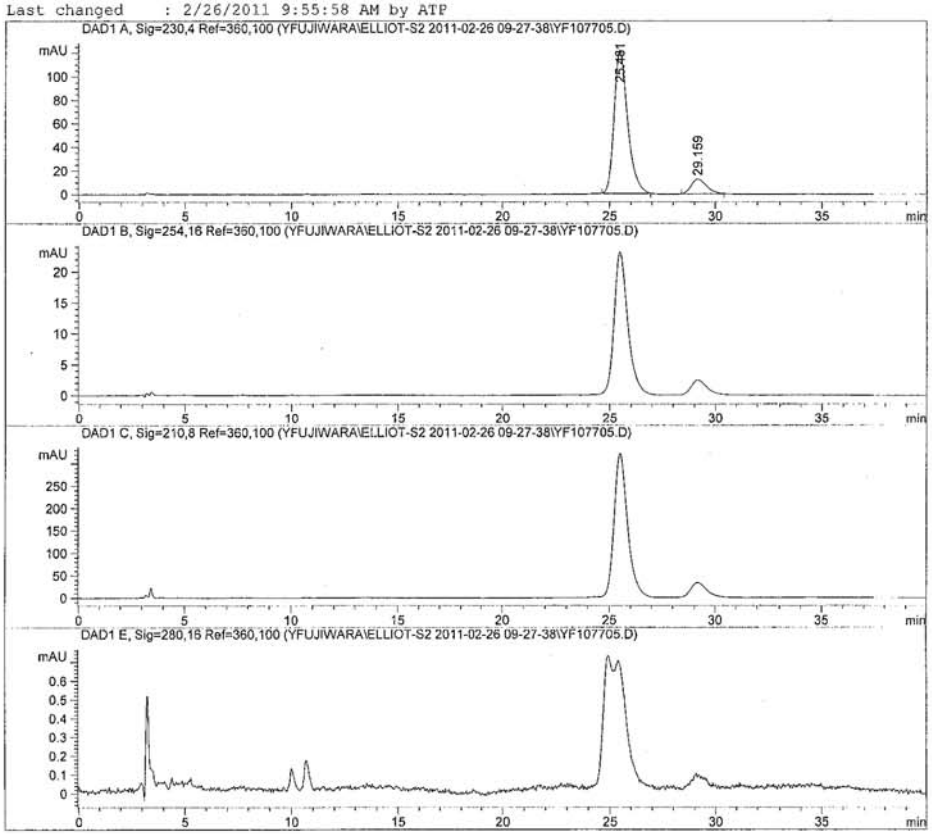


Table 2, entry 4

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF107705.D
ample Name: YF1077 R

Acq. Operator : ATP Seq. Line : 17
Acq. Instrument : Instrument 1 Location : Vial 15
Injection Date : 2/26/2011 6:59:32 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H03-40.M
Last changed : 2/26/2011 9:29:04 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 9:55:58 AM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF107705.D
Sample Name: YF1077 R

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.481	BB	0.6640	5354.84473	122.01455	89.5248
2	29.159	BB	0.7317	626.56525	12.39701	10.4752
Totals :				5981.40997	134.41156	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

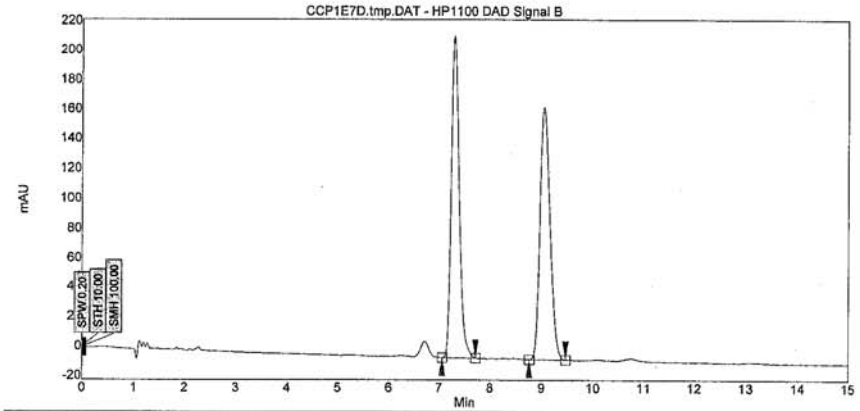
Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 2, entry 4

with (*R*)-catalyst

YF1137rac1 Vial 19 Method: IC 20.0% MeOH



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	7.06	7.29	7.71	0.00	50.66	217.5	39.2	50.661
2	UNKNOWN	8.77	9.04	9.47	0.00	49.34	169.9	38.1	49.339
Total						100.00	387.5	77.3	100.000

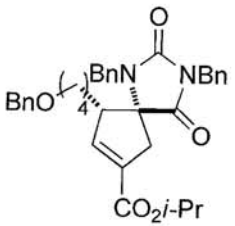
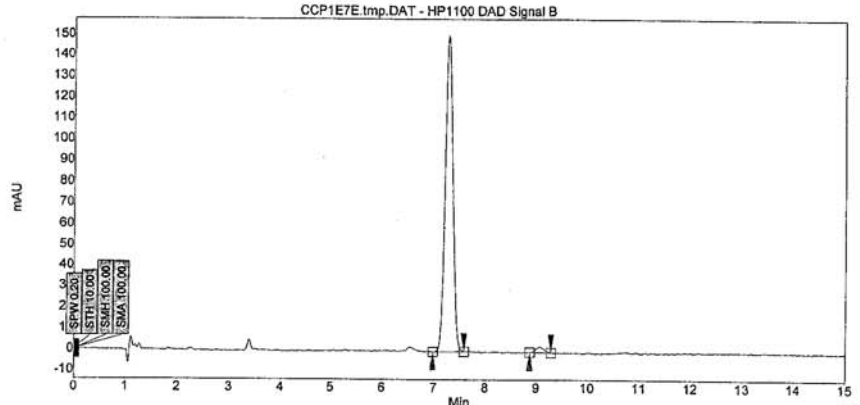


Table 2, entry 5

racemic sample

YF1137S1 Vial 20 Method: IC 20.0% MeOH



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.98	7.27	7.59	0.00	98.07	150.6	26.0	98.069
2	UNKNOWN	8.88	9.08	9.30	0.00	1.93	2.8	0.5	1.931
Total						100.00	153.4	26.5	100.000

96 %ee

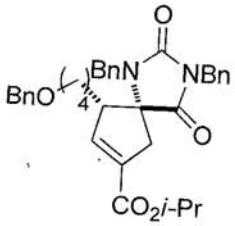
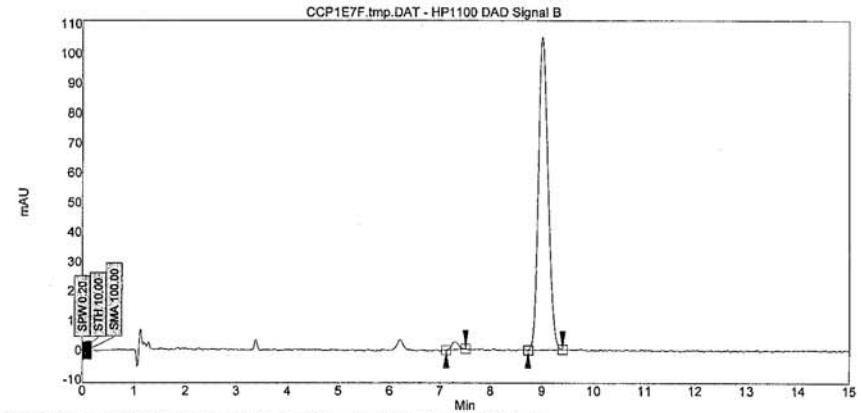


Table 2, entry 5

with (*S*)-catalyst

YF1138R1 Vial 21 Method: IC 20.0% MeOH

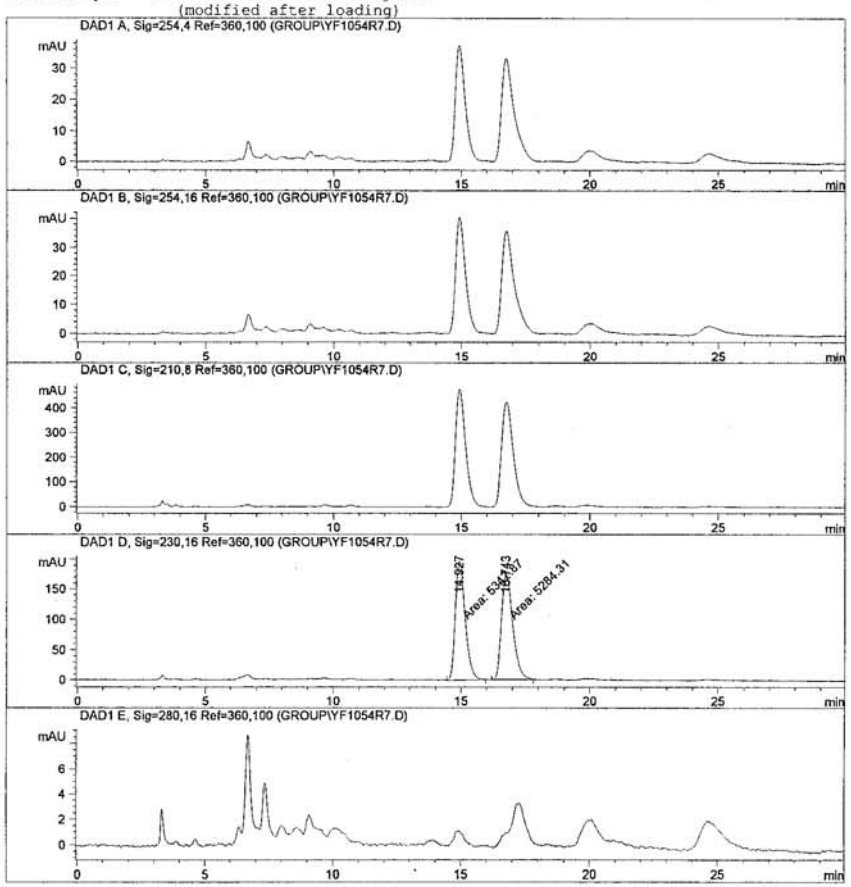


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	7.12	7.31	7.51	0.00	1.80	2.6	0.4	1.805
2	UNKNOWN	8.74	9.01	9.40	0.00	98.20	105.3	23.2	98.195
Total						100.00	108.0	23.6	100.000

Table 2, entry 5

with (*R*)-catalyst

```
Injection Date  : 3/3/2011 9:37:20 AM          Seq. Line :   2
Sample Name     : YF1054 RAC                    Location : Vial 62
Acq. Operator   : JTM                           Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\ADH-1030.M
Last changed    : 3/3/2011 9:01:50 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AD-0020.M
Last changed    : 5/3/2011 12:30:35 PM by JTM
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.927	MM	0.4506	5347.87061	197.79718	50.2989
2	16.743	MM	0.5054	5284.30957	174.26401	49.7011
Totals :				1.06322e4	372.06119	

```
 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

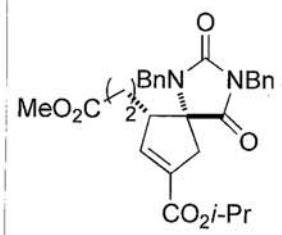
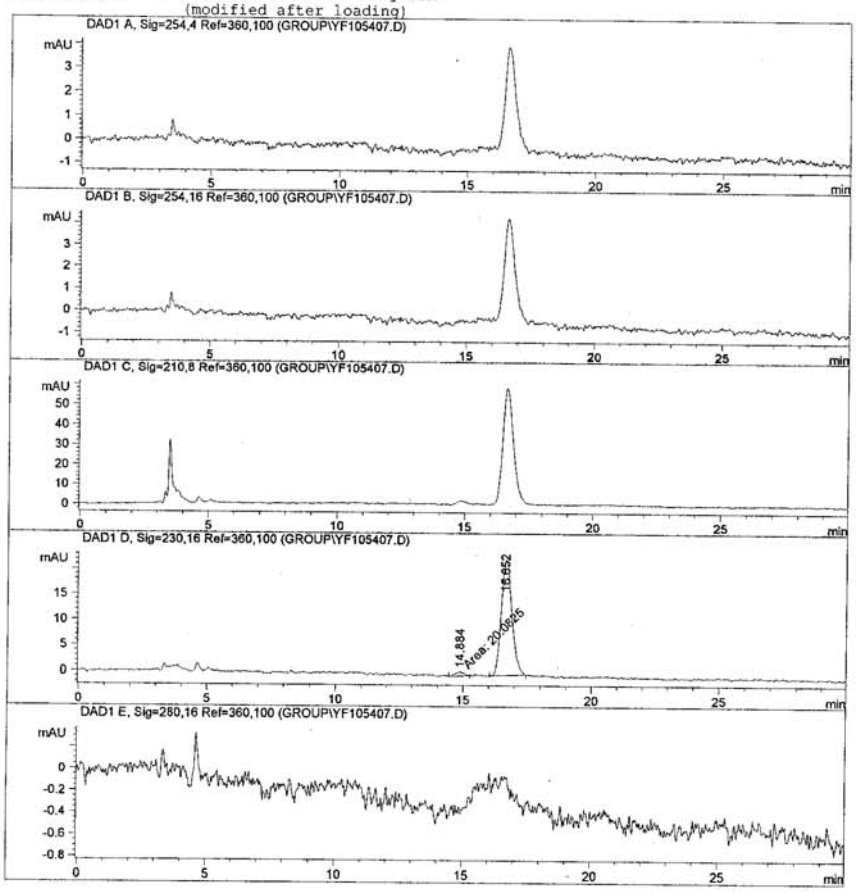


Table 2, entry 6

racemic sample

Data File C:\HPCHEM\1\DATA\GROUP\YF105407.D Sample Name: YF1054 S-cat

Injection Date : 3/3/2011 10:08:42 AM Seq. Line : 3
Sample Name : YF1054 S-cat Location : Vial 63
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\ADH-1030.M
Last changed : 3/3/2011 9:01:50 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AD-0020.M
Last changed : 5/3/2011 12:30:35 PM by JTM
(modified after loading)



Data File C:\HPCHEM\1\DATA\GROUP\YF105407.D Sample Name: YF1054 S-cat

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.884	MM	0.4105	20.08250	8.15349e-1	3.0016
2	16.652	BB	0.4253	648.96741	22.71846	96.9984
Totals :				669.04991	23.53381	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

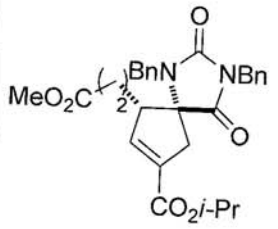
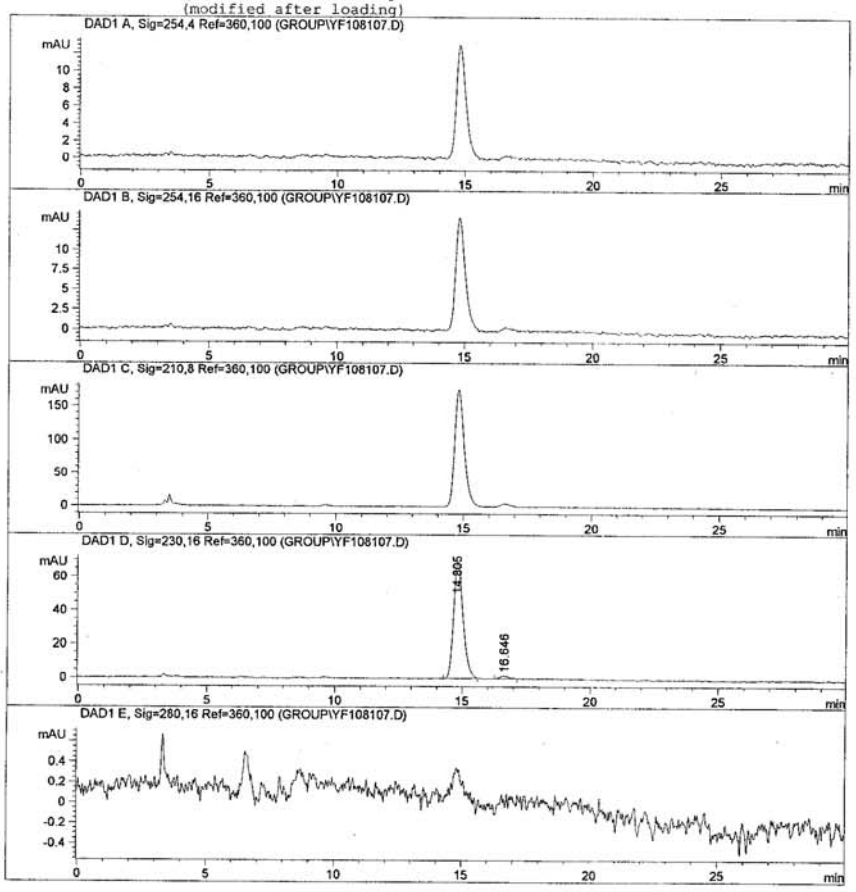


Table 2, entry 6

with (*S*)-catalyst

Data File C:\HPCHEM\1\DATA\GROUP\YF108107.D Sample Name: YF1081 R-cat

Injection Date : 3/3/2011 10:40:02 AM Seq. Line : 4
Sample Name : YF1081 R-cat Location : Vial 64
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\ADH-1030.M
Last changed : 3/3/2011 9:01:50 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AD-0020.M
Last changed : 5/3/2011 12:30:35 PM by JTM
(modified after loading)



Data File C:\HPCHEM\1\DATA\GROUP\YF108107.D Sample Name: YF1081 R-cat

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.805	VB	0.3963	1812.85266	69.50313	97.4552
2	16.646	PV	0.3237	47.33741	1.78352	2.5448
Totals :				1860.19007	71.28664	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

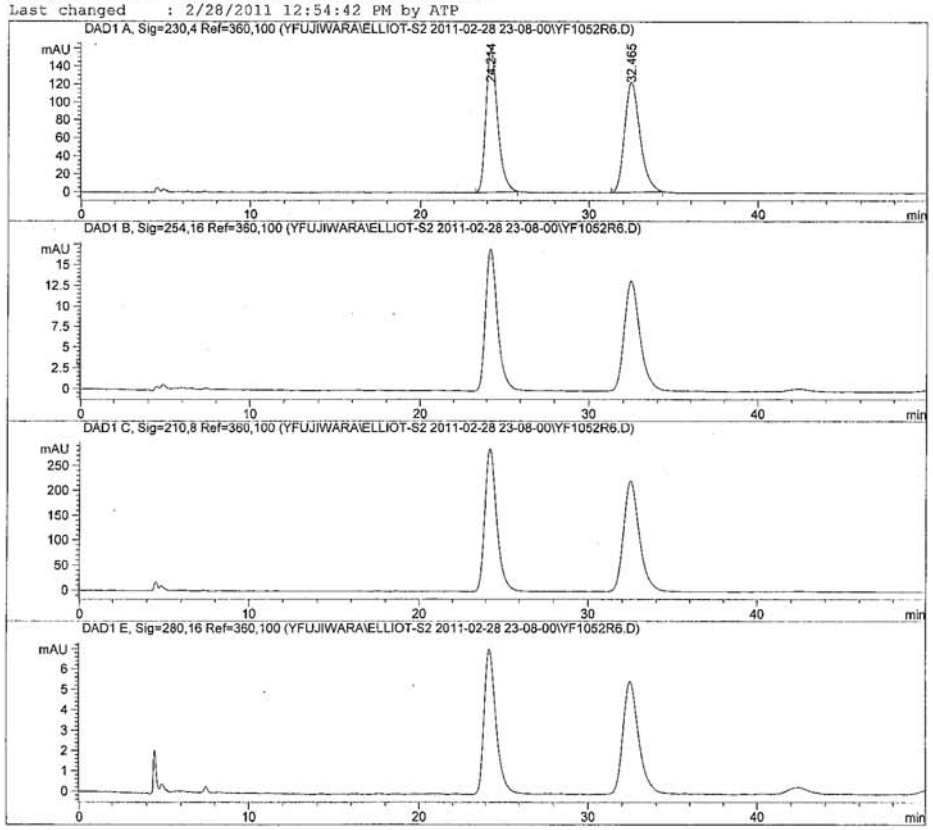
*** End of Report ***

Table 2, entry 6

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF1052R6.D
ample Name: YF1052R RAC

Acq. Operator : ATP Seq. Line : 10
Acq. Instrument : Instrument 1 Location : Vial 10
Injection Date : 3/1/2011 4:11:16 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\AD-H25-50.M
Last changed : 2/26/2011 9:40:59 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF1052R6.D
Sample Name: YF1052R RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.214	BB	0.7386	7749.02881	158.44400	50.1115
2	32.465	BB	0.9519	7714.53271	122.63400	49.8885
Totals :				1.54636e4	281.07800	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

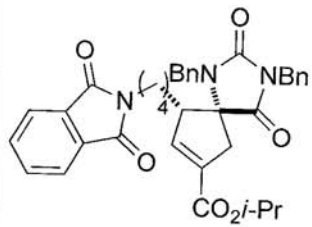


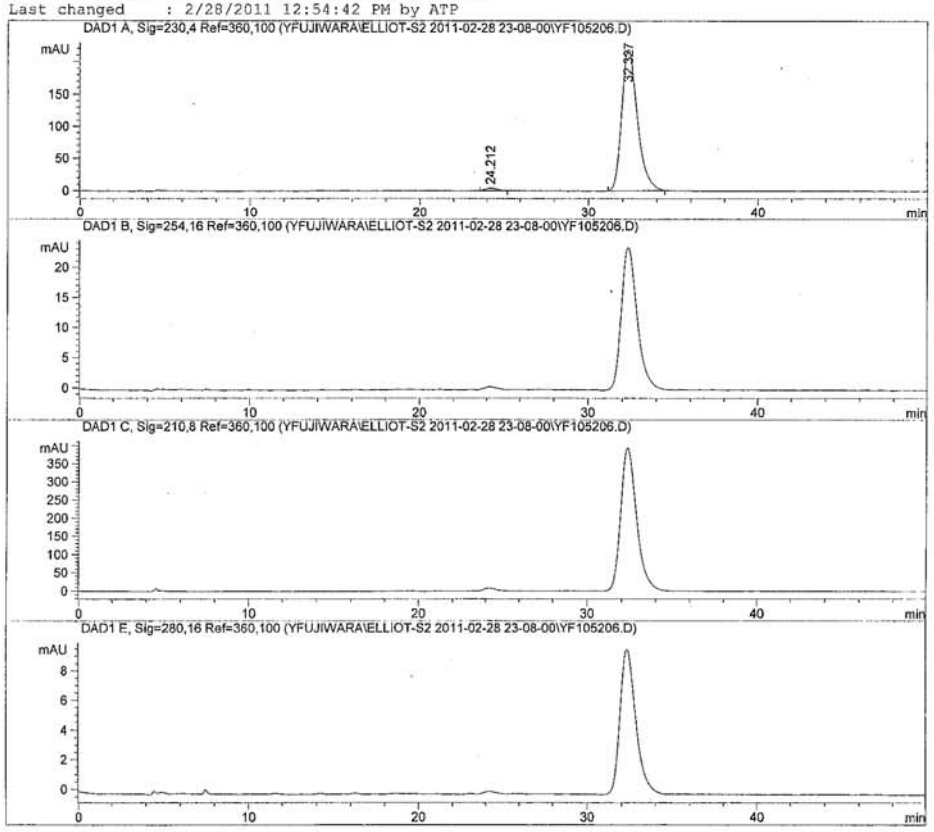
Table 2, entry 7

racemic sample

Instrument 1 3/1/2011 9:56:41 AM ATP

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF105206.D
ample Name: YF1052 R

Acq. Operator : ATP Seq. Line : 11
Acq. Instrument : Instrument 1 Location : Vial 11
Injection Date : 3/1/2011 5:02:35 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\AD-H25-50.M
Last changed : 2/26/2011 9:40:59 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF105206.D
Sample Name: YF1052 R

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.212	BB	0.5537	195.58586	4.29127	1.3787
2	32.327	BB	0.9760	1.39902e4	218.78810	98.6213
Totals :				1.41858e4	223.07937	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

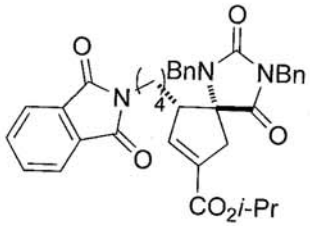
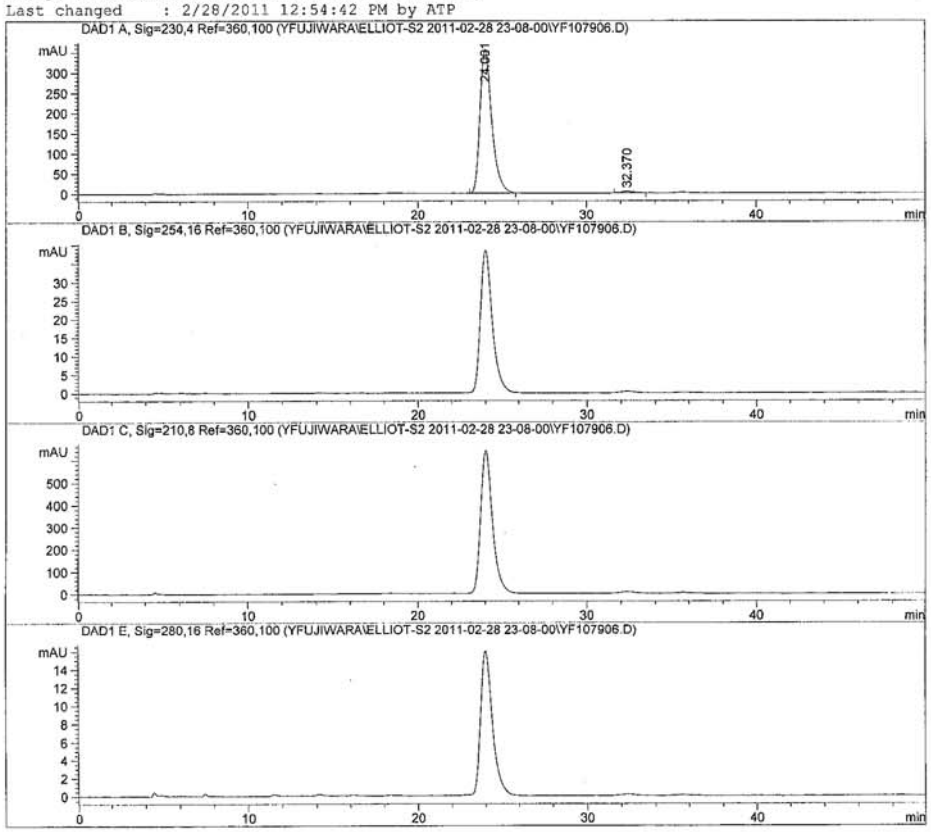


Table 2, entry 7

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF107906.D
ample Name: YF1079 S

Acq. Operator : ATP Seq. Line : 12
Acq. Instrument : Instrument 1 Location : Vial 12
Injection Date : 3/1/2011 5:53:48 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\AD-H25-50.M
Last changed : 2/26/2011 9:40:59 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 23-08-00\YF107906.D
Sample Name: YF1079 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.001	BB	0.7426	1.73538e4	356.09384	98.8965
2	32.370	BB	0.6360	193.64005	3.63180	1.1035
Totals :				1.75475e4	359.72564	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

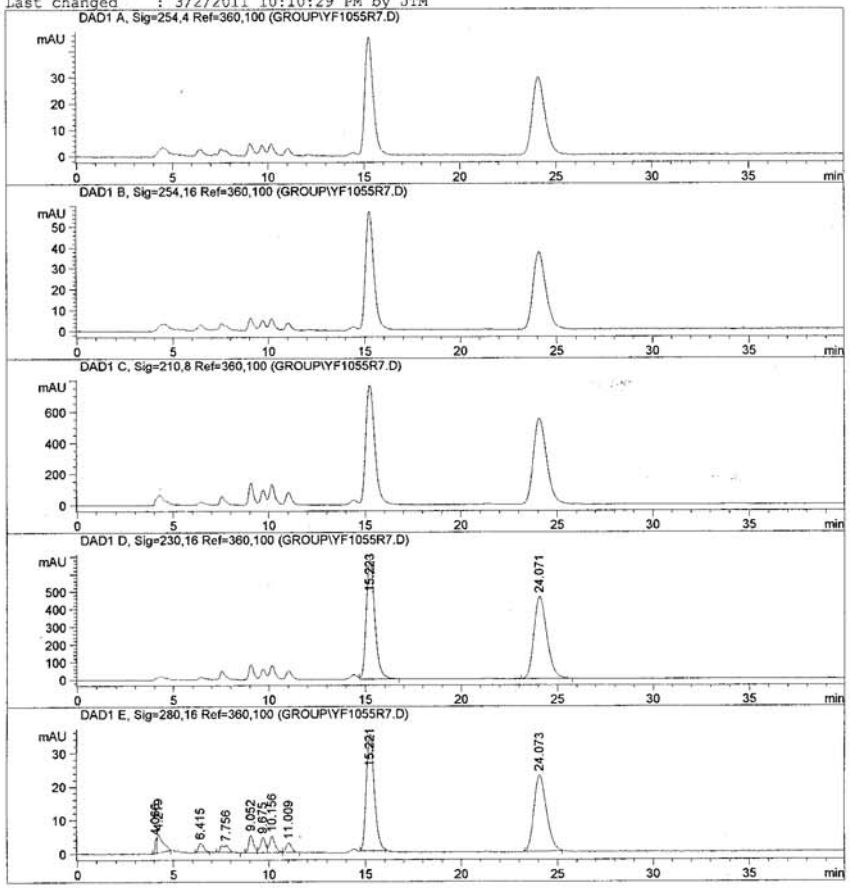
Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 2, entry 7

with (*R*)-catalyst

Injection Date : 3/3/2011 5:09:31 AM Seq. Line : 13
Sample Name : YF1055 RAC Location : Vial 59
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed : 3/2/2011 10:08:40 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed : 3/2/2011 10:10:29 PM by JTM



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.223	VB	0.4830	2.11890e4	680.99597	49.2733
2	24.071	BB	0.7298	2.18140e4	464.59079	50.7267
Totals :				4.30030e4	1145.58676	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.066	PV	0.1040	30.14036	4.39330	1.1480
2	4.219	VB	0.2682	114.53835	5.56414	4.3625
3	6.415	BB	0.2701	53.75902	2.65620	2.0475
4	7.756	PP	0.3575	61.82261	2.08771	2.3547
5	9.052	BV	0.2642	90.52500	5.17082	3.4479
6	9.675	VV	0.2540	82.54912	4.45956	3.1441
7	10.156	VB	0.2772	96.98419	4.89322	3.6939
8	11.009	BB	0.2677	58.52027	2.84825	2.2289
9	15.221	PB	0.4461	1002.95801	34.81258	38.2001
10	24.073	BB	0.6293	1033.73816	22.78539	39.3725
Totals :				2625.53508	89.67117	

Results obtained with enhanced integrator!

*** End of Report ***

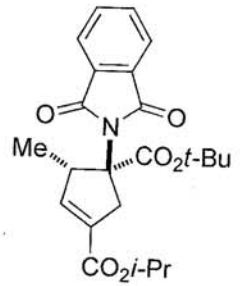
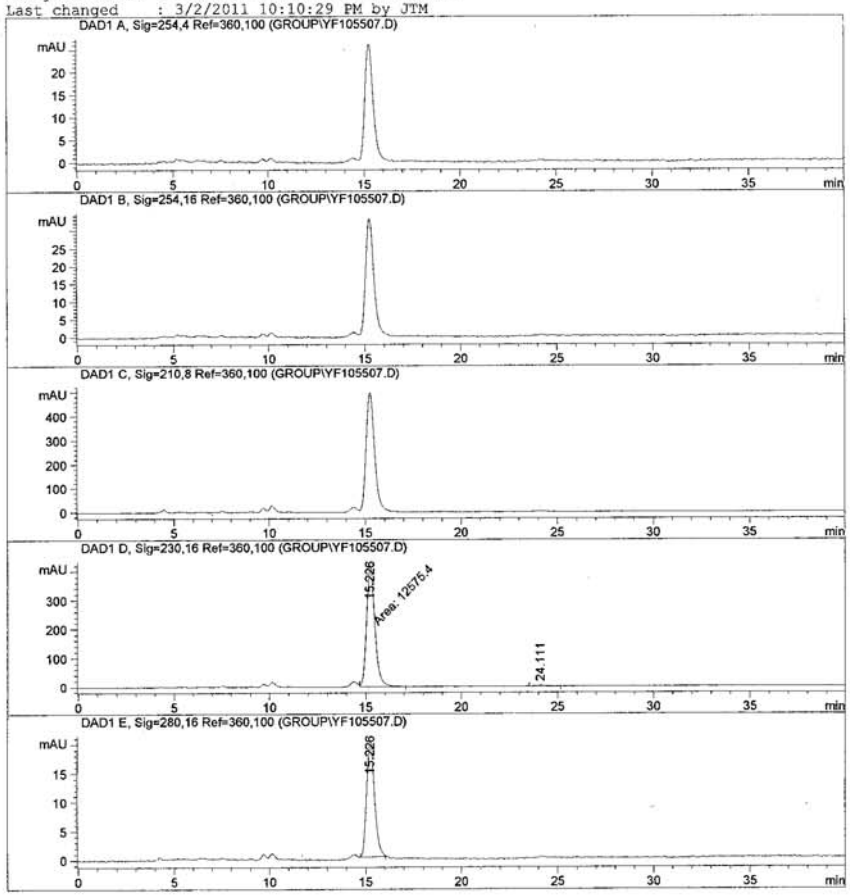


Table 3, entry 1

racemic sample

```
Injection Date  : 3/3/2011 5:50:47 AM          Seq. Line :  14
Sample Name     : YF1055 S-cat                  Location : Vial 60
Acq. Operator   : JTM                             Inj :   1
Acq. Instrument : Instrument 1                Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 3/2/2011 10:08:40 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1 15.226 FM    0.5056 1.25754e4   414.52951  98.9273
   2 24.111 BP    0.5213  136.36325    3.11167   1.0727

Totals :                  1.27118e4   417.64118

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1 15.226 PB    0.4305  571.15997   19.91845 100.0000

Totals :                   571.15997   19.91845

 Results obtained with enhanced integrator!

                    *** End of Report ***
```

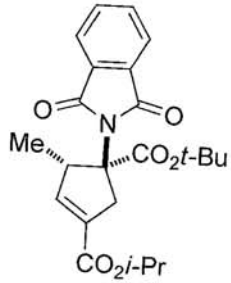
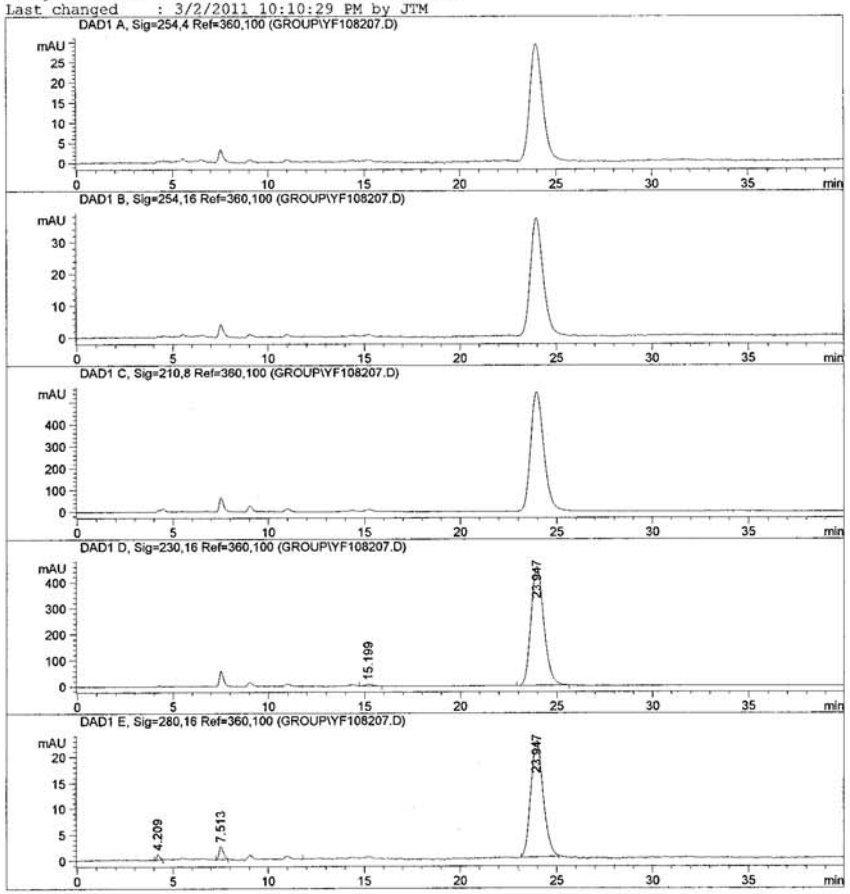


Table 3, entry 1

with (*S*)-catalyst

```
Injection Date  : 3/3/2011 6:32:03 AM          Seq. Line :  15
Sample Name     : YF1082 R-cat                  Location : Vial 61
Acq. Operator   : JTM                           Inj :  1
Acq. Instrument : Instrument 1                  Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 3/2/2011 10:08:40 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.199 VB    0.4034  220.70259    7.32709   1.0262
   2  23.947 BB    0.7194 2.12867e4   458.71677  98.9738

Totals :                  2.15074e4   466.04386

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.209 PB    0.1711   12.81015    1.12246   1.2004
   2   7.513 BB    0.2204   39.69534    2.53864   3.7198
   3  23.947 BB    0.6220 1014.62317   22.50602  95.0797

Totals :                  1067.12865   26.16712

 Results obtained with enhanced integrator!

                  *** End of Report ***
```

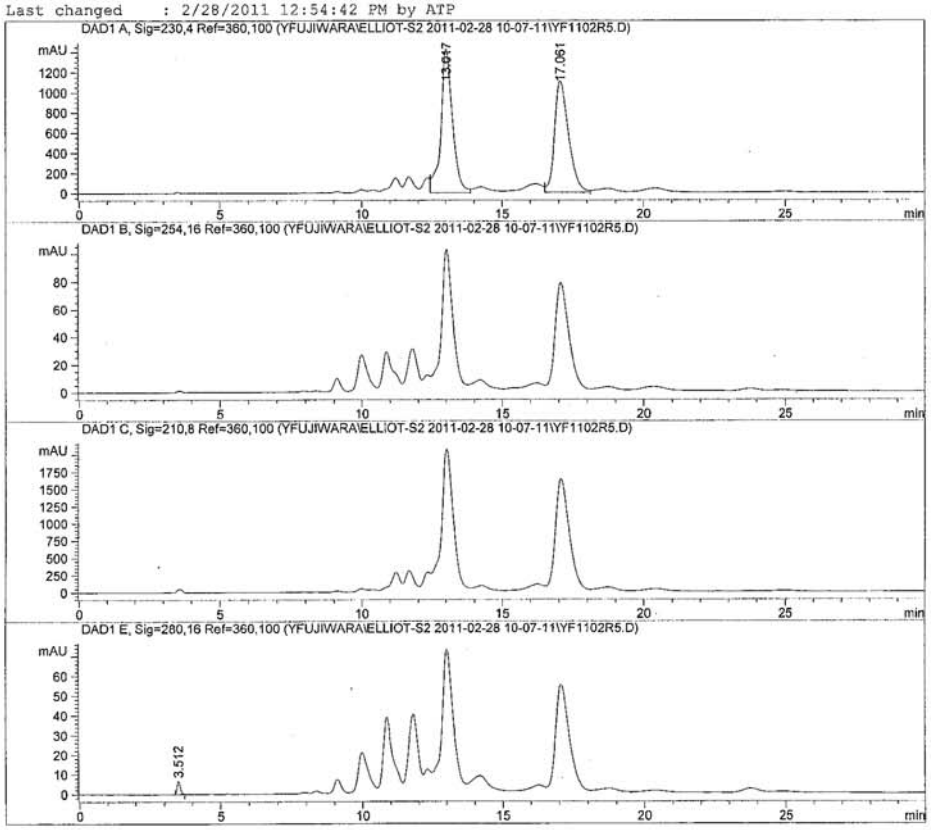
Table 3, entry 1

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF1102R5.D
ample Name: YF1102 RAC

Acq. Operator : ATP Seq. Line : 6
Acq. Instrument : Instrument 1 Location : Vial 21
Injection Date : 2/28/2011 1:20:07 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\~~AD~~-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP

IA column used



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF1102R5.D
Sample Name: YF1102 RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.017	VV	0.4267	4.11534e4	1426.09290	51.9759
2	17.061	VV	0.5132	3.80244e4	1111.35950	48.0241
Totals :				7.91779e4	2537.45239	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.512	BB	0.1251	51.71578	6.48241	100.0000
Totals :				51.71578	6.48241	

*** End of Report ***

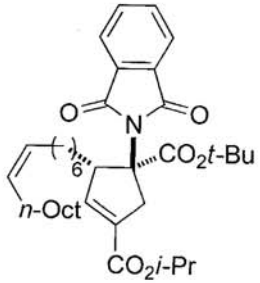
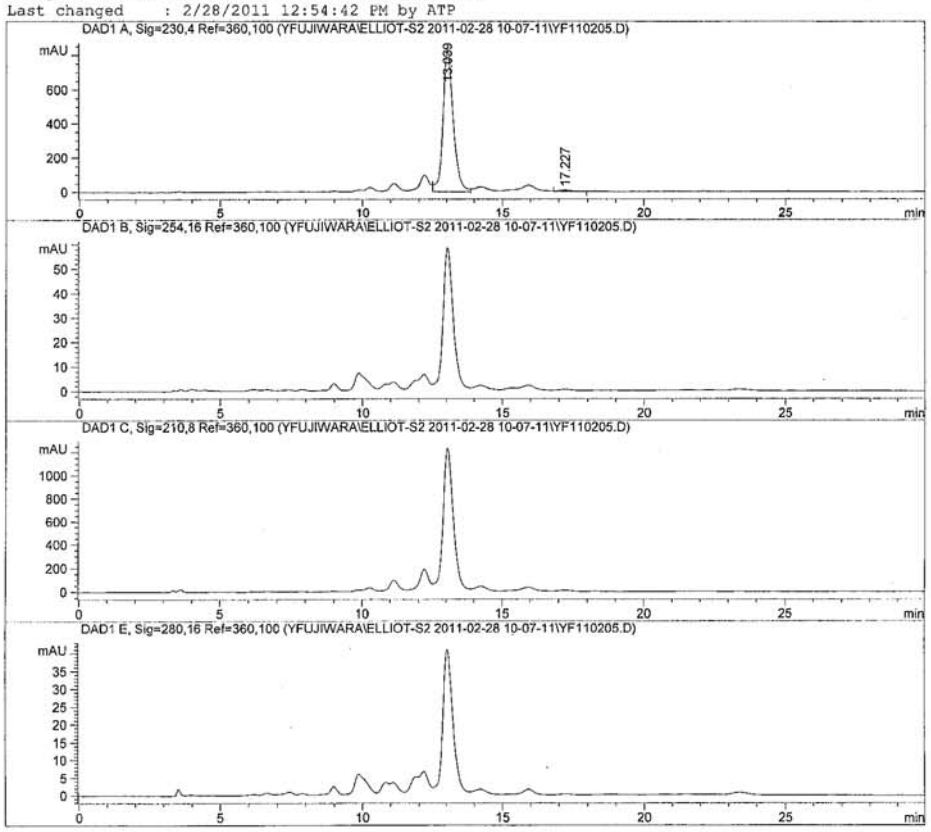


Table 3, entry 2

racemic sample

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF110205.D
ample Name: YF1102 S-1

Acq. Operator : ATP Seq. Line : 7
Acq. Instrument : Instrument 1 Location : Vial 22
Injection Date : 2/28/2011 1:51:26 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 10 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF110205.D
Sample Name: YF1102 S-1

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.039	VV	0.3903	2.14791e4	828.97296	98.8464
2	17.227	VB	0.4734	250.67580	8.04837	1.1536
Totals :				2.17298e4	837.02133	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

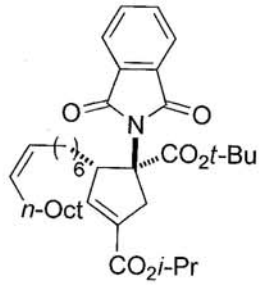


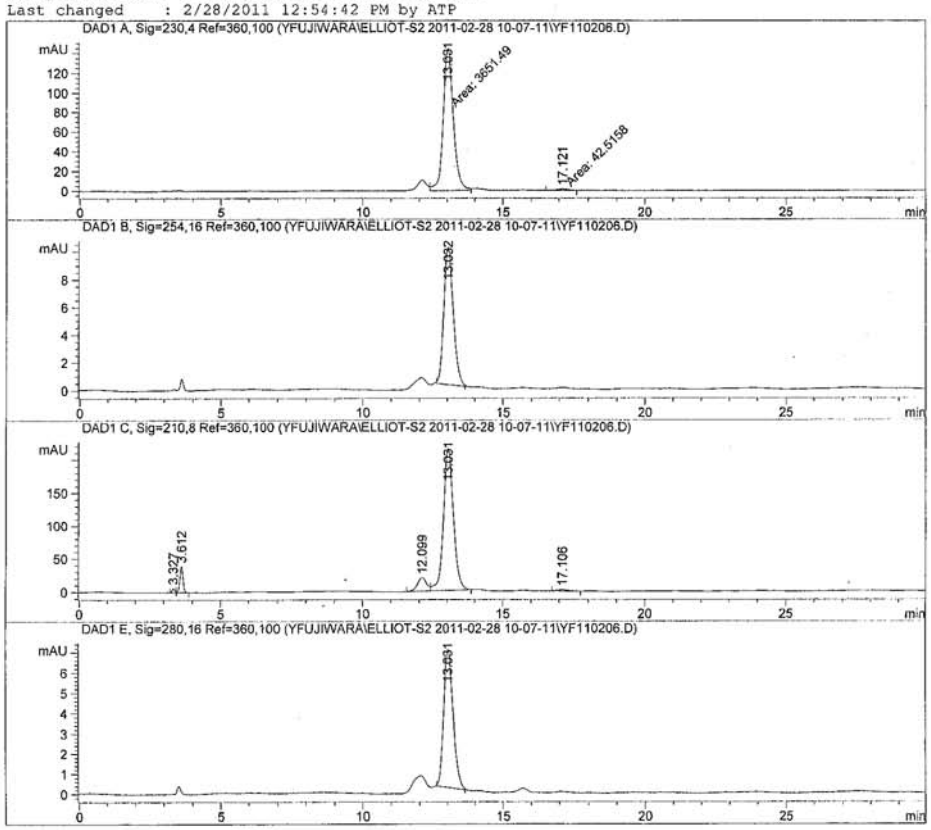
Table 3, entry 2

with (*S*)-catalys

Before prep HPLC purification

ta File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF110206.D
mple Name: YF1102 S-2

Acq. Operator : ATP Seq. Line : 8
Acq. Instrument : Instrument 1 Location : Vial 23
Injection Date : 2/28/2011 2:22:49 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF110206.D
Sample Name: YF1102 S-2

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.031	MF	0.4219	3651.49316	144.26373	98.8491
2	17.121	MM	0.5224	42.51578	1.35652	1.1509
Totals :				3694.00894	145.62026	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.032	BB	0.3628	232.70863	9.87988	100.0000
Totals :				232.70863	9.87988	

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.327	BV	0.0994	41.46928	6.41283	0.6728
2	3.612	VB	0.1166	296.33112	39.02552	4.8077
3	12.099	BV	0.3427	457.83014	20.17720	7.4278
4	13.031	VB	0.3781	5319.20215	213.94739	86.2987
5	17.106	BB	0.3337	48.87917	1.82966	0.7930
Totals :				6163.71185	281.39260	

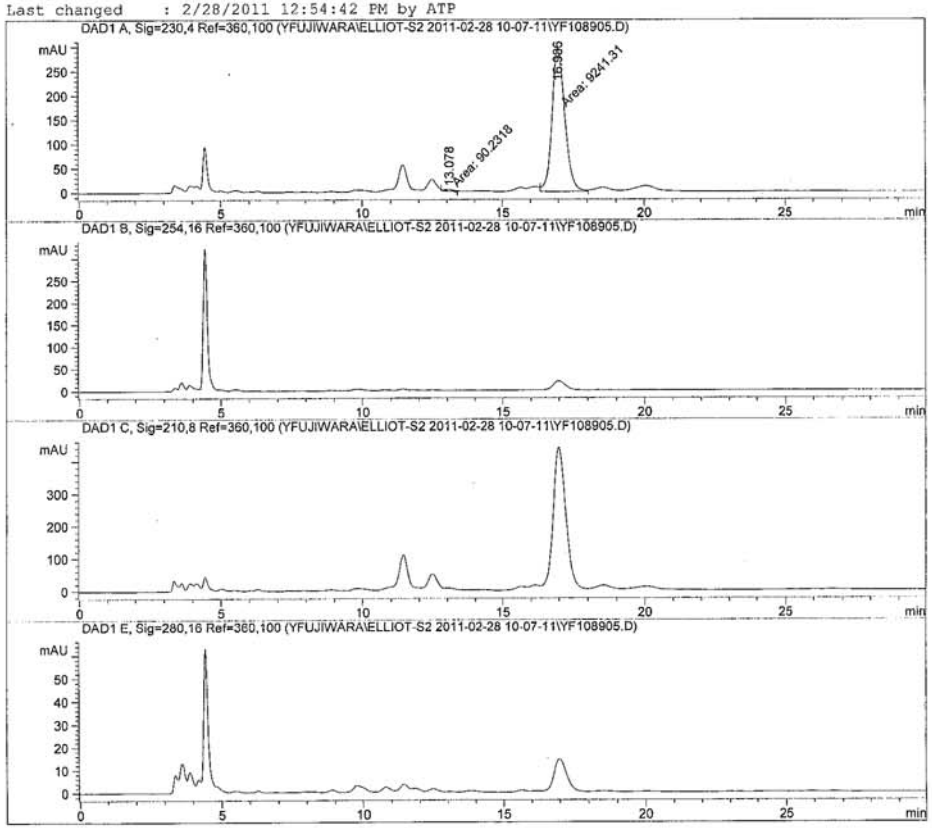
Signal 4: DAD1 E, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.031	BB	0.3533	159.41580	6.80607	100.0000
Totals :				159.41580	6.80607	

After prep HPLC purification

ta File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF108905.D
mple Name: YF1089 R-1

Acq. Operator : ATP
Acq. Instrument : Instrument 1
Injection Date : 2/28/2011 2:54:09 PM
Seq. Line : 9
Location : Vial 24
Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 10 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF108905.D
Sample Name: YF1089 R-1

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.078	MM	0.4284	90.23175	3.51029	0.9670
2	16.986	FM	0.5209	9241.30566	295.70801	99.0330
Totals :				9331.53741	299.21830	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

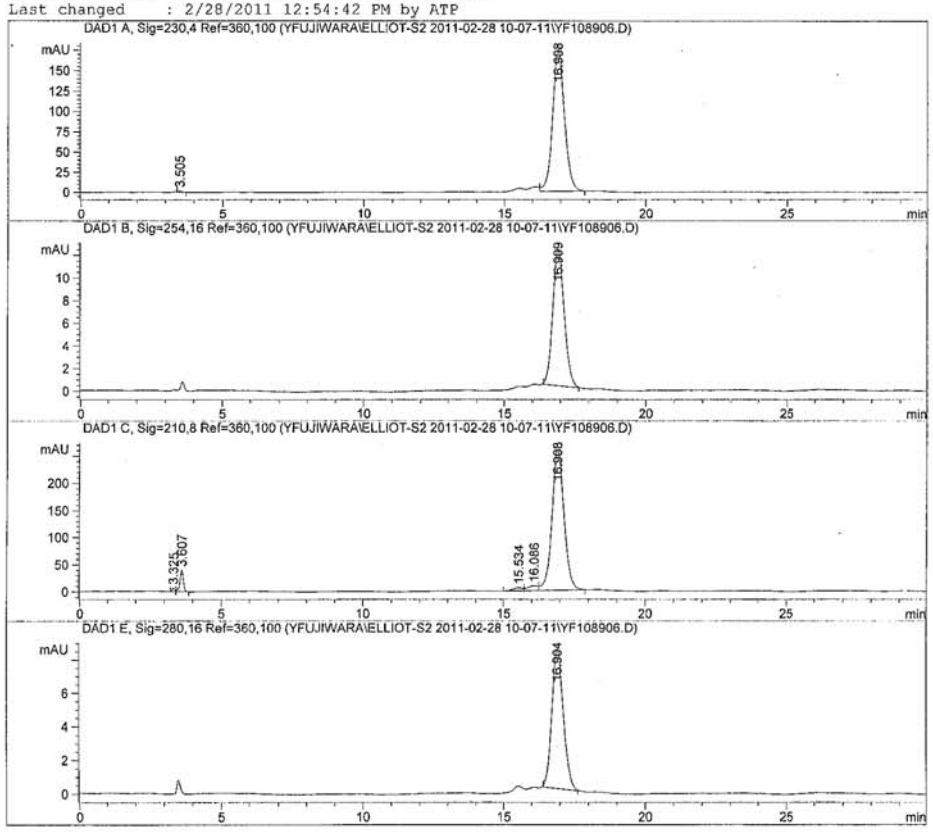
Table 3, entry 2

with (*R*)-catalyst

Before prep HPLC purification

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF108906.D
ample Name: YF1089 R-2

Acq. Operator : ATP Seq. Line : 10
Acq. Instrument : Instrument 1 Location : Vial 25
Injection Date : 2/28/2011 3:25:30 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF108906.D
Sample Name: YF1089 R-2

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.505	VB	0.1292	12.88167	1.51572	0.2469
2	16.908	VB	0.4554	5204.52979	174.76656	99.7531
Totals :				5217.41146	176.28228	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.909	BB	0.4355	344.60764	12.05645	100.0000
Totals :				344.60764	12.05645	

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.325	BV	0.0964	37.07005	5.97647	0.4371
2	3.607	VB	0.1162	305.81046	39.53893	3.6055
3	15.534	BV	0.3472	139.89638	5.68369	1.6494
4	16.086	VV	0.3578	226.79286	9.19268	2.6739
5	16.908	VB	0.4566	7772.15869	260.14874	91.6341
Totals :				8481.72844	320.54052	

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

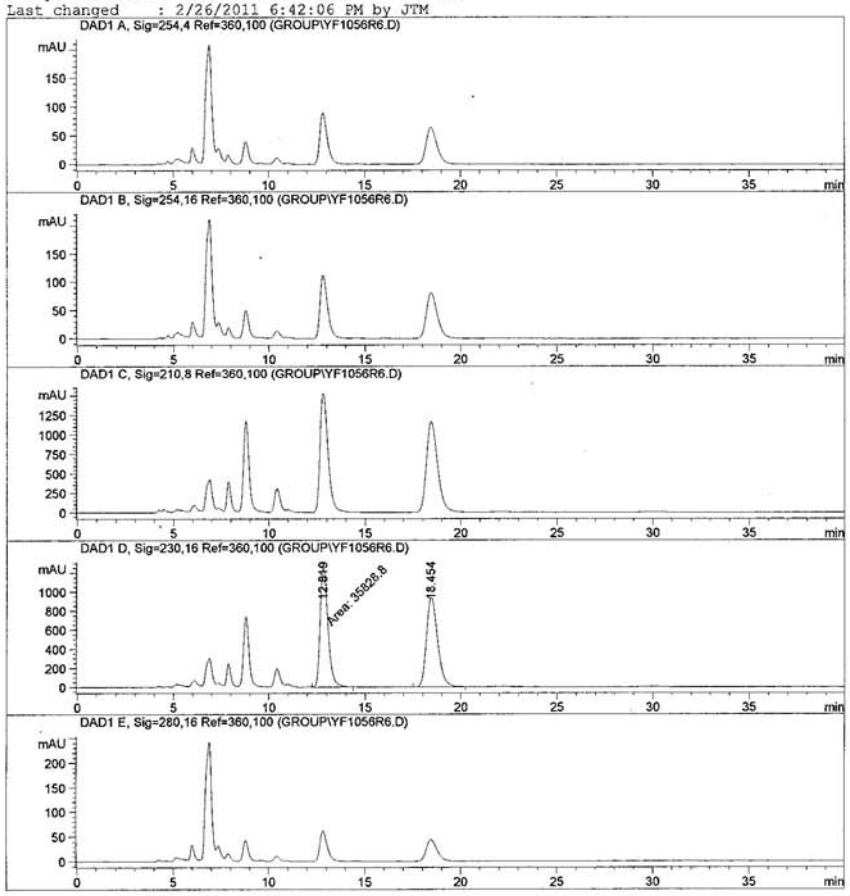
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.904	BB	0.4366	237.20107	8.32063	100.0000
Totals :				237.20107	8.32063	

Table 3, entry 2

with (*R*)-catalyst

After prep HPLC purification

```
Injection Date  : 2/26/2011 12:04:03 PM        Seq. Line :  21
Sample Name     : YF1056 RAC                    Location : Vial 54
Acq. Operator   : JTM                           Inj :  1
Acq. Instrument : Instrument 1                  Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 2/4/2011 9:13:33 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ASH-1010.M
Last changed    : 2/26/2011 6:42:06 PM by JTM
```



Data File C:\HPCHEM\1\DATA\GROUP\YF1056R6.D Sample Name: YF1056 RAC

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.819 MM    0.4752 3.58288e4  1256.57361  48.4542
   2  18.454 BB    0.6298 3.81148e4   938.47461  51.5458

Totals :                  7.39436e4  2195.04822

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

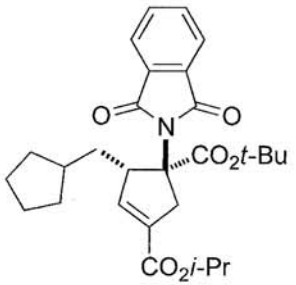
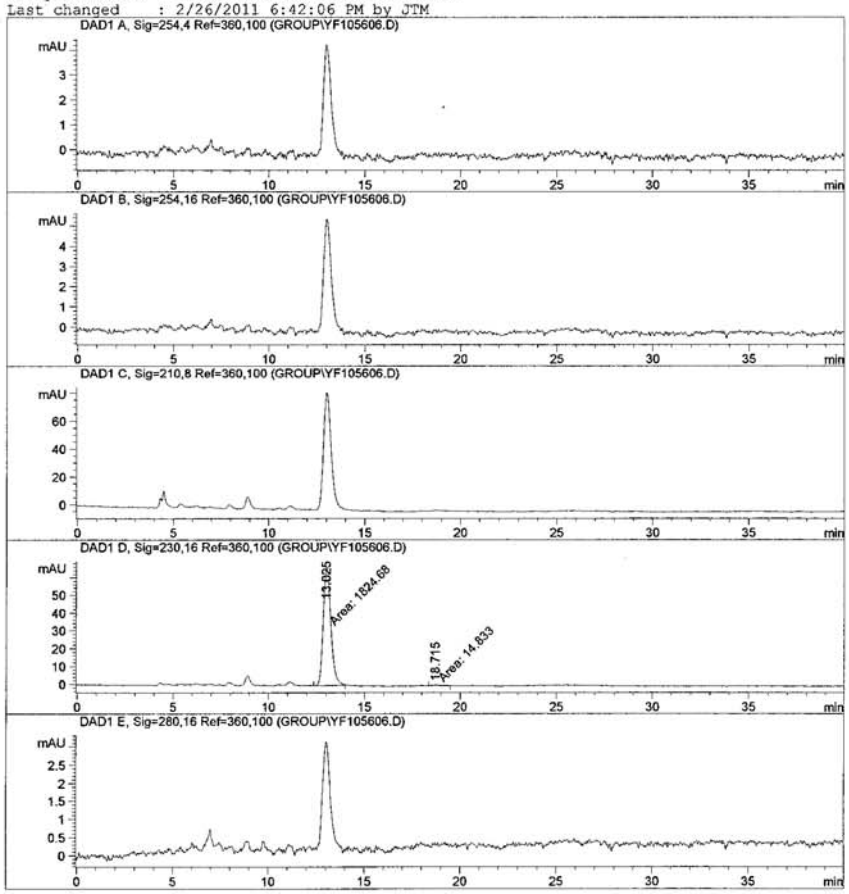


Table 3, entry 3

racemic sample

```
Injection Date  : 2/26/2011 12:45:20 PM        Seq. Line :  22
Sample Name     : YF1056 R1                     Location : Vial 55
Acq. Operator   : JTM                              Inj :  1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 2/4/2011 9:13:33 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ASH-1010.M
Last changed    : 2/26/2011 6:42:06 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  13.025 MM    0.4563 1824.67590   66.65190  99.1936
   2  18.715 MM    0.4902   14.83295 5.04354e-1   0.8064

Totals :                  1839.50886   67.15626

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

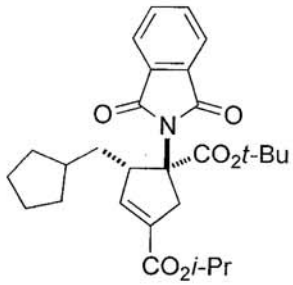
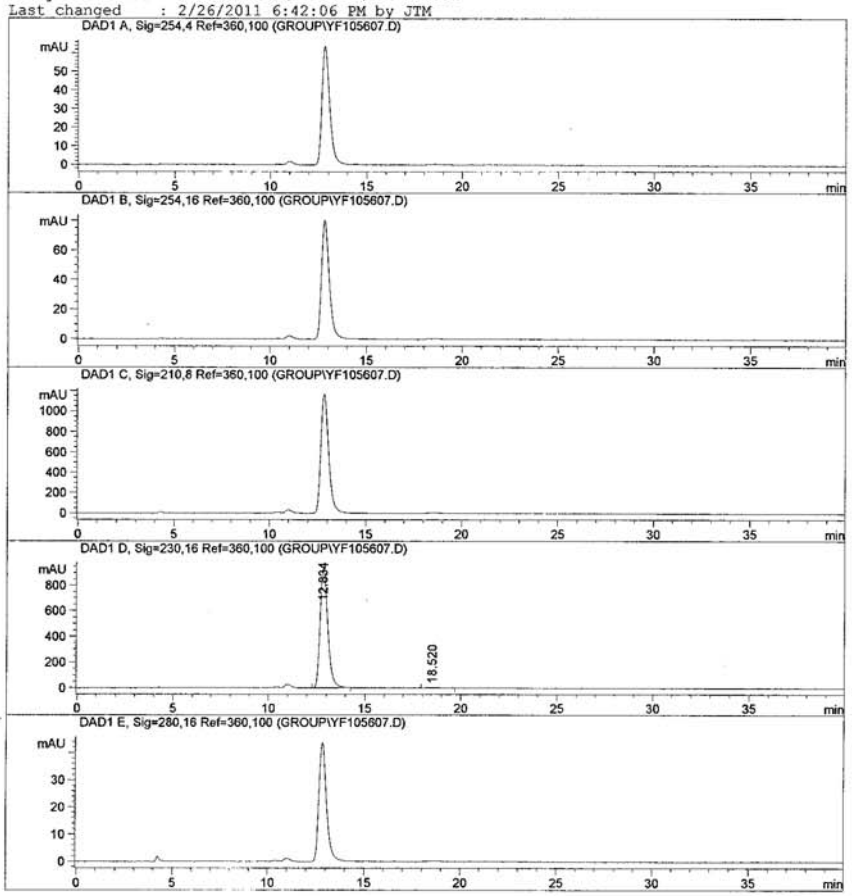


Table 3, entry 3

with (*S*)-catalyst

Before prep HPLC purification

```
Injection Date  : 2/26/2011 1:26:37 PM          Seq. Line :  23
Sample Name     : YF1056 R2                      Location : Vial 56
Acq. Operator   : JTM                            Inj :  1
Acq. Instrument : Instrument 1                   Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 2/4/2011 9:13:33 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ASH-1010.M
Last changed    : 2/26/2011 6:42:06 PM by JTM
```



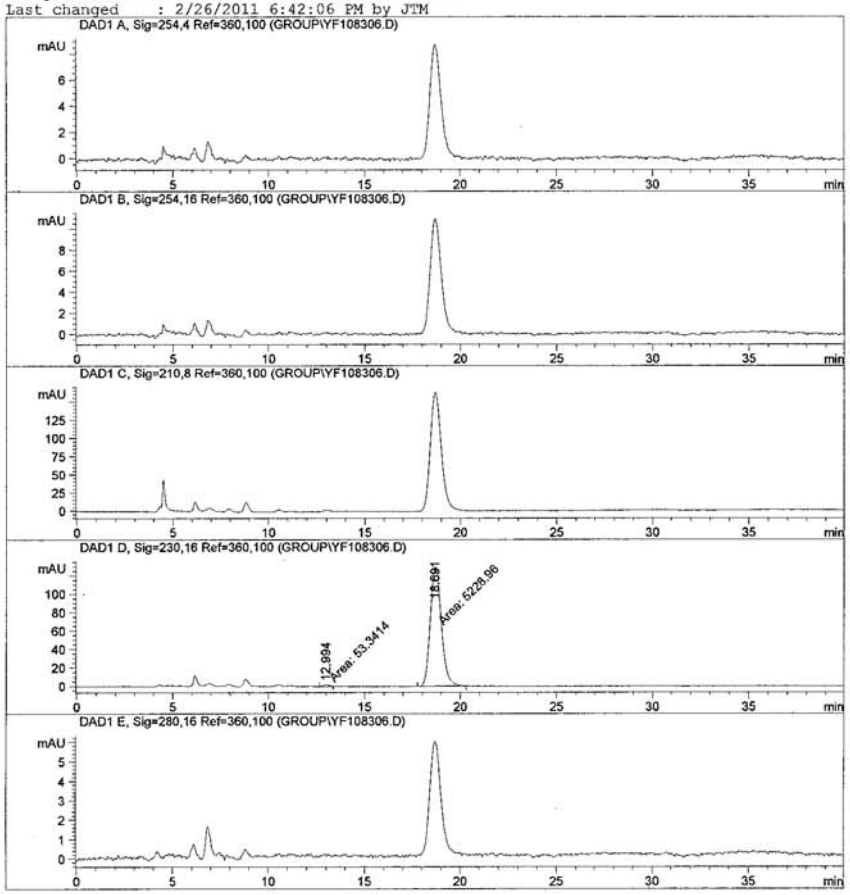
Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|------|----|-------|----------|----------|--------|
   1  12.834 BB    0.4282 2.59324e4   933.27240  99.1146
   2  18.520 BB    0.4787  231.65501    5.79120   0.8854

Totals :                  2.61640e4   939.06360

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

After prep HPLC purification

```
Injection Date  : 2/26/2011 2:07:55 PM          Seq. Line :  24
Sample Name     : YF1083 S1                     Location : Vial 57
Acq. Operator   : JTM                              Inj :  1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed    : 2/4/2011 9:13:33 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ASH-1010.M
Last changed    : 2/26/2011 6:42:06 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.994 MM    0.4289   53.34139    2.07268   1.0098
   2  18.691 MM    0.6706 5228.95703  129.95149  98.9902

Totals :                  5282.29842  132.02417

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

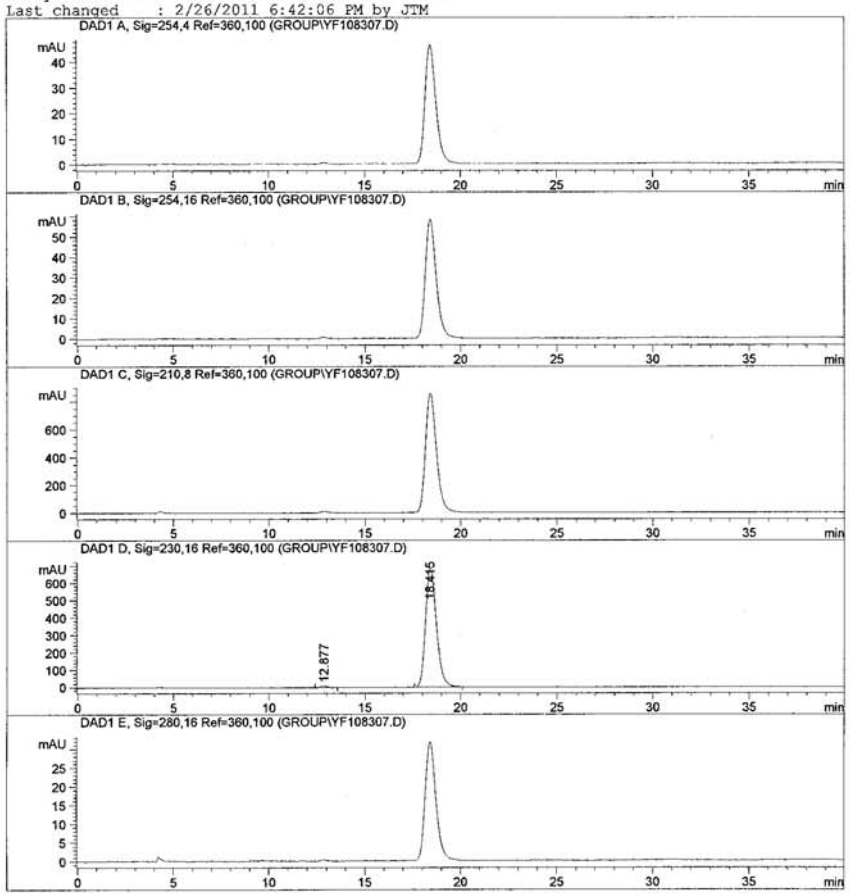
*** End of Report ***

Table 3, entry 3

with (*R*)-catalyst

Before prep HPLC purification

Injection Date : 2/26/2011 2:49:14 PM Seq. Line : 25
Sample Name : YF1083 S2 Location : Vial 58
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IC-3040.M
Last changed : 2/4/2011 9:13:33 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ASH-1010.M
Last changed : 2/26/2011 6:42:06 PM by JTM



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.877	BB	0.3377	224.49306	8.56744	0.8176
2	18.415	BB	0.6122	2.72324e4	687.34766	99.1824
Totals :				2.74569e4	695.91510	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

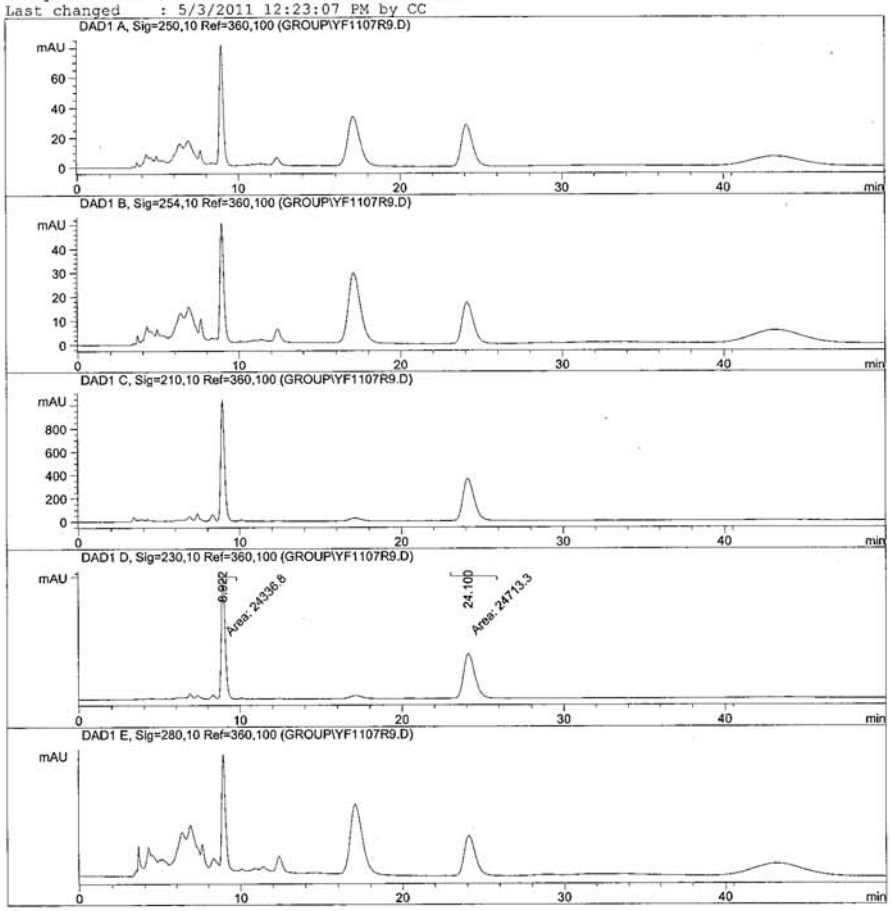
*** End of Report ***

Table 3, entry 3

with (*R*)-catalyst

After prep HPLC purification

```
Injection Date  : 5/3/2011 9:01:57 AM          Seq. Line :  53
Sample Name     : YF1107 8 RAC                  Location : Vial 1
Acq. Operator   : NB                               Inj :  1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-10-50.M
Last changed    : 4/23/2011 8:41:10 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed    : 5/3/2011 12:23:07 PM by CC
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]   [mAU*s]      [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.922 FM    0.2880 2.43368e4  1408.30347  49.6163
   2  24.100 MM    0.8012 2.47133e4   514.06177  50.3837

Totals :                  4.90501e4  1922.36523

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100
```

*** End of Report ***

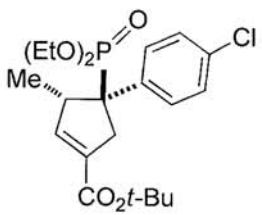
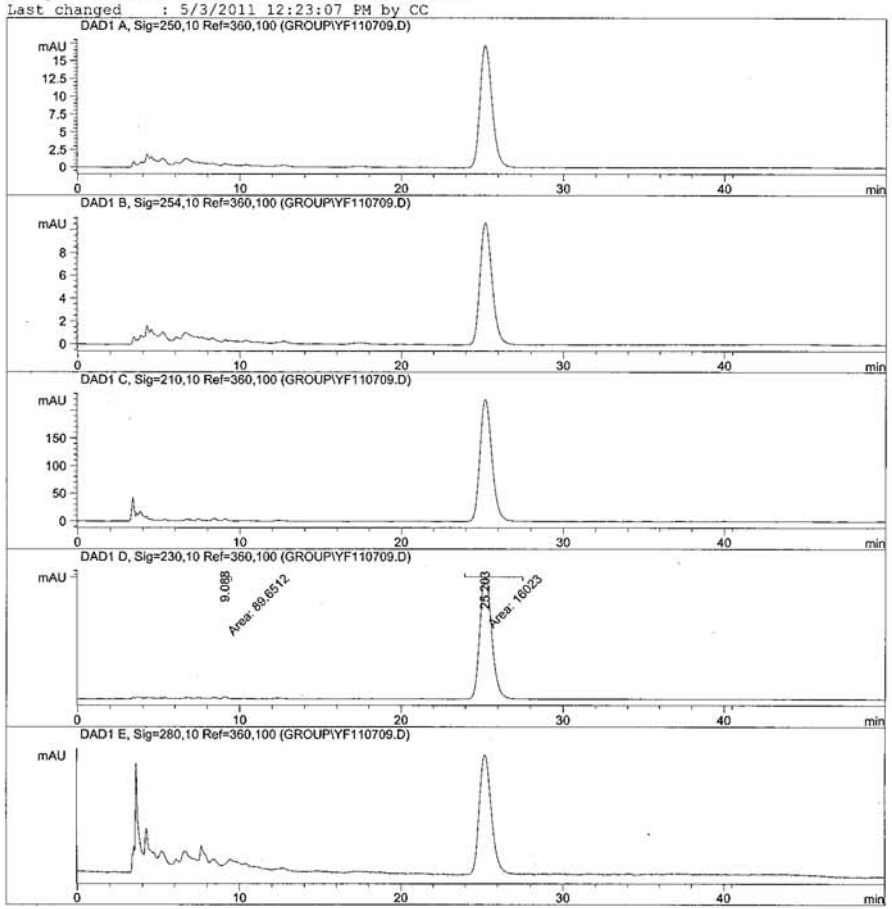


Table 4, entry 1

racemic sample

```
Injection Date  : 5/3/2011 9:53:12 AM          Seq. Line :  54
Sample Name     : YF1107                      Location : Vial 2
Acq. Operator   : NB                             Inj :   1
Acq. Instrument : Instrument 1               Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-10-50.M
Last changed    : 4/23/2011 8:41:10 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed    : 5/3/2011 12:23:07 PM by CC
```



Data File C:\HPCHEM\1\DATA\GROUP\YF110709.D Sample Name: YF1107

Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.088	MM	0.2821	89.65121	5.29612	0.5564
2	25.203	MM	0.8480	1.60230e4	314.91232	99.4436
Totals :				1.61126e4	320.20845	

```
 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

*** End of Report ***
```

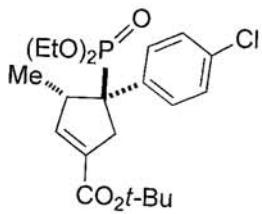
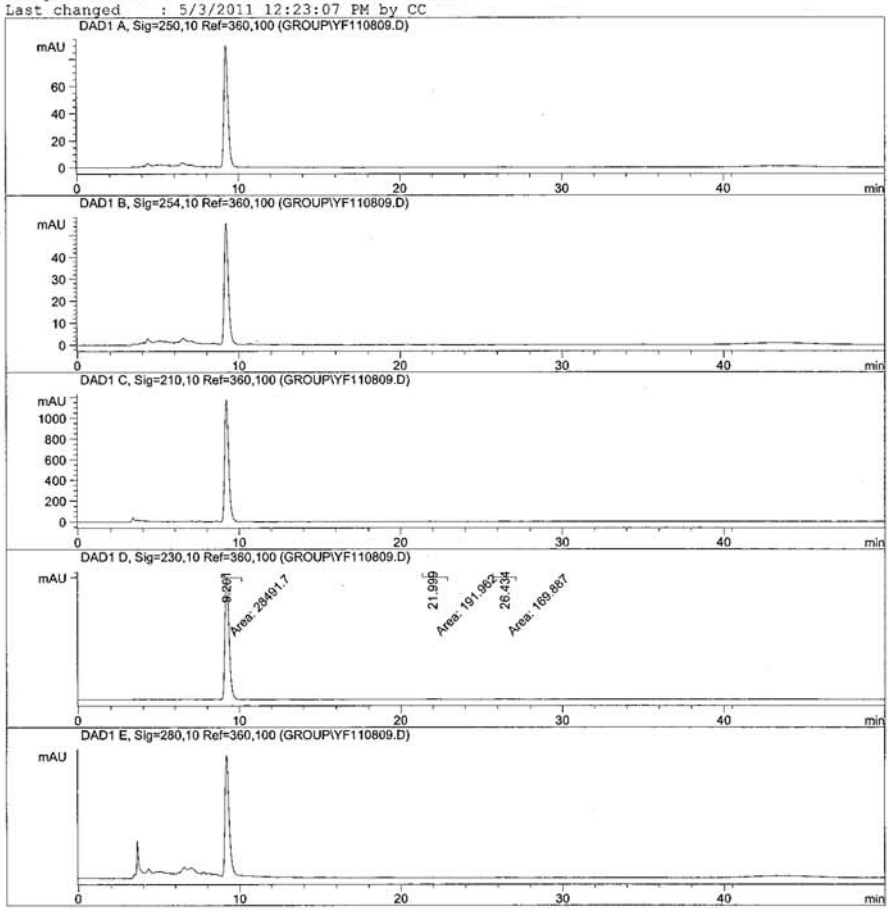


Table 4, entry 1

with (*S*)-catalyst

Injection Date : 5/3/2011 10:44:24 AM Seq. Line : 55
Sample Name : YF1108 Location : Vial 3
Acq. Operator : NB Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 15 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\AD-10-50.M
Last changed : 4/23/2011 8:41:10 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed : 5/3/2011 12:23:07 PM by CC



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.201	MM	0.3074	2.84917e4	1544.52637	98.7459
2	21.999	MM	0.8982	191.96202	3.56179	0.6653
3	26.434	MM	0.8723	169.88744	3.24591	0.5888
Totals :				2.88536e4	1551.33407	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

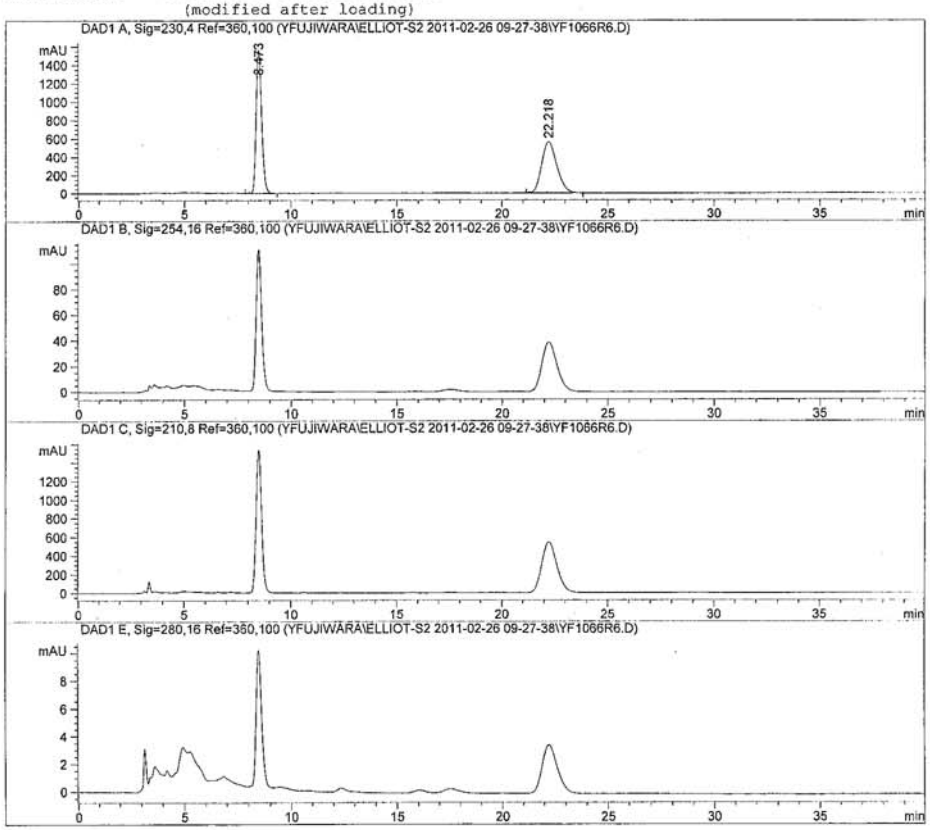
*** End of Report ***

Table 4, entry 1

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1066R6.D
ample Name: YF1066RAC

Acq. Operator : ATP Seq. Line : 35
Acq. Instrument : Instrument 1 Location : Vial 7
Injection Date : 2/27/2011 8:13:26 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-40.M
Last changed : 2/26/2011 8:52:21 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1066R6.D
Sample Name: YF1066RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.473	BB	0.2766	2.79823e4	1565.02124	50.1835
2	22.218	BB	0.7696	2.77777e4	559.15961	49.8165
Totals :				5.57600e4	2124.18085	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

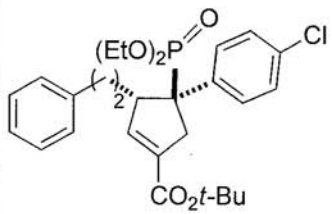
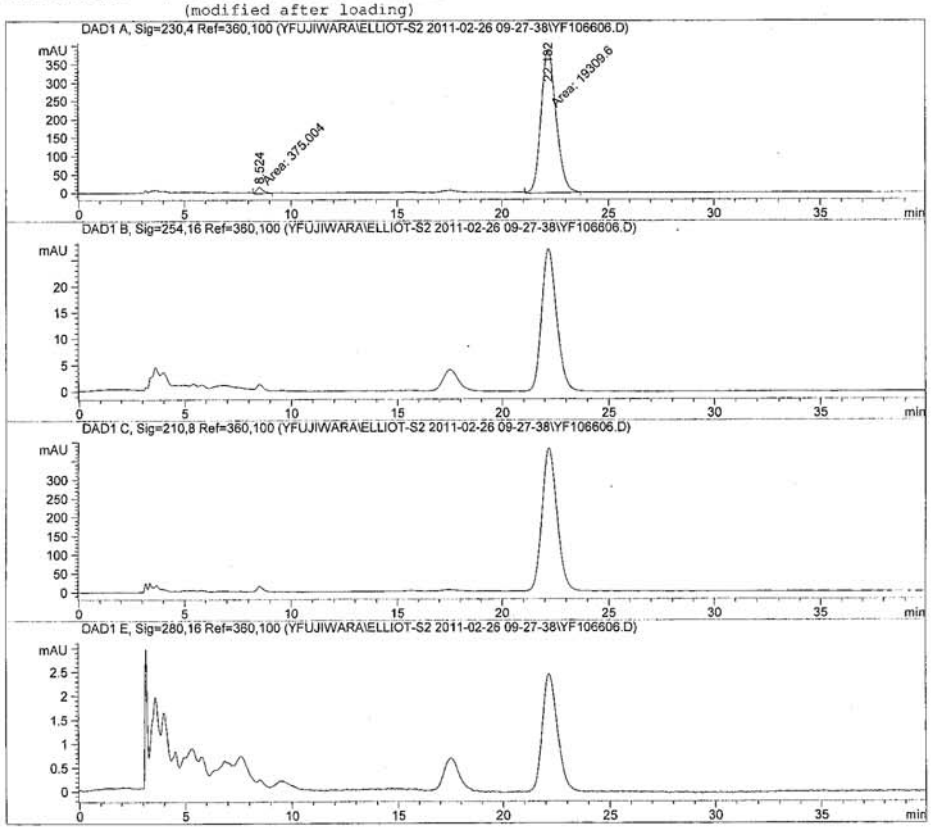


Table 4, entry 2

racemic sample

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF106606.D
ample Name: YF1066 S

Acq. Operator : ATP Seq. Line : 36
Acq. Instrument : Instrument 1 Location : Vial 8
Injection Date : 2/27/2011 8:54:45 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-40.M
Last changed : 2/26/2011 8:52:21 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF106606.D
Sample Name: YF1066 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.524	MM	0.3904	375.00385	16.01004	1.9051
2	22.182	MM	0.8225	1.93096e4	391.29907	98.0949
Totals :				1.96846e4	407.30911	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

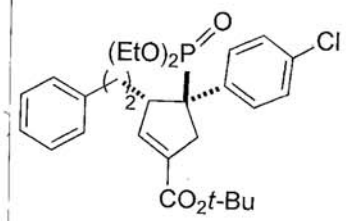
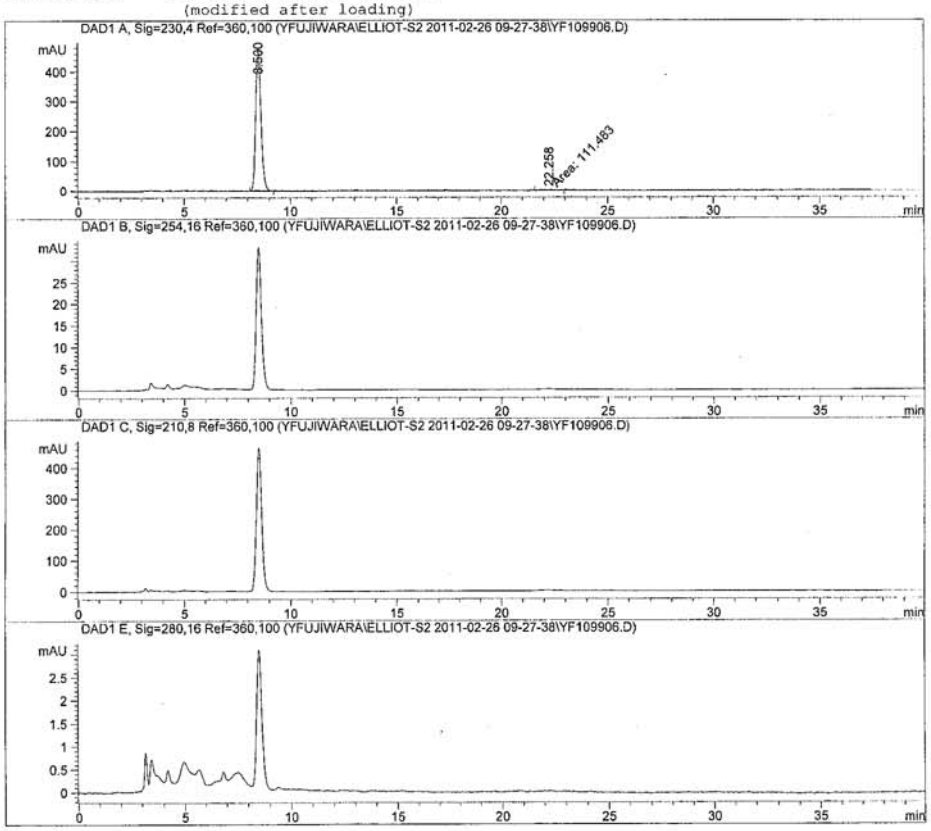


Table 4, entry 2

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF109906.D
ample Name: YF1099 S

Acq. Operator : ATP Seq. Line : 37
Acq. Instrument : Instrument 1 Location : Vial 9
Injection Date : 2/27/2011 9:36:03 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-40.M
Last changed : 2/26/2011 8:52:21 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF109906.D
Sample Name: YF1099 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.500	BB	0.2695	8285.64160	475.08841	98.6724
2	22.258	MM	0.8139	111.48270	2.28288	1.3276
Totals :				8397.12430	477.37129	

Table 4, entry 2

with (*R*)-catalyst

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

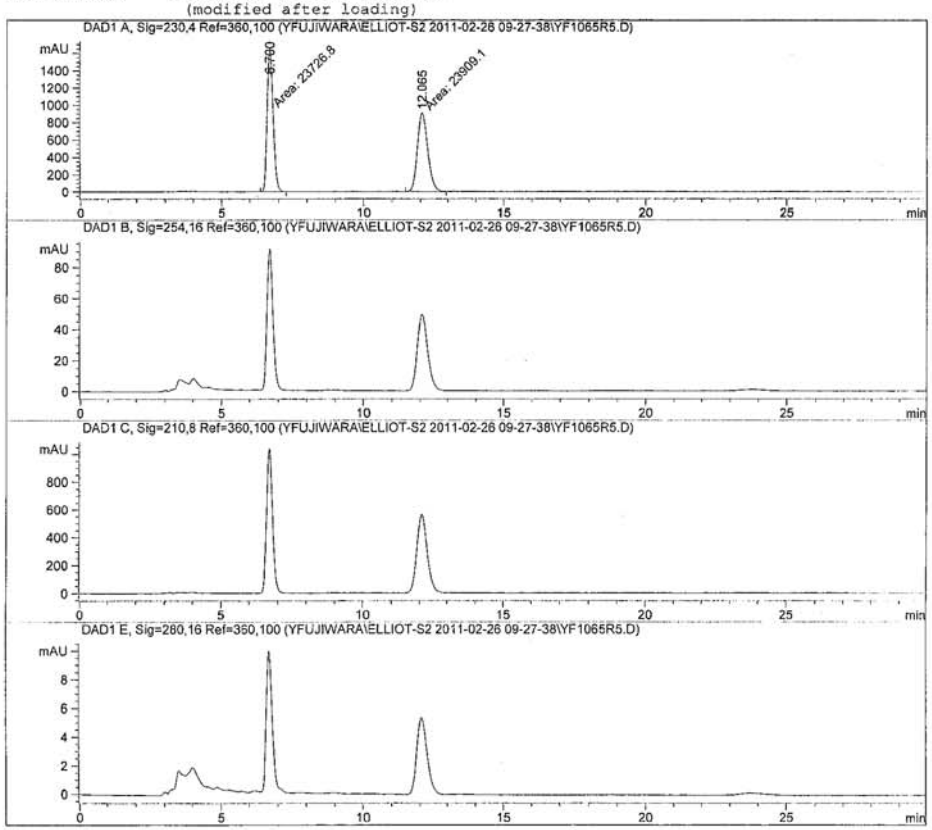
Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1065R5.D
ample Name: YF1065RAC

Acq. Operator : ATP Seq. Line : 5
Acq. Instrument : Instrument 1 Location : Vial 4
Injection Date : 2/26/2011 11:33:57 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-30.M
Last changed : 2/26/2011 8:52:00 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1065R5.D
Sample Name: YF1065RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.700	MM	0.2394	2.37268e4	1652.04541	49.8087
2	12.065	MM	0.4380	2.39091e4	909.70343	50.1913
Totals :				4.76359e4	2561.74884	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

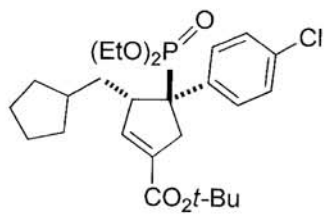
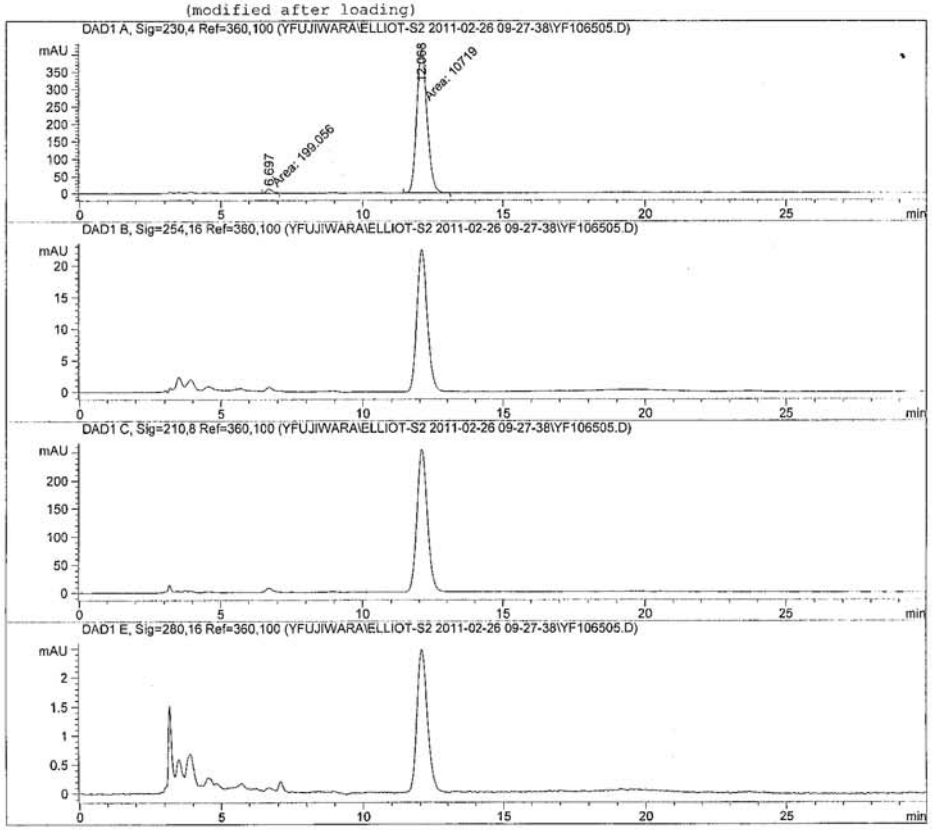


Table 4, entry 3

racemic sample

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF106505.D
ample Name: YF1065 S

Acq. Operator : ATP Seq. Line : 6
Acq. Instrument : Instrument 1 Location : Vial 5
Injection Date : 2/26/2011 12:05:11 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-30.M
Last changed : 2/26/2011 8:52:00 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF106505.D
Sample Name: YF1065 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.697	MM	0.2661	199.05574	12.46568	1.8232
2	12.068	MM	0.4323	1.07190e4	413.23291	98.1768
Totals :				1.09181e4	425.69859	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

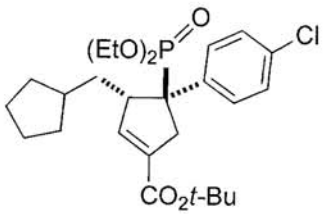
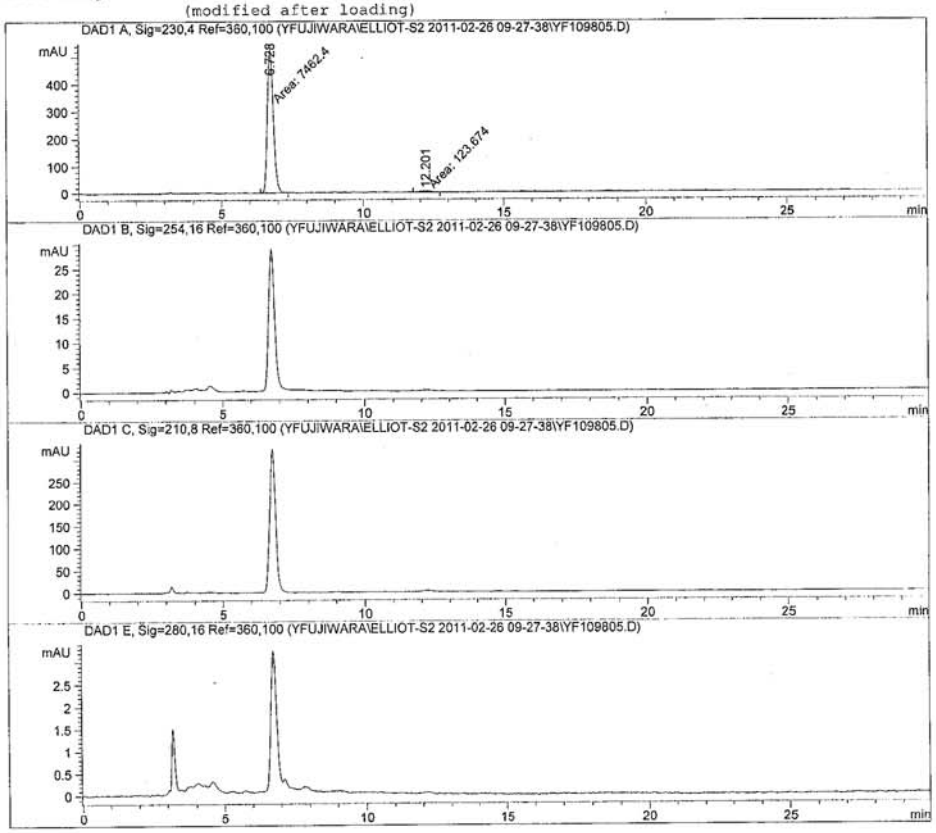


Table 4, entry 3

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF109805.D
ample Name: YF1098 S

```
Acq. Operator   : ATP                              Seq. Line :   7
Acq. Instrument : Instrument 1                      Location : Vial 6
Injection Date  : 2/26/2011 12:36:29 PM                Inj :   1
                                                   Inj Volume : 1 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H10-30.M
Last changed    : 2/26/2011 8:52:00 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed    : 2/26/2011 8:39:08 PM by ATP
                  (modified after loading)
```



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF109805.D
Sample Name: YF1098 S

Area Percent Report

```
Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.728 MM    0.2370 7462.39600  524.88641  98.3697
   2  12.201 MM    0.4653  123.67419    4.42983   1.6303

Totals :                  7586.07019  529.31625


Signal 2: DAD1 B, Sig=254,16 Ref=360,100


Signal 3: DAD1 C, Sig=210,8 Ref=360,100


Signal 4: DAD1 E, Sig=280,16 Ref=360,100
```

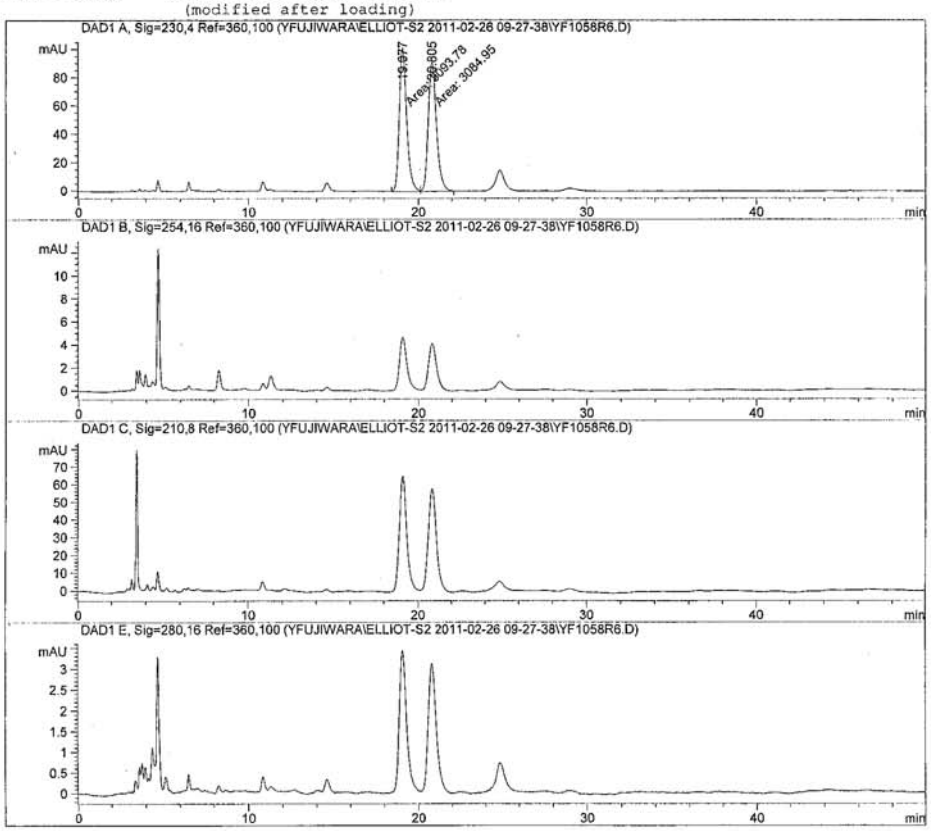
*** End of Report ***

Table 4, entry 3

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1058R6.D
ample Name: YF1058 RAC

Acq. Operator : ATP Seq. Line : 31
Acq. Instrument : Instrument 1 Location : Vial 19
Injection Date : 2/27/2011 5:08:00 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H01-50.M
Last changed : 2/26/2011 9:30:42 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF1058R6.D
Sample Name: YF1058 RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.077	MM	0.5079	3093.77808	101.52602	50.0714
2	20.805	MM	0.5638	3084.95190	91.18791	49.9286
Totals :				6178.72998	192.71394	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

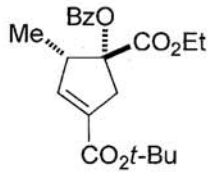
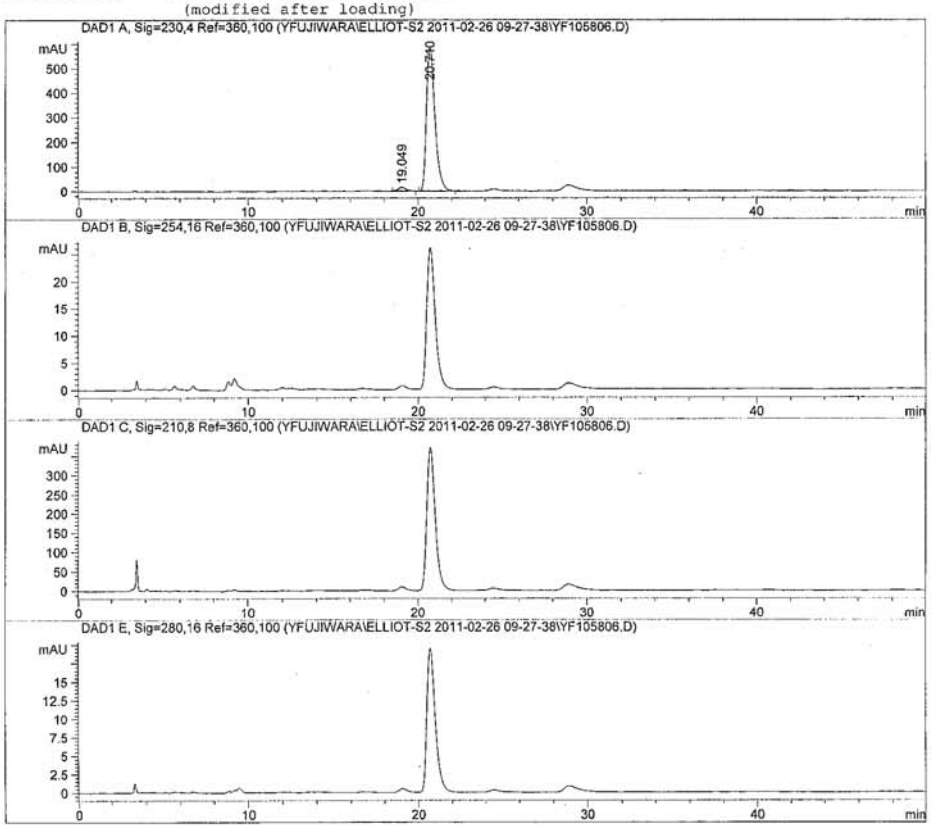


Table 5, entry 1

racemic sample

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF105806.D
ample Name: YF1058 S

Acq. Operator : ATP Seq. Line : 32
Acq. Instrument : Instrument 1 Location : Vial 20
Injection Date : 2/27/2011 5:59:16 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H01-50.M
Last changed : 2/26/2011 9:30:42 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF105806.D
Sample Name: YF1058 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.049	BB	0.4751	499.30032	15.95282	2.4126
2	20.710	BB	0.5287	2.01960e4	582.27618	97.5874
Totals :				2.06953e4	598.22901	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

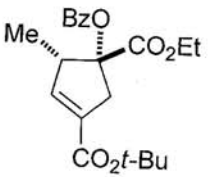
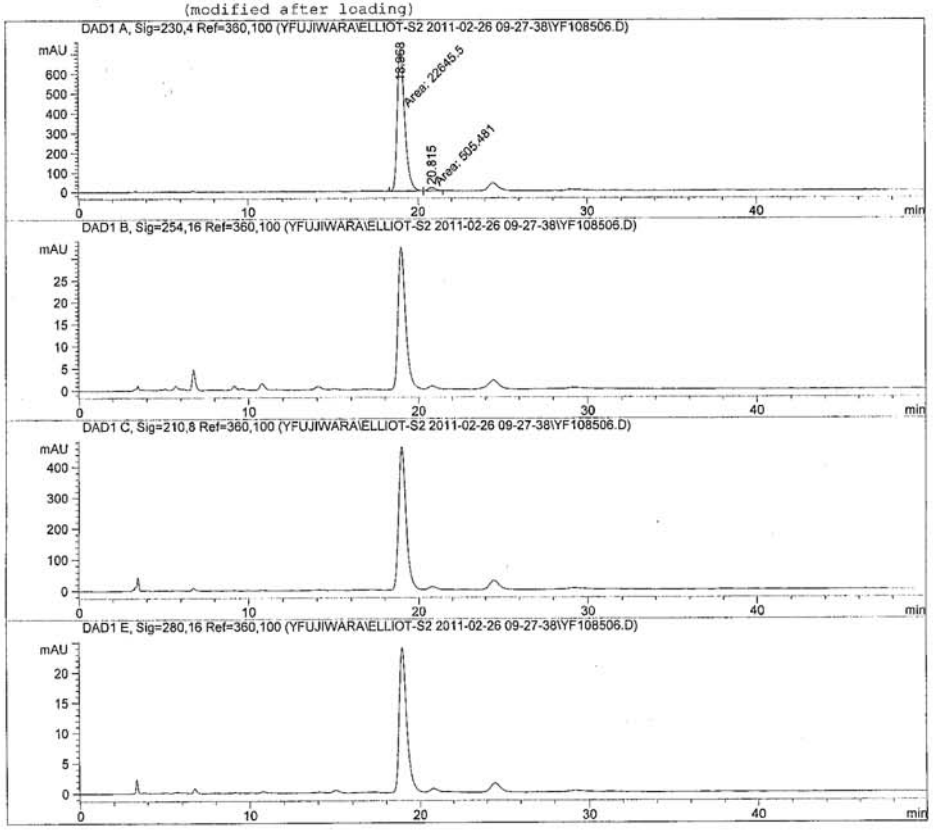


Table 5, entry 1

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF108506.D
ample Name: YF1085 R

Acq. Operator : ATP Seq. Line : 33
Acq. Instrument : Instrument 1 Location : Vial 21
Injection Date : 2/27/2011 6:50:39 AM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\AD-H01-50.M
Last changed : 2/26/2011 9:30:42 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H02-60.M
Last changed : 2/26/2011 8:39:08 PM by ATP
(modified after loading)



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-26 09-27-38\YF108506.D
Sample Name: YF1085 R

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.968	MM	0.5207	2.26455e4	724.85608	97.8166
2	20.815	MM	0.5301	505.48083	15.89293	2.1834
Totals :				2.31510e4	740.74901	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

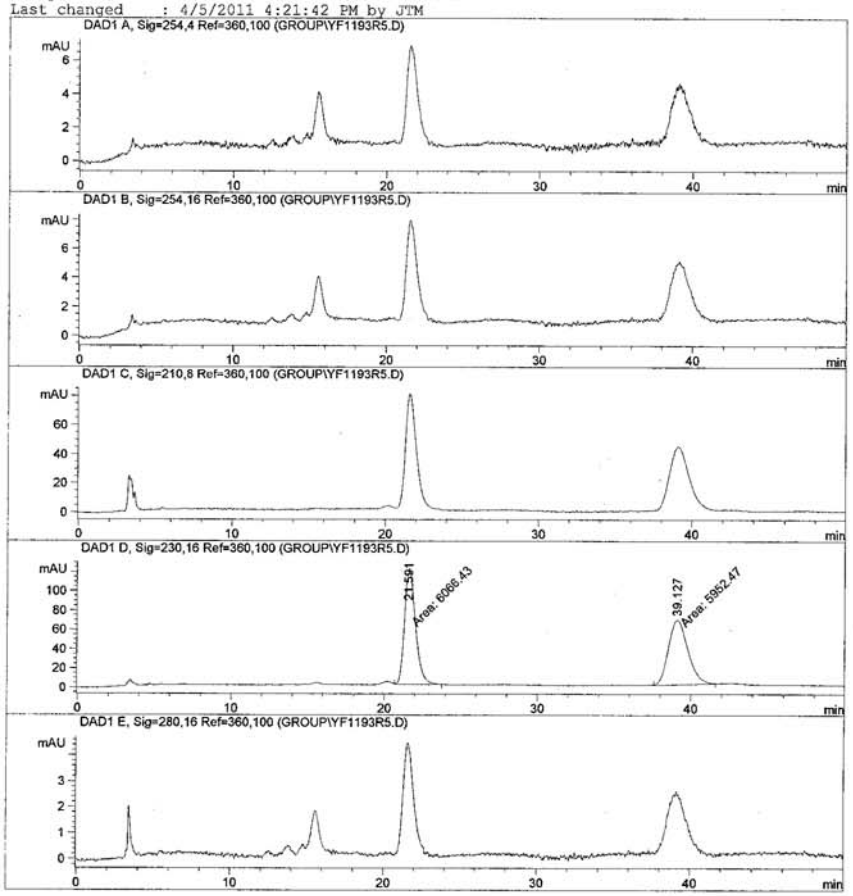
Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 5, entry 1

with (*R*)-catalyst

Injection Date : 4/7/2011 10:48:47 PM Seq. Line : 14
Sample Name : YF1193 RAC Location : Vial 18
Acq. Operator : JTM Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IC-1050.M
Last changed : 3/1/2011 10:19:39 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-0320.M
Last changed : 4/5/2011 4:21:42 PM by JTM



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.591	MM	0.8388	6066.43408	120.53661	50.4741
2	39.127	MM	1.4786	5952.47217	67.09765	49.5259
Totals :				1.20189e4	187.63425	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

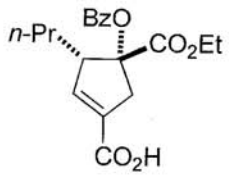
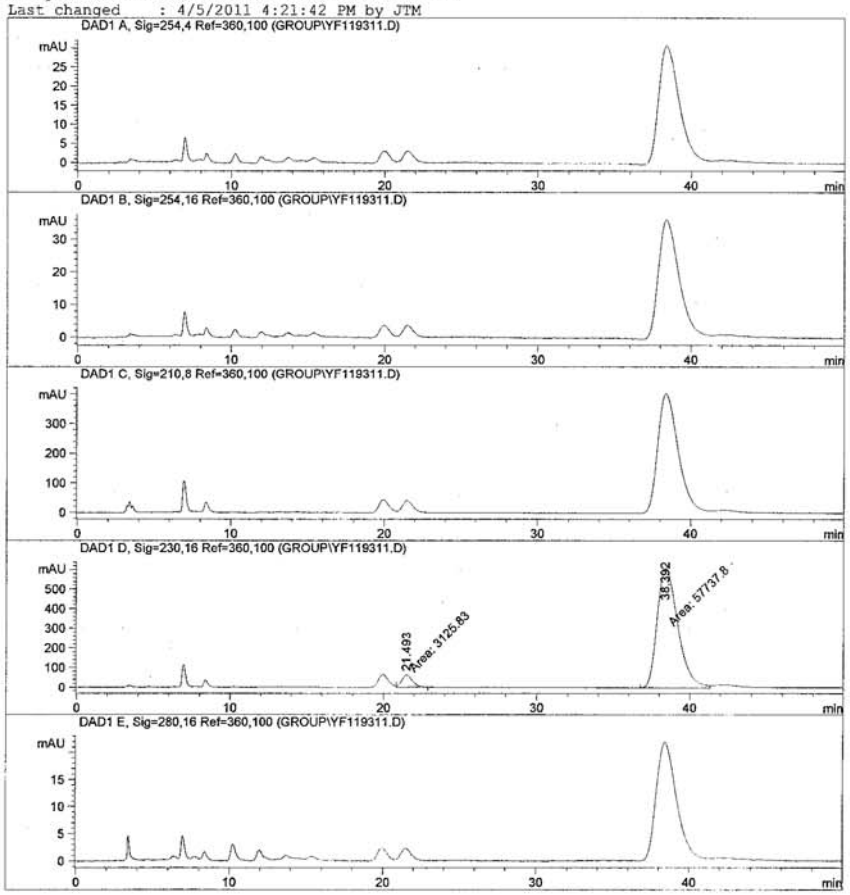


Table 5, entry 2

racemic sample

```
Injection Date  : 4/7/2011 11:40:06 PM          Seq. Line :  15
Sample Name     : YF1193 S-CAT                  Location : Vial 19
Acq. Operator   : JTM                              Inj :  1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-1050.M
Last changed    : 3/1/2011 10:19:39 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-0320.M
Last changed    : 4/5/2011 4:21:42 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  21.493 FM    0.8163 3125.82690   63.81886   5.1358
   2  38.392 MF    1.5706 5.77378e4    612.69031  94.8642

Totals :                  6.08636e4    676.50917

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

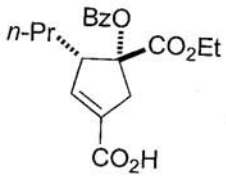
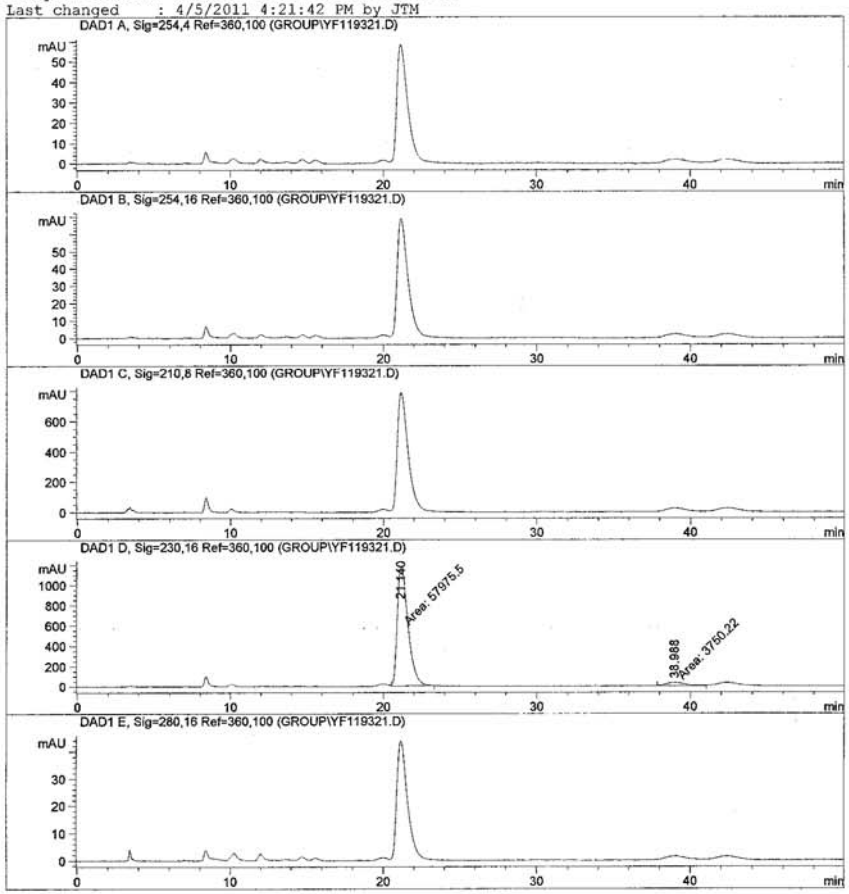


Table 5, entry 2

with (*S*)-catalyst

```
Injection Date  : 4/8/2011 12:31:23 AM          Seq. Line :  16
Sample Name     : YF1193 R-CAT                  Location : Vial 20
Acq. Operator   : JTM                              Inj :  1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-1050.M
Last changed    : 3/1/2011 10:19:39 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-0320.M
Last changed    : 4/5/2011 4:21:42 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.140	FM	0.8197	5.79755e4	1178.73462	93.9244
2	38.988	MM	1.5853	3750.22217	39.42817	6.0756
Totals :				6.17257e4	1218.16279	

Results obtained with enhanced integrator!

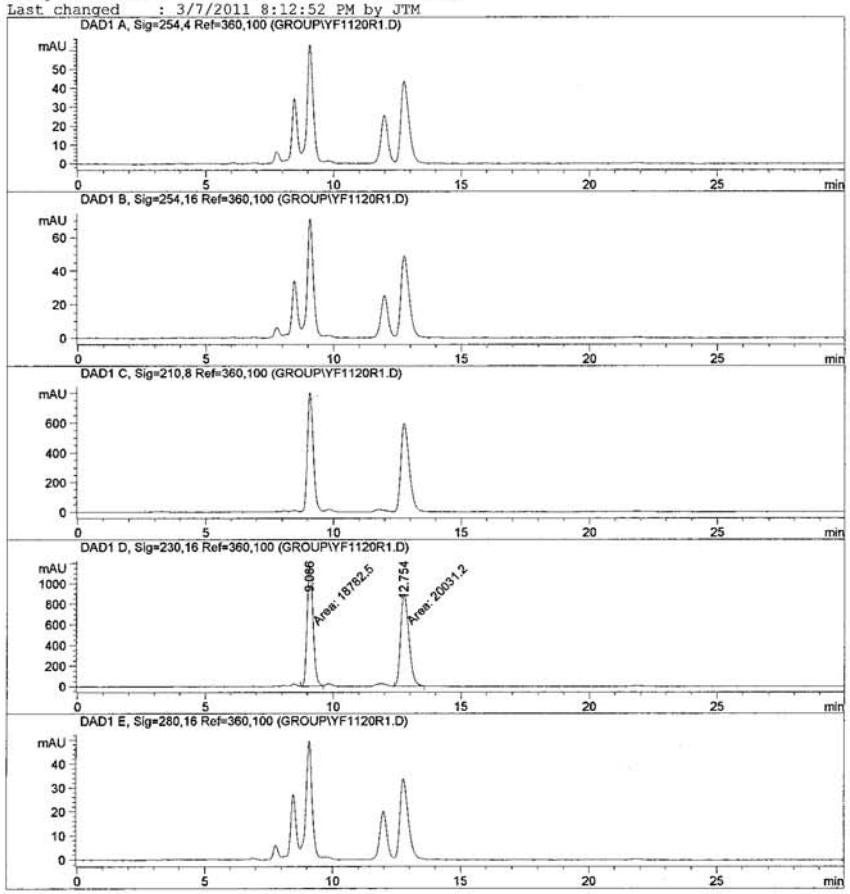
Signal 5: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 5, entry 2

with (*R*)-catalyst

```
Injection Date  : 3/7/2011 8:42:51 PM          Seq. Line :   2
Sample Name     : YF1120 RAC                    Location : Vial 71
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0130.M
Last changed    : 3/5/2011 3:36:54 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-1040.M
Last changed    : 3/7/2011 8:12:52 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.086 MM    0.2690 1.87825e4  1163.57739  48.3913
   2  12.754 MM    0.3732 2.00312e4   894.48456  51.6087

Totals :                  3.88137e4  2058.06195

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

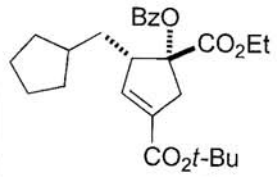
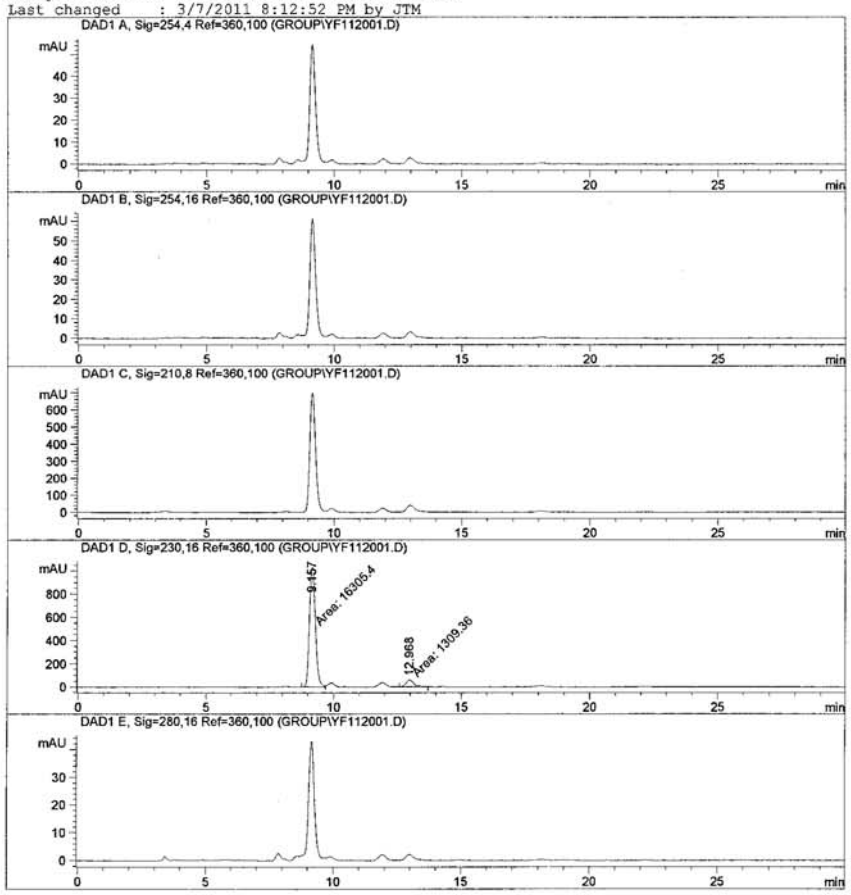


Table 5, entry 3

racemic sample

*** End of Report ***

```
Injection Date  : 3/7/2011 9:14:07 PM          Seq. Line :   3
Sample Name     : YF1120 S CAT                  Location : Vial 72
Acq. Operator   : JTM                             Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0130.M
Last changed    : 3/5/2011 3:36:54 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-1040.M
Last changed    : 3/7/2011 8:12:52 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.157 MF    0.2632 1.63054e4  1032.31580  92.5667
   2  12.968 MM    0.3638 1309.36438   59.98289   7.4333

Totals :                  1.76148e4  1092.29868

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

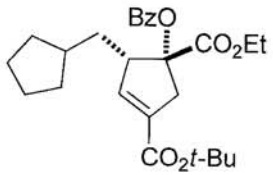
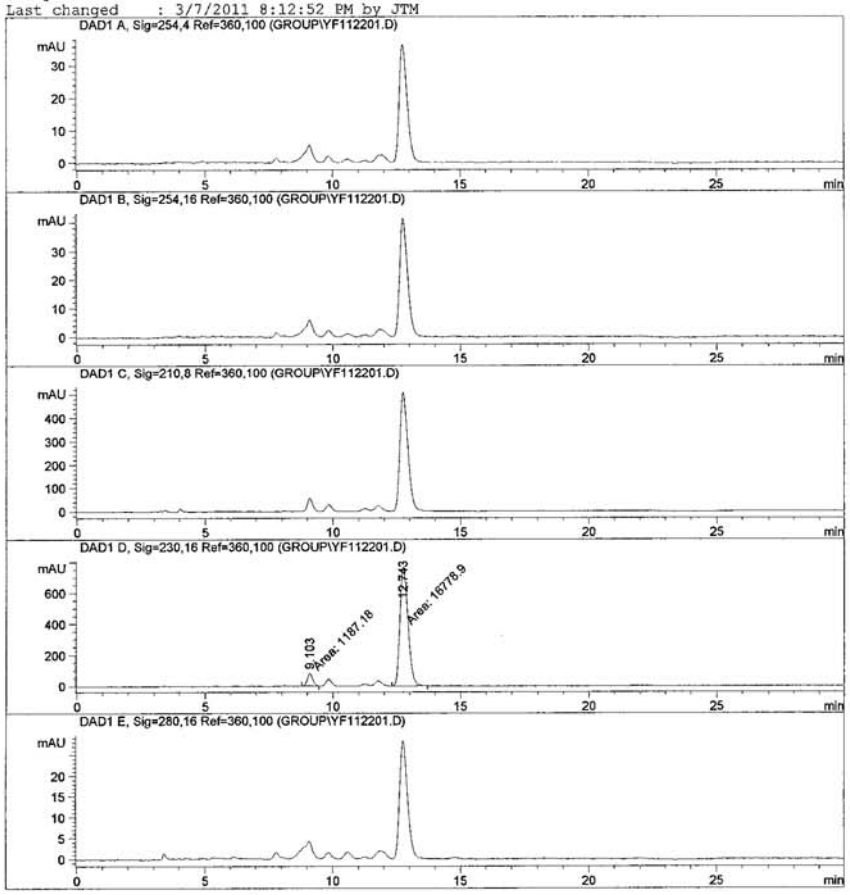


Table 5, entry 3

with (*S*)-catalyst

```
Injection Date  : 3/7/2011 9:45:22 PM          Seq. Line :   4
Sample Name     : YF1120 R CAT                  Location : Vial 73
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0130.M
Last changed    : 3/5/2011 3:36:54 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ODH-1040.M
Last changed    : 3/7/2011 8:12:52 PM by JTM
```



Area Percent Report

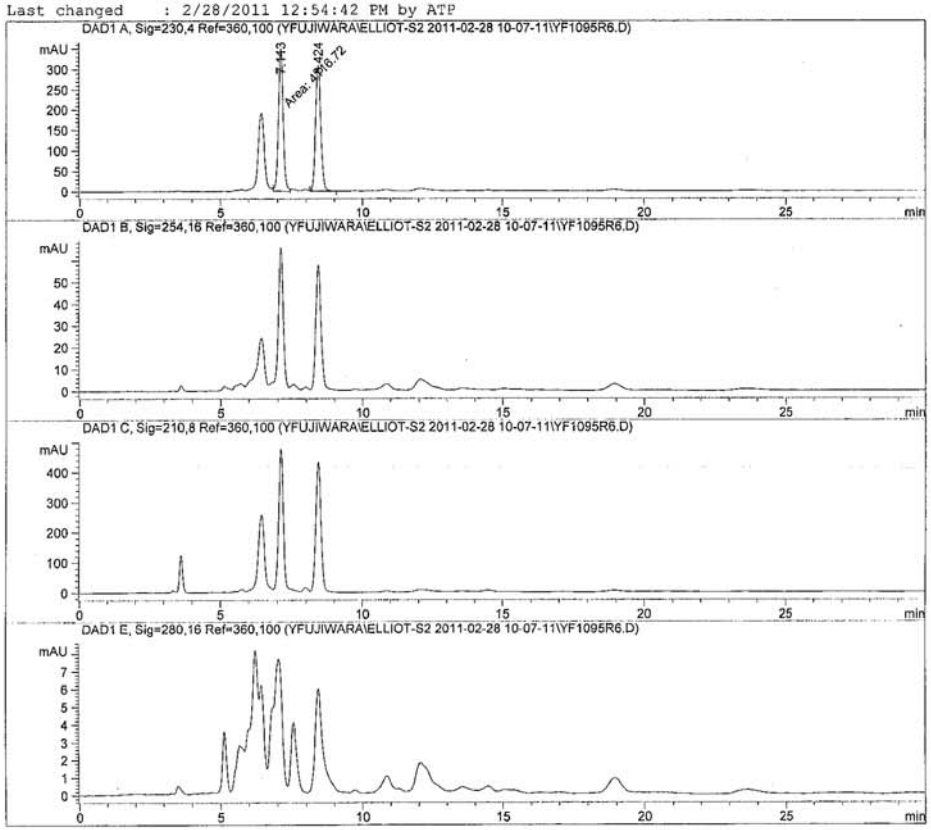
```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.103 MM    0.2422 1187.17957   81.69284   6.6079
   2  12.743 MM    0.3629 1.67789e4    770.67529  93.3921

Totals :                  1.79660e4    852.36813

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

                      *** End of Report ***
```

Table 5, entry 3

with (*R*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF1095R6.D
ample Name: YF1095 RAC

Acq. Operator : ATP Seq. Line : 11
Acq. Instrument : Instrument 1 Location : Vial 26
Injection Date : 2/28/2011 3:56:46 PM Inj : 1
Inj Volume : 1 µl IA column.
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF1095R6.D
Sample Name: YF1095 RAC

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.113	FM	0.1966	4116.71875	348.91183	50.7636
2	8.424	VB	0.2009	3992.86377	308.66205	49.2364
Totals :				8109.58252	657.57388	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

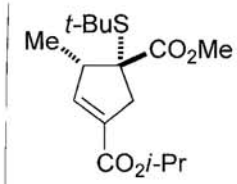


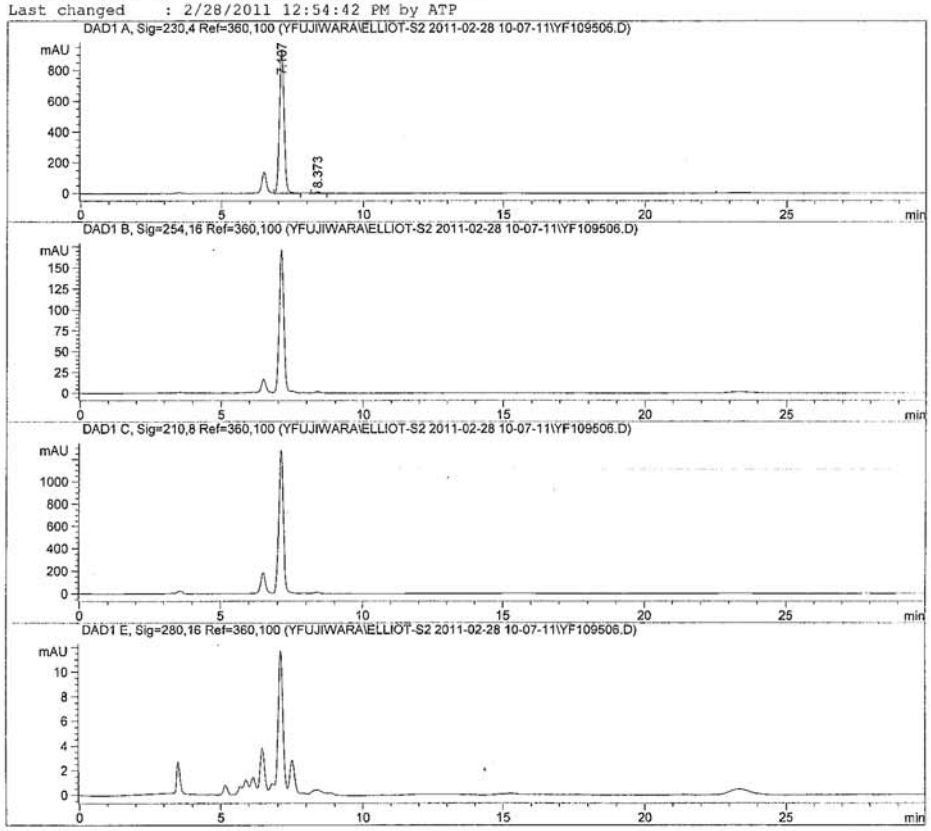
Table 6, entry 1

racemic sample

ta File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF109506.D
mple Name: YF1095 S

Acq. Operator : ATP Seq. Line : 12
Acq. Instrument : Instrument 1 Location : Vial 27
Injection Date : 2/28/2011 4:28:03 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP

IA column



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF109506.D
Sample Name: YF1095 S

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.107	VB	0.1733	1.05289e4	935.58063	98.7731
2	8.373	VB	0.2086	130.78296	9.62103	1.2269
Totals :				1.06597e4	945.20166	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

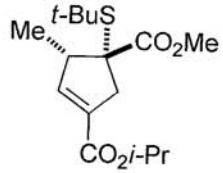
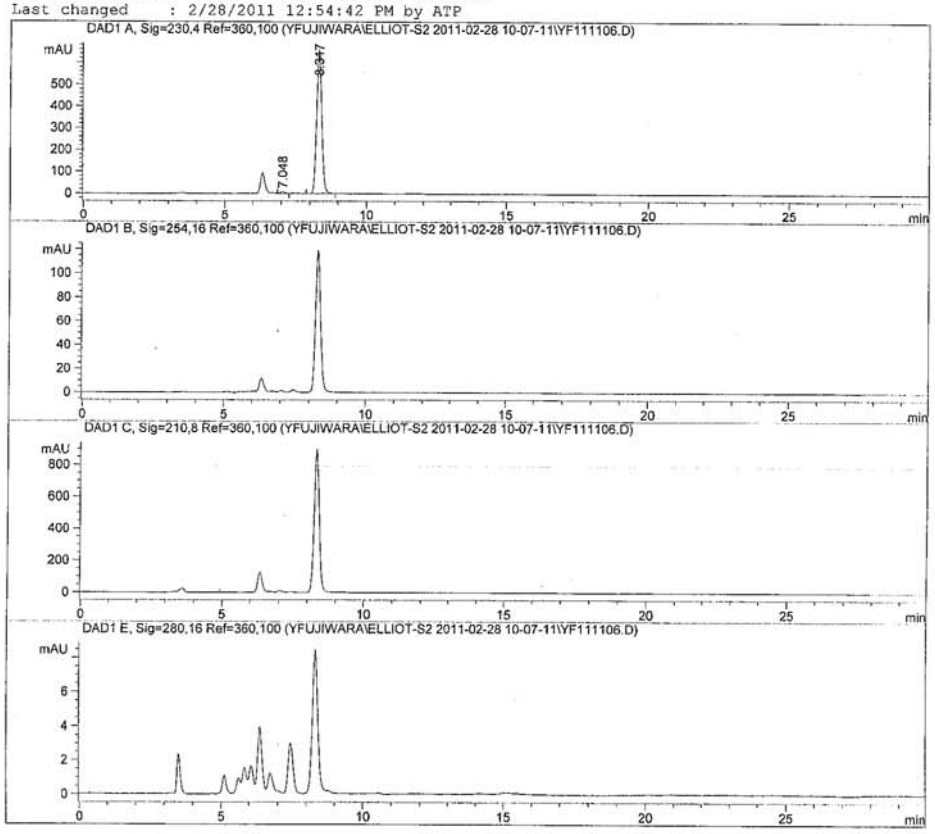


Table 6, entry 1

with (*S*)-catalyst

ata File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF111106.D
ample Name: YF1111 R

Acq. Operator : ATP Seq. Line : 13
Acq. Instrument : Instrument 1 Location : Vial 28
Injection Date : 2/28/2011 4:59:19 PM Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\AD-H01-30.M
Last changed : 2/26/2011 9:31:41 AM by ATP
Analysis Method : C:\CHEM32\1\METHODS\AD-H05-30.M
Last changed : 2/28/2011 12:54:42 PM by ATP



Data File C:\CHEM32\1\DATA\YFUJIWARA\ELLIOT-S2 2011-02-28 10-07-11\YF111106.D
Sample Name: YF1111 R

Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.048	VV	0.1783	96.27586	8.36081	1.1435
2	8.317	VB	0.1963	8323.41406	654.87170	98.8565
Totals :				8419.68993	663.23252	

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

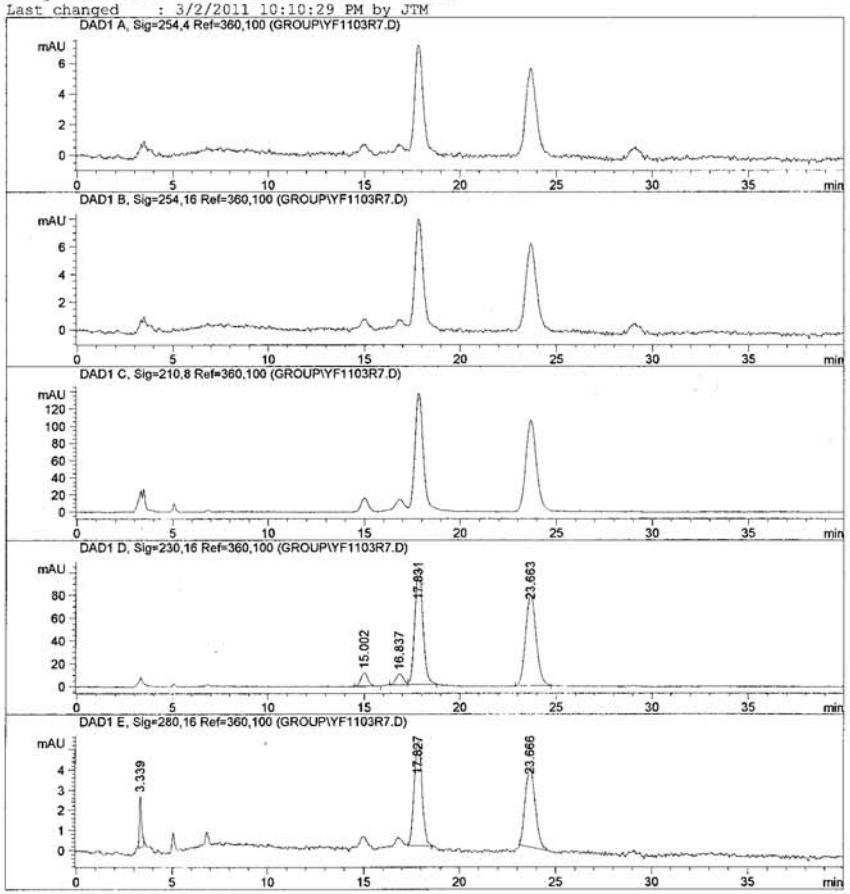
Signal 4: DAD1 E, Sig=280,16 Ref=360,100

*** End of Report ***

Table 6, entry 1

with (*R*)-catalyst

```
Injection Date  : 3/2/2011 11:28:47 PM          Seq. Line :   5
Sample Name     : YF1103 RAC                     Location : Vial 53
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0440.M
Last changed    : 3/2/2011 10:07:23 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.002 BP    0.3640  299.83340   11.89622   4.5204
   2  16.837 BV    0.3665  268.95212    9.61097   4.0549
   3  17.831 VB    0.4462 3007.47852  103.15027  45.3423
   4  23.663 BB    0.5779 3056.56714   79.97822  46.0824

Totals :                  6632.83118  204.63568

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.339 BB    0.1198   20.97638    2.55563   6.7858
   2  17.827 PB    0.4010  145.37054    5.15454  47.0267
   3  23.666 BB    0.4409  142.77673    4.01493  46.1876

Totals :                   309.12365   11.72509

 Results obtained with enhanced integrator!
```

*** End of Report ***

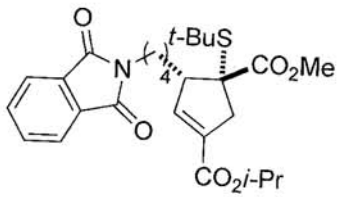
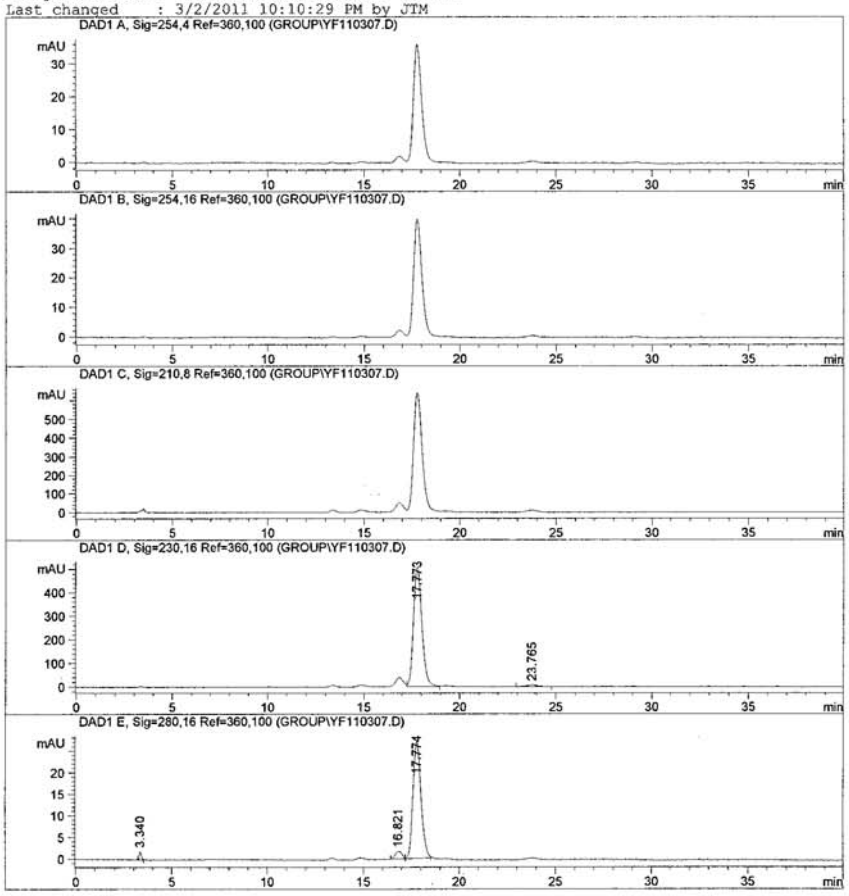


Table 6, entry 2

racemic sample

```
Injection Date  : 3/3/2011 12:10:06 AM          Seq. Line :   6
Sample Name     : YF1103 S-cat                   Location : Vial 54
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0440.M
Last changed    : 3/2/2011 10:07:23 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.773 VB    0.4684 1.54583e4   508.88803  98.0453
   2  23.765 BP    0.4751  308.19495    8.00621   1.9547

Totals :                  1.57665e4   516.89424

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.340 BB    0.1107   13.32599    1.87888   1.5857
   2  16.821 BV    0.3032   42.70980    1.78479   5.0822
   3  17.774 VB    0.4363  784.34705   27.04794  93.3321

Totals :                   840.38284   30.71161

 Results obtained with enhanced integrator!

*** End of Report ***
```

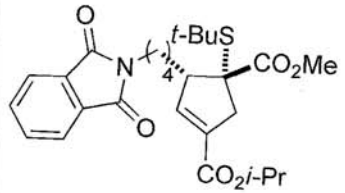
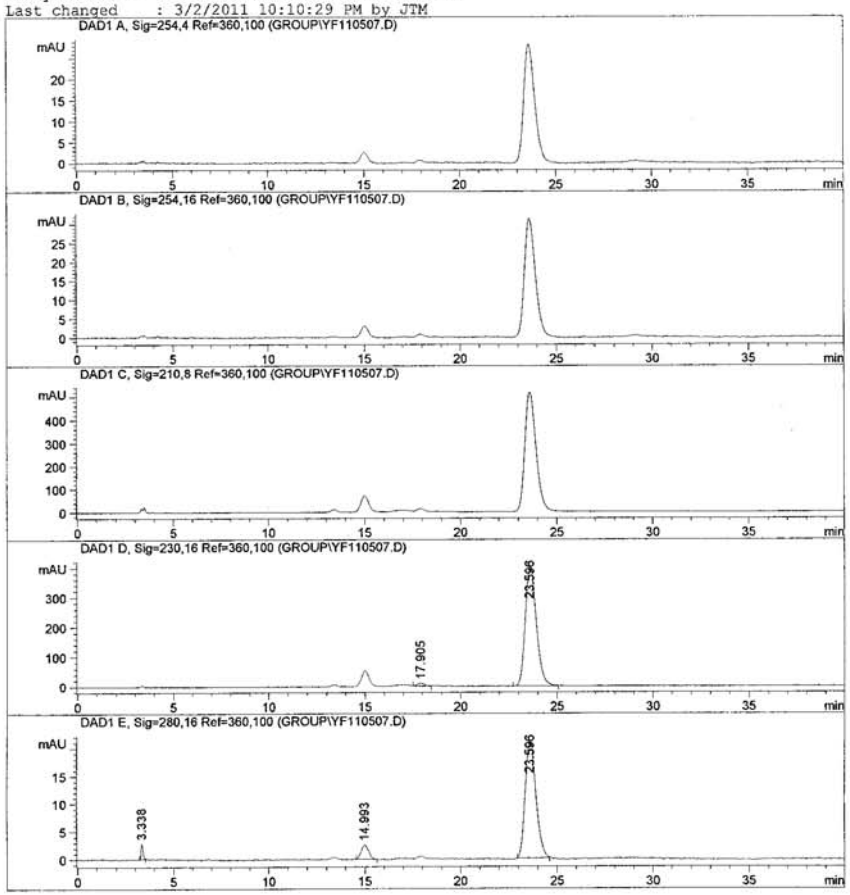


Table 6, entry 2

with (*S*)-catalyst

```
Injection Date  : 3/3/2011 12:51:25 AM          Seq. Line :   7
Sample Name     : YF1103 R-cat                  Location : Vial 55
Acq. Operator   : JTM                             Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IA-0440.M
Last changed    : 3/2/2011 10:07:23 PM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\ADH-1020.M
Last changed    : 3/2/2011 10:10:29 PM by JTM
```



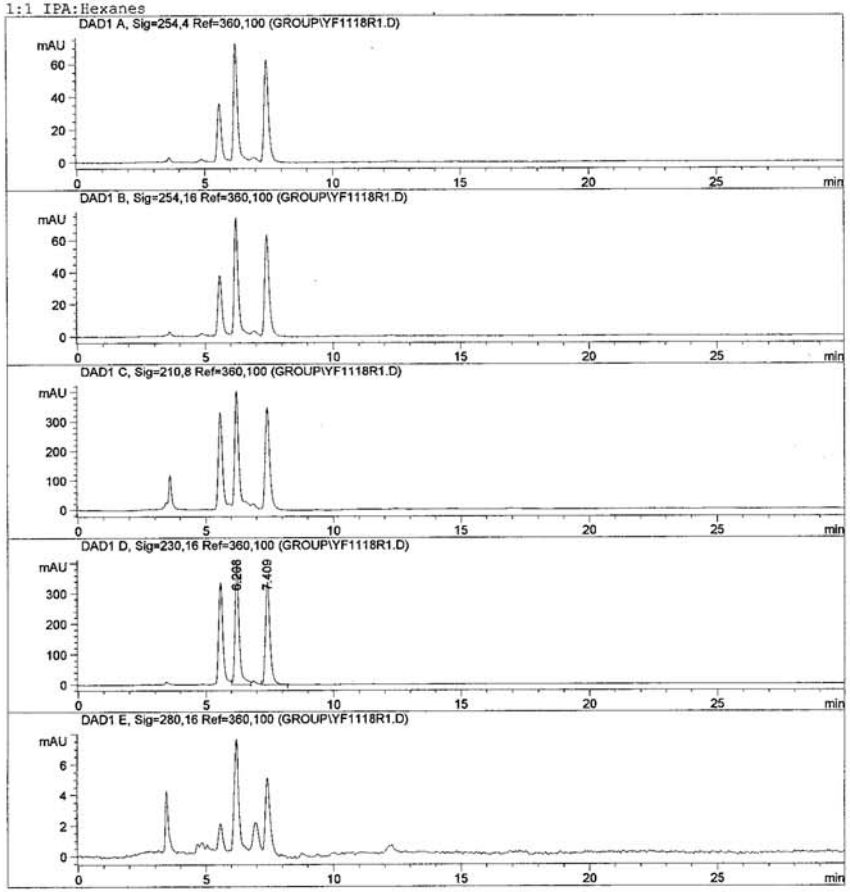
Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.905 VP    0.3508  266.56589    9.75396   1.6419
   2  23.596 PB    0.6066 1.59688e4   402.73621  98.3581

Totals :                  1.62354e4   412.49016

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.338 BB    0.1144   20.84478    2.81426   2.3177
   2  14.993 BP    0.3461   68.26148    2.55201   7.5898
   3  23.596 BB    0.5476  810.27417   21.11805  90.0925

Totals :                   899.38043   26.48432

 Results obtained with enhanced integrator!

                *** End of Report ***
```

Table 6, entry 2

with (*R*)-catalyst

```
Injection Date  : 3/5/2011 11:22:50 PM          Seq. Line :  21
Sample Name     : YF1118 RAC                    Location : Vial 74
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Acq. Method     : C:\HPCHEM\1\METHODS\ADH-0130.M
Last changed    : 1/1/2011 9:04:38 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AS00320.M
Last changed    : 3/6/2011 12:10:21 PM by JTM
1:1 IPA:Hexanes
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.208 VV    0.1700 4454.23926  393.69000  50.7404
   2   7.409 VB    0.1948 4324.23926  339.03305  49.2596

Totals :                  8778.47852  732.72305

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

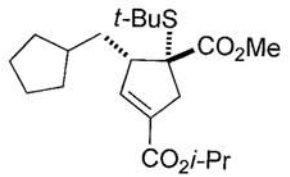
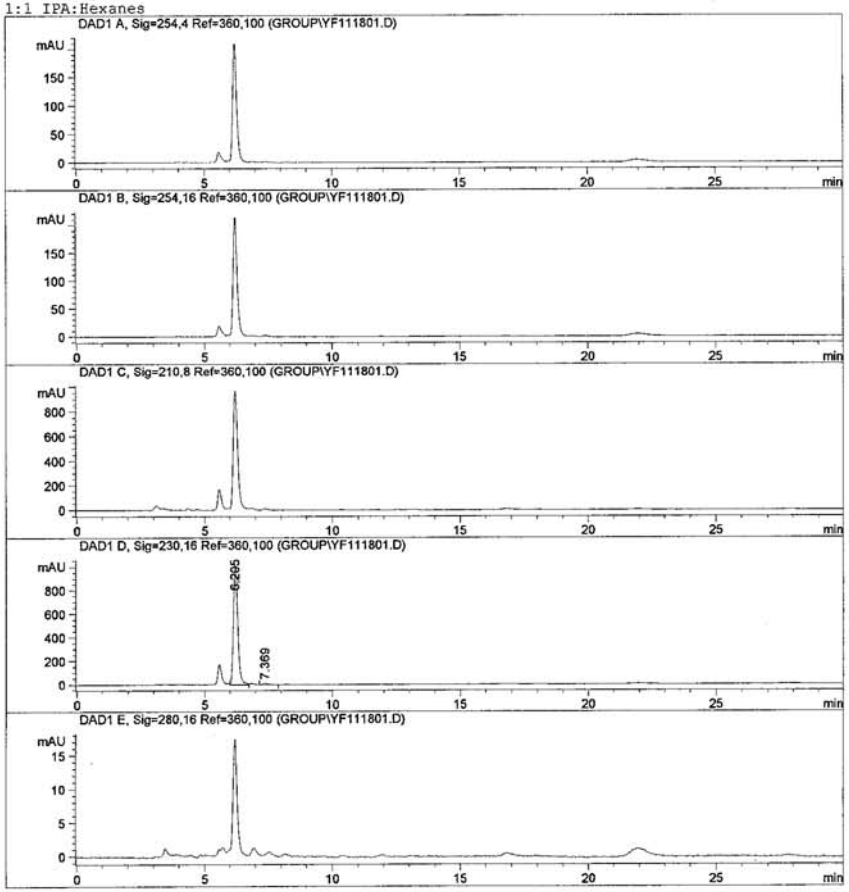


Table 6, entry 3

racemic sample

```
Injection Date  : 3/5/2011 11:54:10 PM          Seq. Line :  22
Sample Name     : YF1118 S-cat                  Location : Vial 75
Acq. Operator   : JTM                              Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Acq. Method     : C:\HPCHEM\1\METHODS\ADH-0130.M
Last changed    : 1/1/2011 9:04:38 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AS00320.M
Last changed    : 3/6/2011 12:10:21 PM by JTM
1:1 IPA:Hexanes
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|------|----|-------|----------|----------|--------|
   1   6.205 BV    0.1794 1.18209e4  1018.26752  98.5926
   2   7.369 VB    0.2095  168.74585   11.61742   1.4074

Totals :                   1.19897e4  1029.88493

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

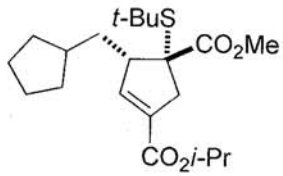
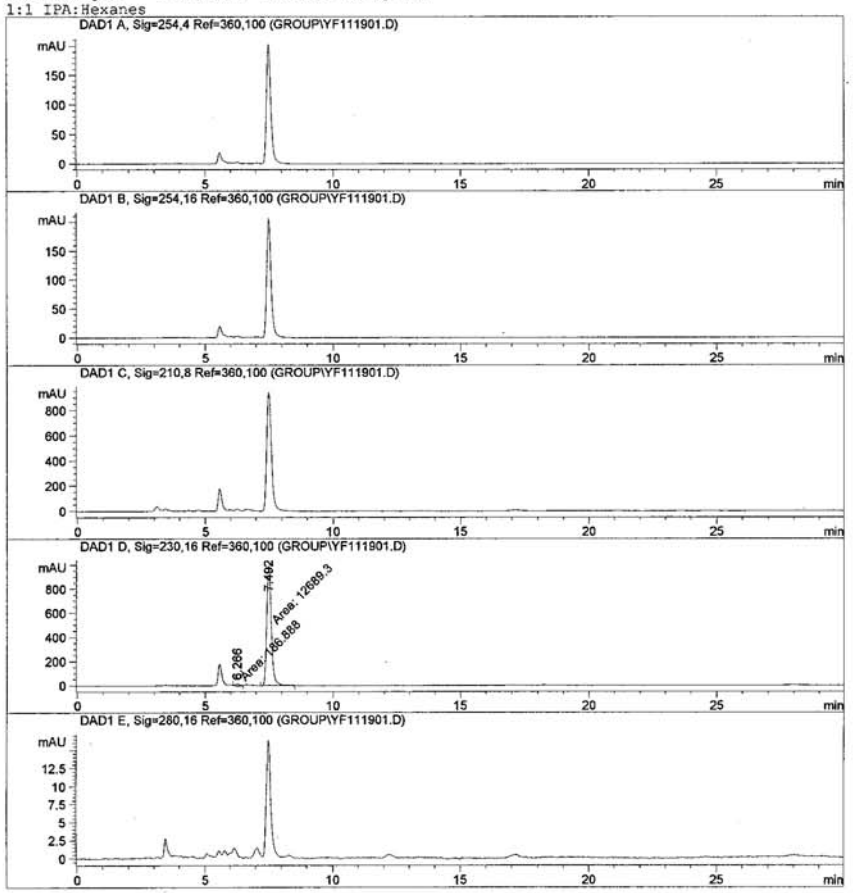


Table 6, entry 3

with (*S*)-catalyst

```
Injection Date  : 3/6/2011 12:25:30 AM          Seq. Line :  23
Sample Name     : YF1119 R-cat                   Location : Vial 76
Acq. Operator   : JTM                               Inj :  1
Acq. Instrument : Instrument 1                  Inj Volume : 5 µl
Acq. Method     : C:\HPCHEM\1\METHODS\ADH-0130.M
Last changed    : 1/1/2011 9:04:38 AM by JTM
Analysis Method : C:\HPCHEM\1\METHODS\AS00320.M
Last changed    : 3/6/2011 12:10:21 PM by JTM
1:1 IPA:Hexanes
```



Area Percent Report

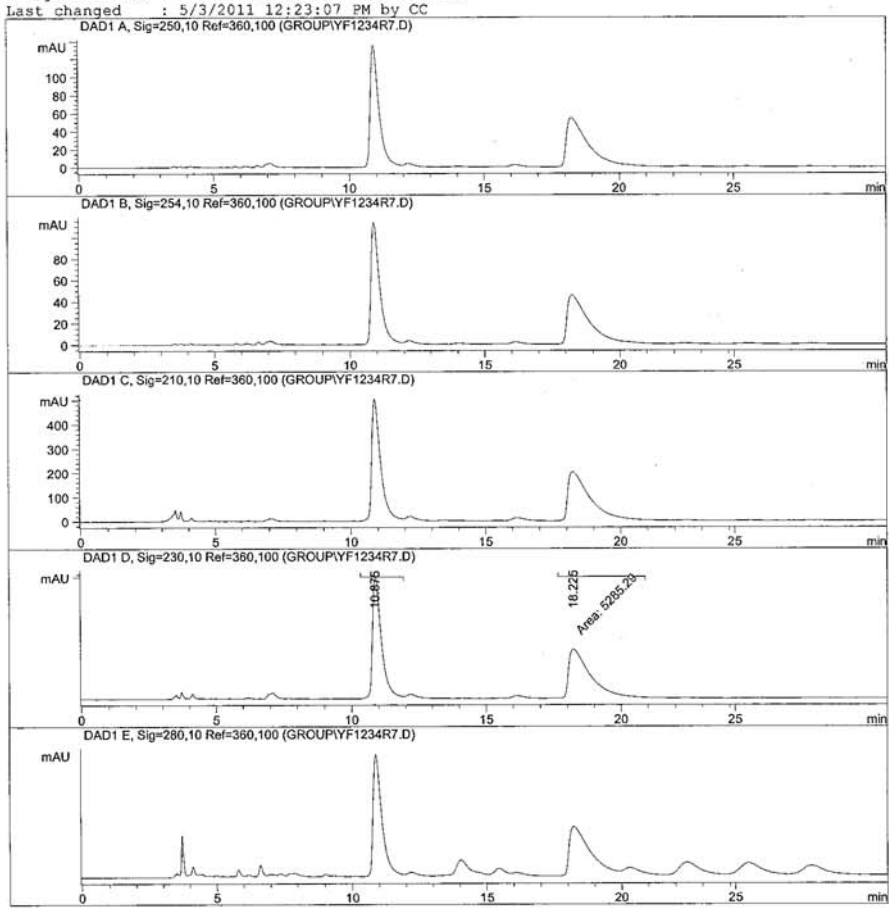
```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Signal 2: DAD1 B, Sig=254,16 Ref=360,100

Signal 3: DAD1 C, Sig=210,8 Ref=360,100

Signal 4: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  6.266 FM    0.1947  186.88757   16.00057   1.4514
   2  7.492 MM    0.2136 1.26893e4   990.24139  98.5486

Totals :                  1.28762e4  1006.24197

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,16 Ref=360,100
```

*** End of Report ***

Table 6, entry 3

with (*R*)-catalyst

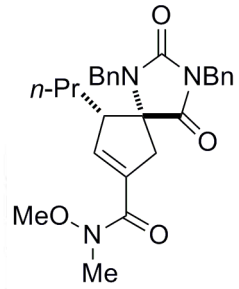
```
Injection Date  : 5/3/2011 12:08:37 PM          Seq. Line :  58
Sample Name     : Weinreb RAC                    Location : Vial 31
Acq. Operator   : NB                                Inj :  1
Acq. Instrument : Instrument 1                Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IB-15-30.M
Last changed    : 4/7/2011 9:46:30 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed    : 5/3/2011 12:23:07 PM by CC
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.875 BB    0.3345 5388.98145  235.95155  50.4857
   2  18.225 MM    0.9319 5285.28564   94.52305  49.5143

Totals :                  1.06743e4   330.47460

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100
```

*** End of Report ***

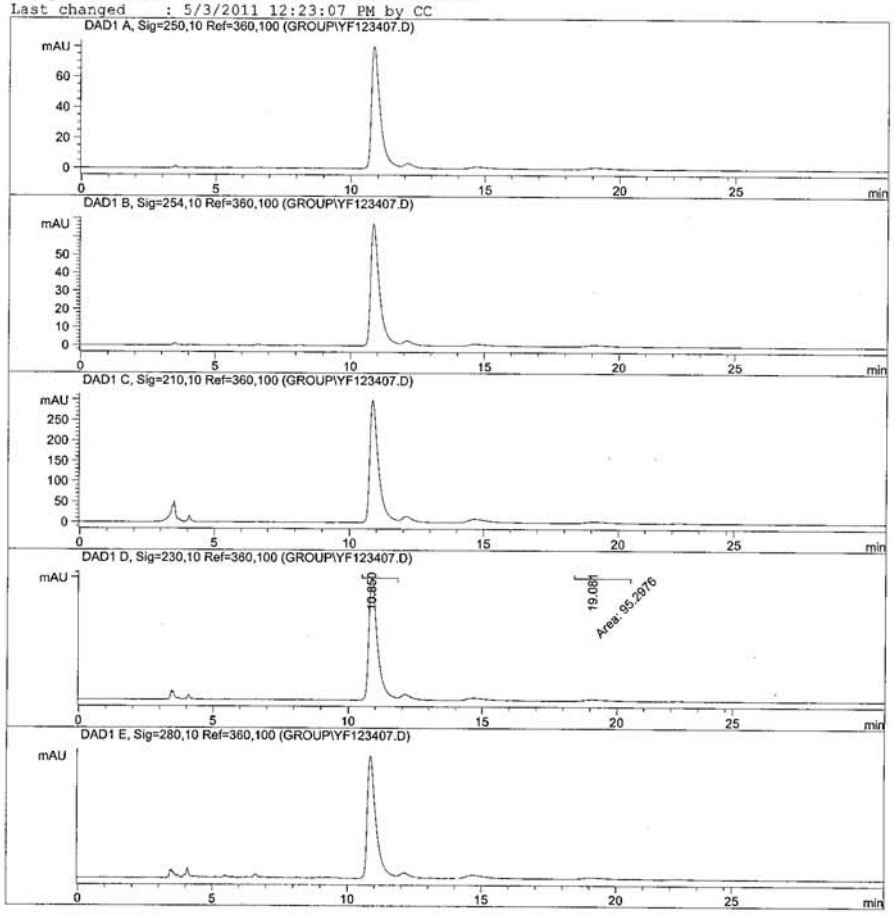


eq 3

racemic sample

Data File C:\HPCHEM\1\DATA\GROUP\YF123407.D Sample Name: Weinreb S

Injection Date : 5/3/2011 12:40:23 PM Seq. Line : 1
Sample Name : Weinreb S Location : Vial 32
Acq. Operator : NB Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 15 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IB-15-30.M
Last changed : 4/7/2011 9:46:30 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed : 5/3/2011 12:23:07 PM by CC



Data File C:\HPCHEM\1\DATA\GROUP\YF123407.D Sample Name: Weinreb S

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

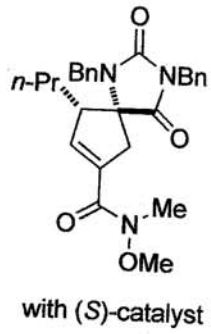
Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.850	BB	0.3304	3104.63135	139.12048	97.0219
2	19.081	MM	0.9713	95.29759	1.63527	2.9781
Totals :				3199.92894	140.75576	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

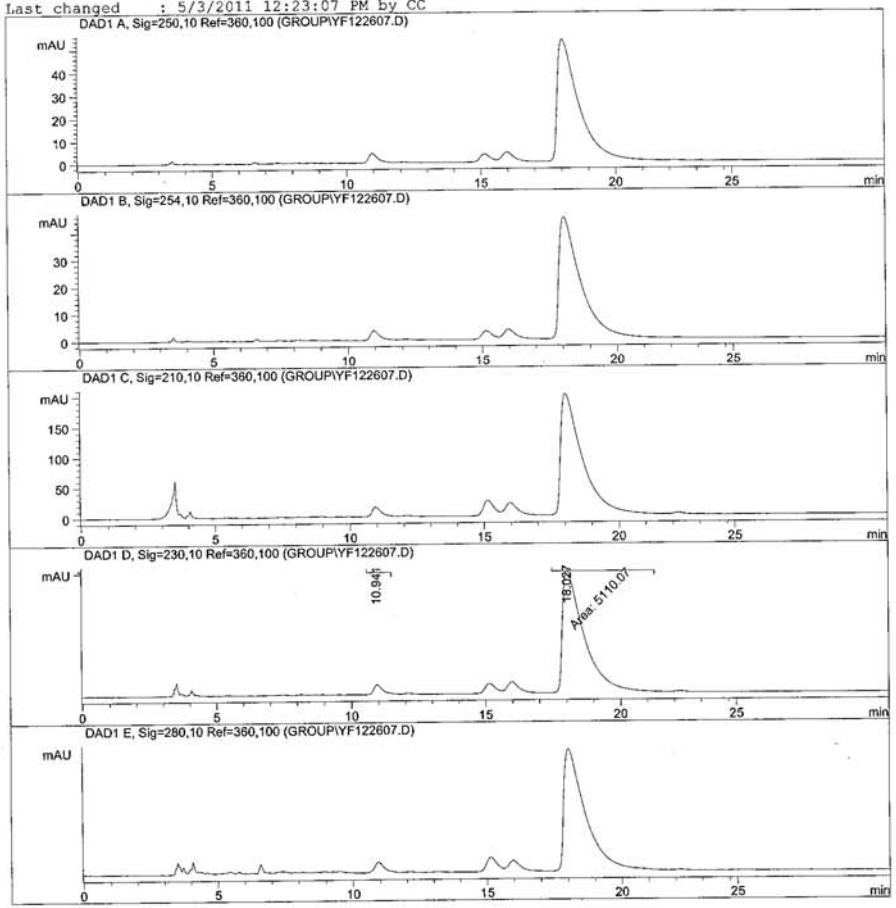
*** End of Report ***



with (*S*)-catalyst

Data File C:\HPCHEM\1\DATA\GROUP\YF122607.D Sample Name: Weinreb F

Injection Date : 5/3/2011 1:11:40 PM Seq. Line : 2
Sample Name : Weinreb R Location : Vial 33
Acq. Operator : NB Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : 15 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\IB-15-30.M
Last changed : 4/7/2011 9:46:30 PM by CC
Analysis Method : C:\HPCHEM\1\METHODS\AS-00730.M
Last changed : 5/3/2011 12:23:07 PM by CC



Data File C:\HPCHEM\1\DATA\GROUP\YF122607.D Sample Name: Weinreb F

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.941	BB	0.3298	157.23886	7.11569	2.9852
2	18.027	MM	0.9154	5110.06934	93.03423	97.0148
Totals :				5267.30820	100.14992	

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

*** End of Report ***

with (*R*)-catalyst