Supporting Information

An In-depth Study on Ring-closing Metathesis of Carbohydrate-derived α-Alkoxyacrylates: Efficient Syntheses of DAH, KDO and 2-Deoxy-β-KDO

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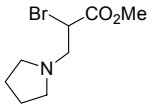
General experimental information

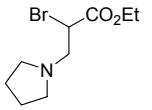
All reactions with air- or moisture-sensitive compounds were performed under an inert atmosphere. Nitrogen and argon were dried over Sicapent, $CaCl_2$ and KOH. CH_2Cl_2 was distilled over CaH_2. THF and Et_2O were distilled over Na. Acetonitrile was distilled and stored on molecular sieves (4 Å). Toluene was distilled over CaH_2 and deoxygenated using the freeze-pump-thaw method. Et_3N was distilled and stored over KOH. All other chemicals were purchased from commercial suppliers and used without further purification. Column chromatography was performed using silica gel (230-400 mesh, 60 Å). ^{1}H and ^{13}C-NMR spectra were recorded on a 200, 300 or 400 MHz spectrometer. Spectra are reported in units of ppm on the δ scale, relative to chloroform (7.25 ppm for ^{1}H-NMR and 77.0 ppm for ^{13}C-NMR). IR measurements were performed on an FTIR spectrometer. 2-Vinylphenol[1] was prepared by a Wittig olefination of salicyl aldehyde, using $Ph_3P{=}CH_2$.

Methyl 2-bromo-3-(pyrrolidin-1-yl)propanoate (4a)



A solution of methyl 2,3-dibromopropanoate (2.01 g, 8.17 mmol) in toluene (130 mL) was cooled to 0 ºC and pyrrolidine (0.68 mL, 8.05 mmol) and Et_3N (1.15 mL, 8.17 mmol) were added. After stirring at 0 ºC for 1 h, the resulting suspension was filtered over Celite, washed with H_2O (25 mL), dried ($MgSO_4$) and concentrated. The resulting crude product was >95% pure according to NMR and therefore directly used in the next step. The yield was 1.72 g (89%). The analytical data were in agreement with those reported earlier.[2] ^{1}H-NMR ($CDCl_3$, 200 MHz): δ 4.33 (dd, J = 6.0, 9.2 Hz, 1H), 3.88 (s, 3H), 3.30 (dd, J = 9.2, 12.9 Hz, 1H), 2.95 (dd, J = 6.0, 12.9 Hz, 1H), 2.72 (m, 4H), 1.84 (m, 4H). ^{13}C-NMR ($CDCl_3$, 300 MHz): δ 169.5, 59.3, 58.2, 54.1, 43.0, 23.6.

Ethyl 2-bromo-3-(pyrrolidin-1-yl)propanoate (4b)

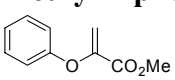


The same procedure was applied as for **4a**, using ethyl 2,3-dibromopropanoate. The crude yield was 1.77 g (92%). ^{1}H NMR ($CDCl_3$, 200 MHz): δ 4.38-4.26 (m, 3H), 3.28 (dd, J = 9.2, 12.7 Hz, 1H), 2.95 (dd, J = 6.0, 12.7 Hz, 1H), 2.62 (m, 4H), 1.76 (m, 4H), 1.37 (t, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.4, 61.8, 59.3, 54.1, 43.0, 23.6, 13.9.

General procedure A for the preparation of α-alkoxyacrylates

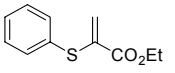
To a cooled (0 ºC) solution of the alcohol (1 equiv) in diethyl ether/DMF (1:1, 0.05M) was added NaH (60% in mineral oil; 2.5 equiv) and the mixture was stirred at 40 ºC for 1 h. After cooling to room temperature, freshly prepared **4a** or **b** (3.5 equiv) was added and the reaction was stirred for 18 h. Next, H_2O was added, the mixture was extracted with diethyl ether (3 ×) and the combined organic layers were concentrated *in vacuo*. The residue was dissolved in (m)ethanol/MeCN (1:1, 0.1M), MeI (10 equiv) and Na_2CO_3 (5 equiv) were added and the reaction mixture was allowed to stir at reflux temperature for 48 h. Next, H_2O was added and the mixture was extracted with CH_2Cl_2 (3 ×). The combined organic layers were dried with $MgSO_4$, concentrated and the product was isolated by column chromatography (EtOAc/heptane, 1:6).

Methyl 2-phenoxyacrylate (9)



This compound was prepared from phenol according to general procedure A. The yield was 62 mg (55%). Analytical data agreed with those reported in literature.[3] ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.32-7.05 (m, 5H), 5.69 (d, J = 2.0 Hz, 1H), 4.88 (d, J = 2.0 Hz, 1H), 3.83 (s, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 162.9, 155.0, 150.4, 129.6, 124.1, 119.1, 103.8, 52.6.

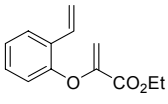
Ethyl 2-(phenylsulfanyl)acrylate (10)



This compound was prepared from thiophenol according to general procedure A. The yield was 26 mg (53%). Analytical data agreed with those reported in literature.[4] ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.45-7.27 (m, 5H), 6.31 (s, 1H), 5.24 (s, 1H), 4.25 (q, J = 7.1

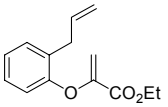
Hz, 2H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 163.9, 138.7, 133.9, 132.8, 129.4, 128.6, 122.3, 61.9, 14.3.

Ethyl 2-(2-vinylphenoxy)acrylate (13)



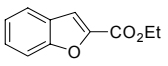
This compound was prepared from 2-vinylphenol according to general procedure A. The yield was 35 mg (61%). ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.57 (d, J = 7.5 Hz, 1H), 7.27-7.12 (m, 2H), 6.98-6.83 (m, 2H), 5.77 (dd, J = 1.1, 17.7 Hz, 1H), 5.57 (d, J = 2.1 Hz, 1H), 5.29 (dd, J = 1.1, 11.0 Hz, 1H), 4.63 (d, J = 2.1 Hz, 1H), 4.30 (q, J = 7.2 Hz, 2H), 1.32 (t, J = 7.2 Hz, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 162.3, 151.7, 150.8, 130.4, 129.5, 128.8, 126.4, 124.8, 120.2, 115.5, 101.8, 61.7, 14.4. HRMS (EI^+): calculated for $C_{13}H_{14}O_3$, $[M]^+$: 218.0943, found: 218.0943.

Ethyl 2-(2-allylphenoxy)acrylate (14)



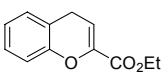
This compound was prepared from 2-allylphenol according to general procedure A. The yield was 7.13 g (78%). ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.26-7.08 (m, 3H), 6.95 (dd, J = 1.4, 7.8 Hz, 1H), 5.94 (m, 1H), 5.57 (d, J = 2.1 Hz, 1H), 5.07 (m, 2H), 4.66 (d, J = 2.1 Hz, 1H), 4.30 (q, J = 7.1 Hz, 2H), 3.36 (d, J = 6.7 Hz, 2H), 1.32 (t, J = 7.1 Hz, 3H).^{13}C-NMR ($CDCl_3$, 75 MHz): δ 162.3, 152.4, 150.7, 136.0, 131.5, 130.3, 127.4, 124.7, 119.7, 116.0, 101.5, 61.6, 34.1, 14.4.HRMS (EI^+): calculated for $C_{14}H_{16}O_3$, $[M]^+$: 232.1100, found: 232.1099.

Ethyl benzofuran-2-carboxylate (15)



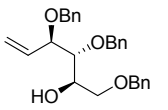
To a solution of **13** (18.5 mg, 84.8 μmol) in toluene (3 mL) was added 5 mol% of (IMes)(PCy_3)Cl_2Ru=CHPh (**A**). The reaction was stirred under an inert atmosphere at 70 ºC for 30 min, followed by removal of the solvent *in vacuo*. The product was purified by column chromatography (EtOAc/heptane, 1:20). The yield was 14.3 mg (89%). Analytical data agreed with those reported in literature.[5] ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.69-7.27 (m, 5H), 4.44 (q, J = 6.9 Hz, 2H), 1.42 (t, J = 6.9 Hz, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 159.3, 155.4, 145.5, 127.3, 126.8, 123.6, 122.6, 113.6, 112.2, 61.6, 14.6.

Ethyl 4*H*-2-chromenecarboxylate (16)



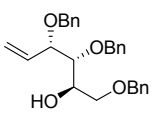
To a solution of **14** (29.7 mg, 128 μmol) in toluene (4 mL) was added 5 mol% of (IMes)(PCy_3)Cl_2Ru=CHPh (**A**). The reaction was stirred under an inert atmosphere at 70 ºC for 30 min, followed by removal of the solvent *in vacuo*. The product was purified by column chromatography (EtOAc/heptane, 1:20). The yield was 24.0 mg (92%).^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.17-6.96 (m, 4H), 6.22 (t, J = 4.1 Hz, 1H), 4.30 (q, J = 7.1 Hz, 2H), 3.55 (d, J = 4.1 Hz, 2H), 1.35 (t, J = 7.1 Hz, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 161.3, 150.8, 141.5, 128.7, 127.7, 123.7, 118.0, 116.9, 110.0, 61.4, 24.7, 14.4. HRMS (EI^+): calculated for $C_{12}H_{12}O_3$, $[M]^+$: 204.0787, found: 204.0787.

(2*R*,3*R*,4*R*)-1,3,4-Tris(benzyloxy)hex-5-en-2-ol (21)



This compound was synthesized according to known procedures, analytical data agreed with those reported in literature.[6] The yield was 856 mg (86%). ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.38-7.23 (m, 15H), 6.00-5.89 (m, 1H), 5.30 (m, 2H), 4.53 (m, 4H), 4.40 (d_{AB}, J = 12.0 Hz, 2H), 4.07 (dd, J = 3.9, 7.2 Hz, 1H), 4.00 (m, 1H), 3.52 (m, 3H), 2.82 (d, J = 4.9 Hz). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 138.0, 137.9, 137.6, 134.9. 128.2 (2), 128.1, 127.9 (2), 127.7, 127.5, 127.4, 118.8, 80.5, 80.2, 74.1, 73.4, 70.9, 70.7, 70.4.

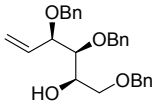
(2*R*,3*R*,4*S*)-1,3,4-Tris(benzyloxy)hex-5-en-2-ol (22)



This compound was synthesized according to known procedures, analytical data agreed with those reported in literature.[7] The yield was 180 mg (28%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.31-7.17 (m, 15H), 5.99-5.87 (m, 1H), 5.34 (m, 2H), 4.64-4.48 (m, 4H), 4.57 (d_{AB}, J = 11.7 Hz, 2H), 4.14 (dd, J = 3.9, 7.8 Hz, 1H), 3.87-3.78 (m, 1H), 3.70 (m, 1H),

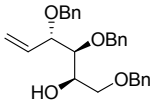
3.61 (m, 2H), 2.67 (d, J = 4.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 138.2(2), 137.8, 134.9, 128.2, 128.1(3), 127.9, 127.6, 127.5, 127.4(2), 127.3, 119.5, 82.0, 80.9, 74.1, 73.4, 70.8, 70.4.

(2*R*,3*S*,4*R*)-1,3,4-Tris(benzyloxy)hex-5-en-2-ol (23)



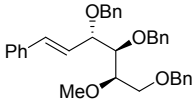
This compound was synthesized according to known procedures, analytical data agreed with those reported in literature.[8] The yield was 281 mg (46%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.35-7.18 (m, 15H), 5.96 (m, 1H), 5.36 (m, 2H), 4.70-4.52 (m, 4H), 4.52 (d_{AB}, J = 11.5 Hz, 2H), 4.09 (dd, J = 3.9, 7.8 Hz, 1H), 3.77-3.57 (m, 4H), 2.83 (br d, J = 5.7 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 138.2, 138.0(2), 135.4, 128.2(2), 128.1(2), 127.8, 127.5(3), 127.4, 119.5, 81.4, 80.6, 79.6, 74.4, 73.2, 71.1, 70.3.

(2*R*,3*S*,4*S*)-1,3,4-Tris(benzyloxy)hex-5-en-2-ol (24)



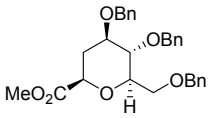
This compound was synthesized according to known procedures, analytical data agreed with those reported in literature.[6] The yield was 271 mg (75%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.31-7.16 (m, 15H), 5.85 (m, 1H), 5.35 (m, 2H), 4.63-4.39 (m, 4H), 4.61 (d_{AB}, J = 11.4 Hz,, 2H), 4.08 (dd, J = 6.6, 7.5 Hz, 1H), 3.91 (m, 1H), 3.60 (dd, J = 2.6, 6.5 Hz, 1H), 3.41 (dd, J = 3.3, 6.0 Hz, 2H), 2.42 (d, J = 6.8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 138.1(2), 137.8, 135.0, 128.2, 128.1, 128.0(2), 127.7(2), 127.6, 127.5, 127.3, 119.2, 82.1, 80.2, 75.0, 73.3, 71.2, 70.7, 70.0.

((2*R*,3*R*,4*S*,*E*)-2-Methoxy-6-phenylhex-5-ene-1,3,4-triyl)tris(oxy)tris(methylene)-tribenzene (36)



To a solution of **35**[9] (4.4 mg, 10.2 μmol) in toluene (1 mL) was added (IMes)(PCy_3)Cl_2Ru=CHPh (**A**, 8.7 mg, 1.0 equiv) and the mixture was stirred under an inert atmosphere at 80 °C for 18 h. The reaction was exposed to air and the solvent was removed *in vacuo*. The product was purified by column chromatography (EtOAc/heptane, 1:10). The isolated yield of **36** was 74%. ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.40-7.23 (m, 20H), 6.61 (d, J = 16.2 Hz, 1H), 6.19 (dd, J = 8.2, 16.2 Hz), 4.88-4.61 (m, 3H), 4.39 (m, 3H), 4.27 (m, 1H), 3.71 (d, J = 6.2 Hz, 1H), 3.53 (m, 3H), 3.38 (s, 3H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 138.8, 138.5, 138.1, 136.5, 133.7, 128.6, 128.5, 128.3 (2), 128.2, 128.0, 127.9, 127.8, 127.6, 127.5, 127.1, 126.6, 81.9, 81.5, 80.1, 75.3, 73.3, 70.7, 69.2. $[\alpha]^{22}_D$ = +10.3 (*c* 0.3, $CHCl_3$). HRMS (CI^+): calculated for $C_{34}H_{37}O_4$, [M^++H]: 509.2692, found: 509.2708.

(2*R*,4*R*,5*S*,6*R*)-Methyl 4,5-di(benzyloxy)-6-[(benzyloxy)methyl]tetrahydro-2*H*-pyran-2-carboxylate (37)



A solution of **29a** (63 mg, 0.129 mmol) in EtOAc/MeOH/Et_3N (50:50:1; 10 ml) was treated with 10% Pd/C (20 mg) and H_2 (1 atm) for 1 h. The mixture was filtered over Celite, concentrated *in vacuo* and the product was purified by column chromatography (EtOAc/heptane, 1:4). The yield was 60 mg (95%). The analytical data agreed with those reported in literature.[10] ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.36-7.17 (m, 15H), 4.90-4.53 (m, 6H), 4.01 (dd, J = 2.0, 12.1 Hz, 1H), 3.80 (s, 3H), 3.78-3.65 (m, 3H), 3.55-3.45 (m, 2H), 2.49 (ddd, J = 2.0, 4.9, 12.8 Hz, 1H), 1.71 (q, J = 12.2 Hz, 1H). ^{13}C-NMR ($CDCl_3$, 75 MHz): δ 170.0, 138.0, 128.2, 128.1 (2), 127.8, 127.7, 127.5 (2), 127.4, 127.3, 80.5, 79.3, 77.8, 75.1, 74.4, 73.4, 71.5, 69.1, 52.4, 34.0. $[\alpha]^{22}_D$ = +10.6 (*c* 0.5, CH_2Cl_2).

References for experimental section:

(1) Bettach, N.; Le Bigot, Y.; Mouloungui, Z.; Delmas, M.; Gaset, A. *Synth. Commun.* **1992**, *22*, 513.

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(3) Campbell, M.; McLeish, M. J.; Lynch, D. E.; Smith, G.; Byriel, K. A.; Kennard, C. H. L. *Aust. J. Chem.* **1992**, 45, 2061.

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(5) Ashram, M. *J. Chem. Soc. Perkin Trans. 2* **2002**, *10*, 1662.

(6) Pearson, W. H.; Hines, J. V. *J. Org. Chem.* **2000**, *65*, 5785.

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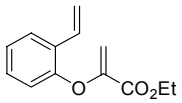
(9) Compound **35** was synthesized by reacting **28** with NaH and MeI in DMF.

(10) Barnes, N. J.; Probert, M. A.; Wightman, R. H. *J. Chem. Soc. Perking Trans. 1* **1996**, 431.

NMR spectra



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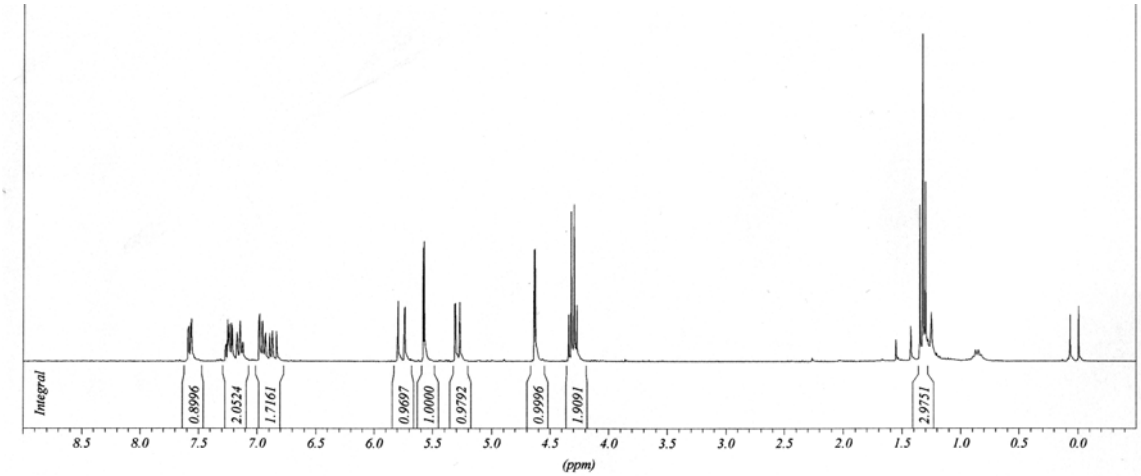

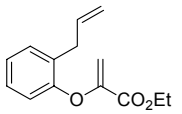

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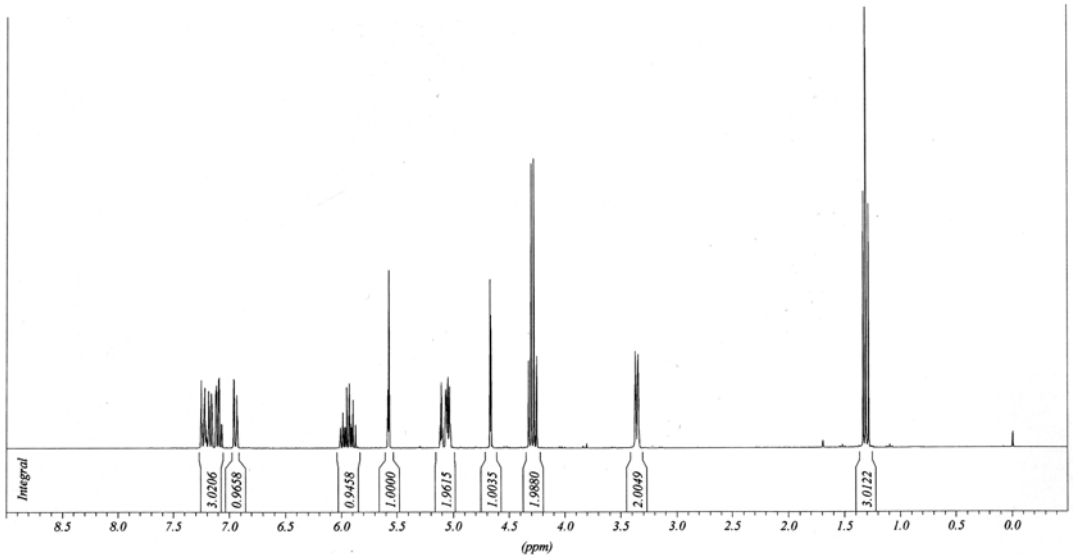

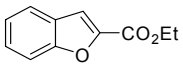
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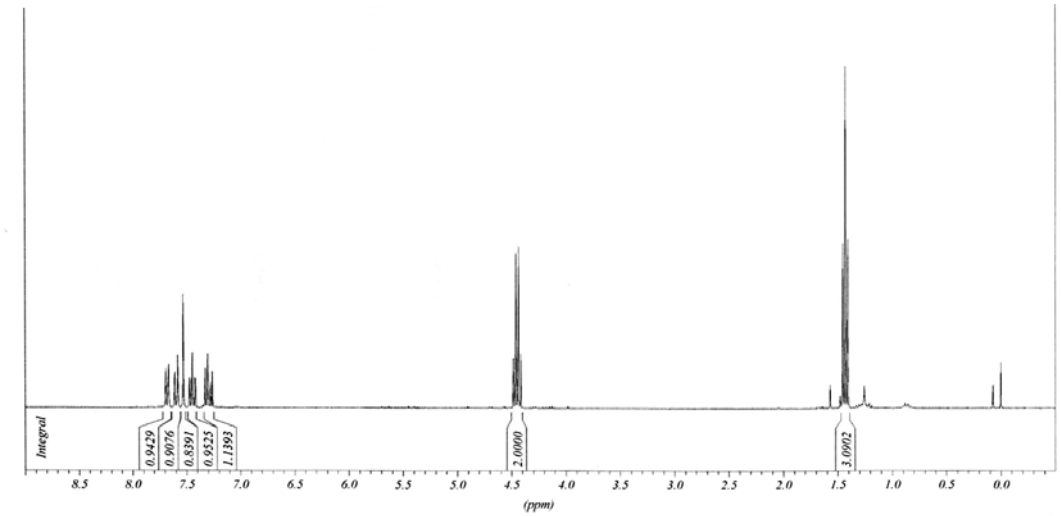
O

15


Integral
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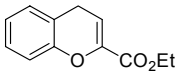
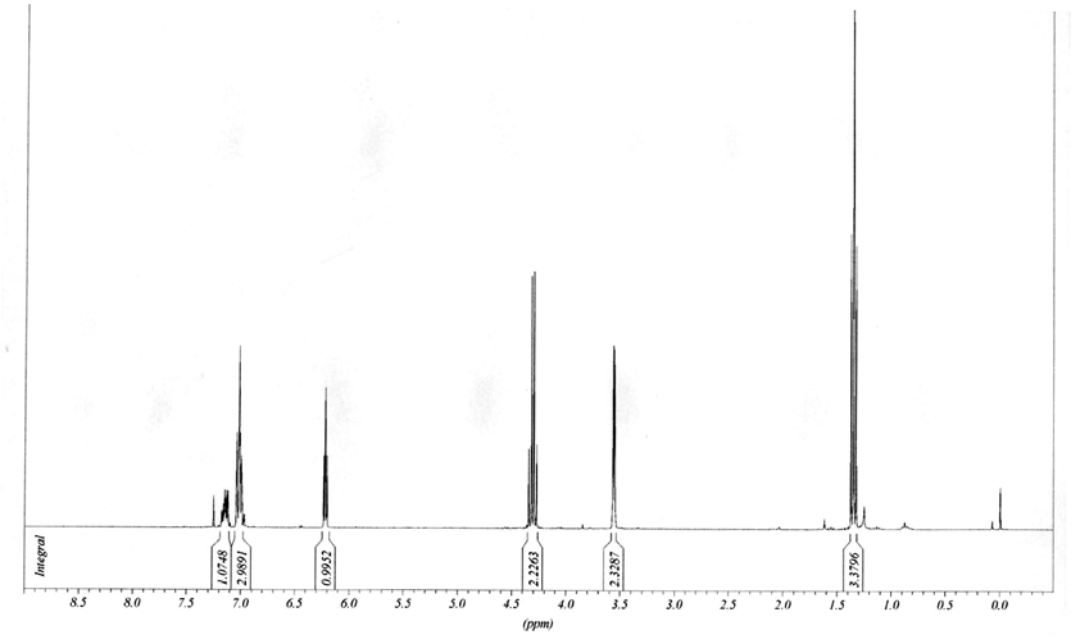
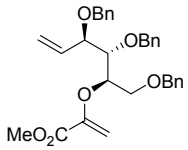
3.0992
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

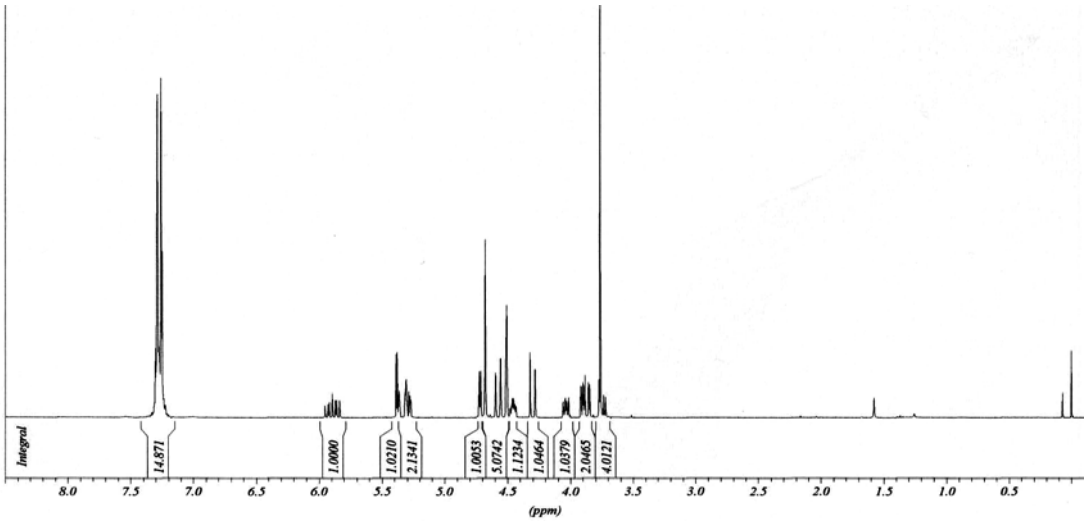

O
CO2Et

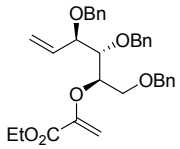
16


Integral
1.0748
2.9891
0.9952
2.2263
2.3287
3.3796
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

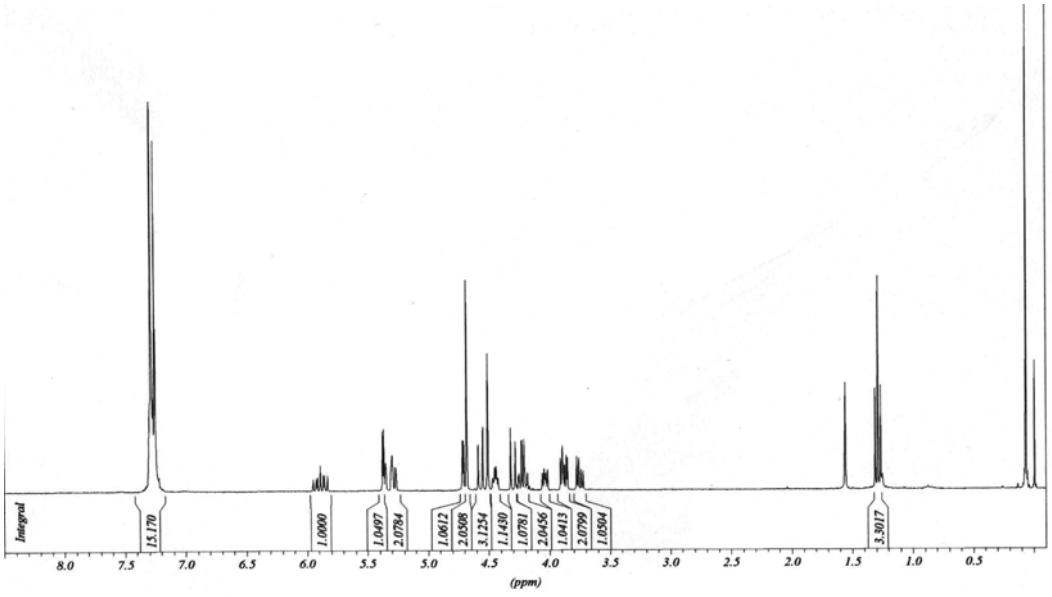

OBn
OBn
OBn
O
MeO2C

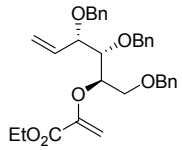
25a


Integral
14.871
1.0000
1.0210
2.1341
1.0053
5.0742
1.1234
1.0464
1.0379
2.0465
4.0121
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

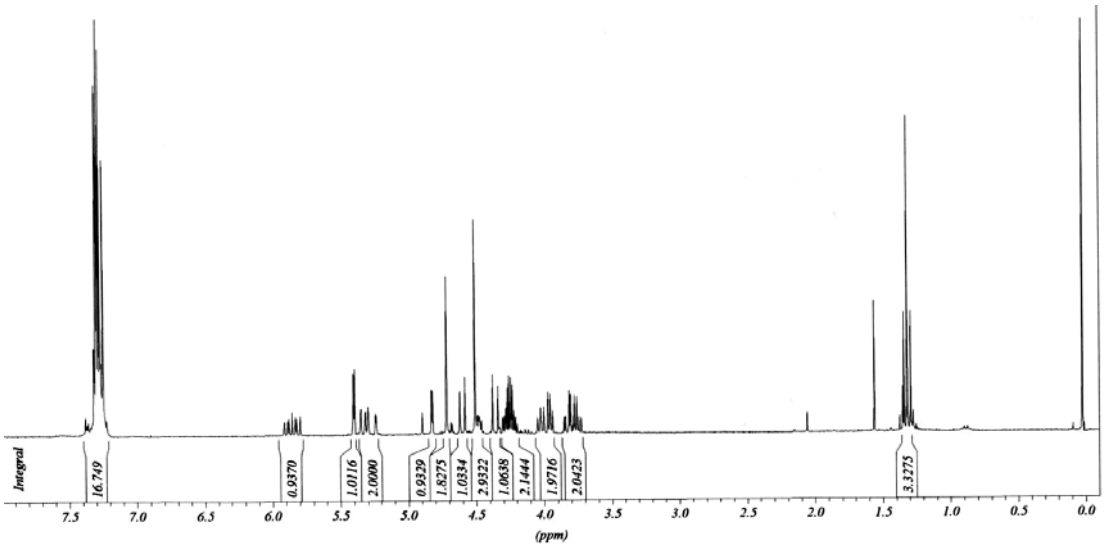

OBn
OBn
OBn
O
EtO2C

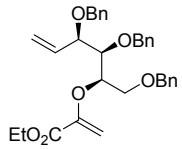
25b


Integral
15.170
1.0000
1.0497
2.0784
1.0612
2.0308
3.1254
1.1430
1.0781
2.0456
1.0413
2.0799
1.0504
5.3017
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

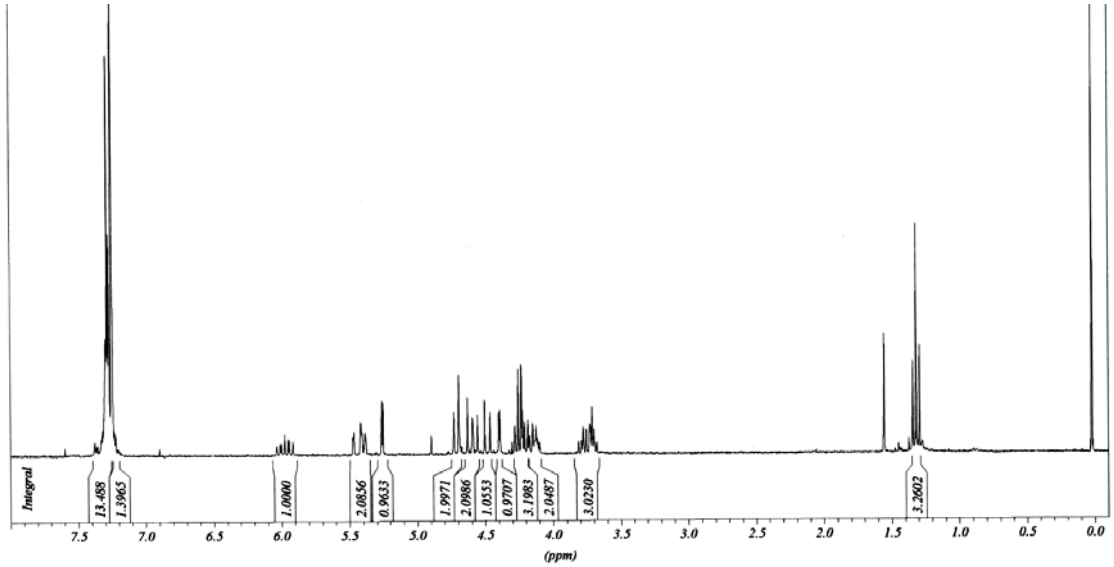

OBn
OBn
OBn
O
EtO2C

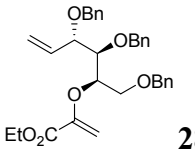
26


Integral
16.749
0.9370
1.0116
2.0000
0.9339
1.8275
1.0334
2.9322
1.0638
2.1444
1.9716
2.0423
3.3275
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

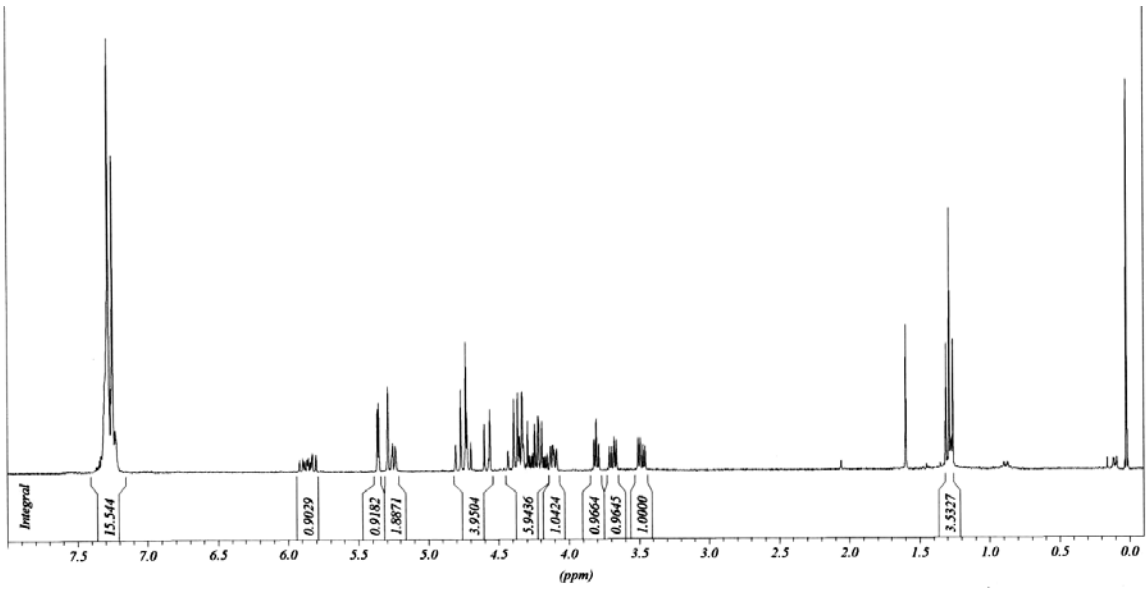

OBn
OBn
OBn
O
EtO2C

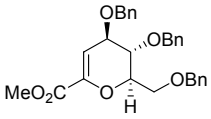
27


Integral
13.488
1.3965
1.0000
2.0856
0.9633
1.9971
2.0986
1.0553
0.9707
3.1983
2.0487
3.0230
3.2602
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

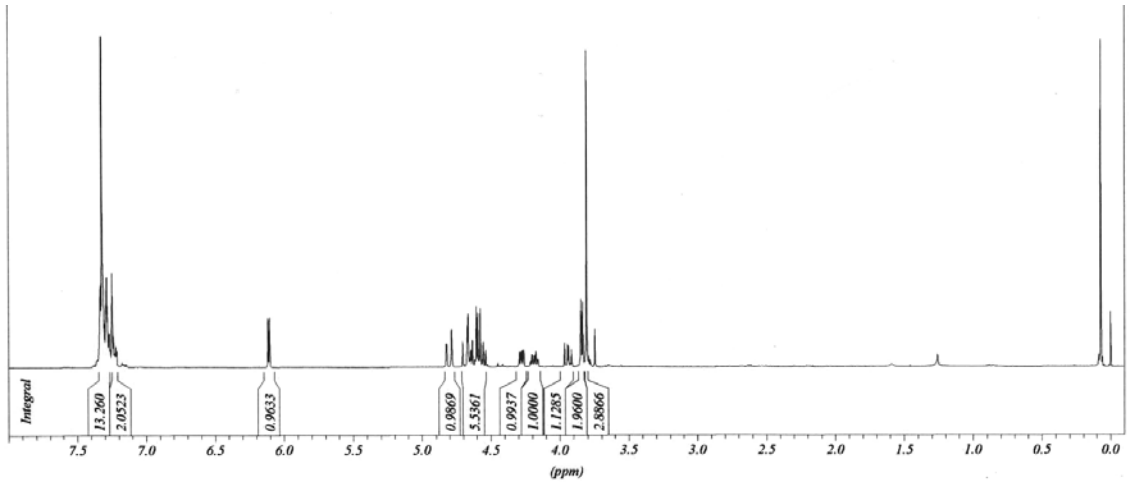

OBn
OBn
OBn
O
EtO2C

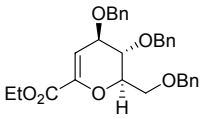
28


Integral
15.544
0.9029
0.9182
1.5871
3.9504
5.9436
1.0424
0.9664
0.9645
1.0000
3.5327
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

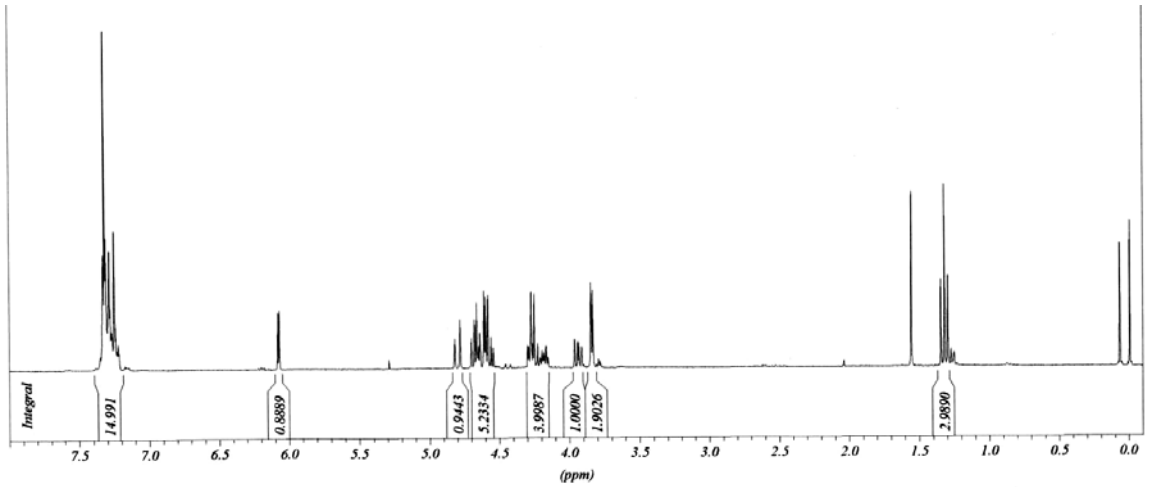

OBn
OBn
OBn
MeO2C
O
H

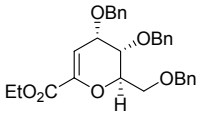
29a


Integral
13.260
2.0523
0.9633
0.9869
5.5361
0.9937
1.0000
1.1285
1.9600
2.8866
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

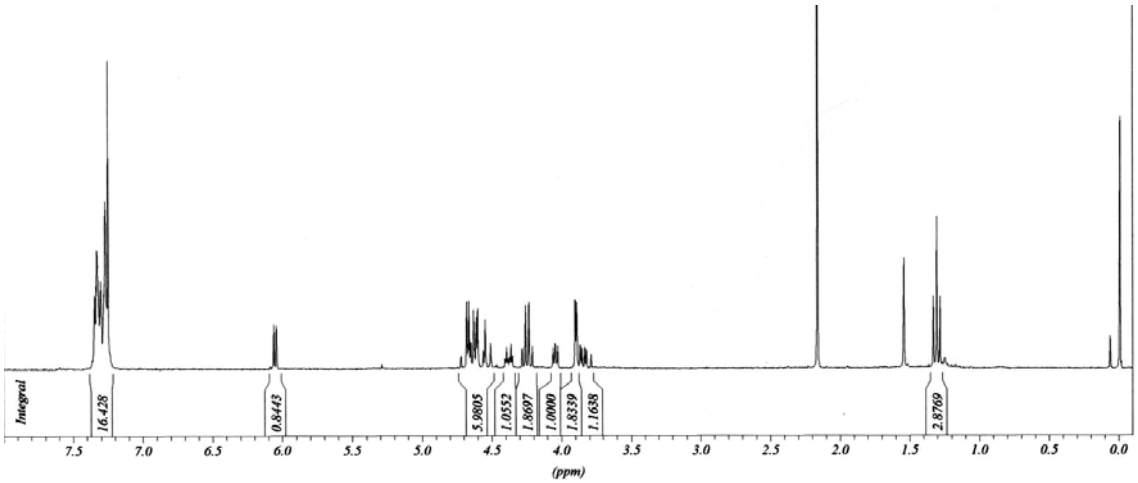

OBn
OBn
OBn
EtO2C
O
H

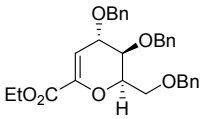
29b


Integral
14.991
0.8889
0.9443
5.2334
3.9987
1.0000
1.9026
2.9890
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

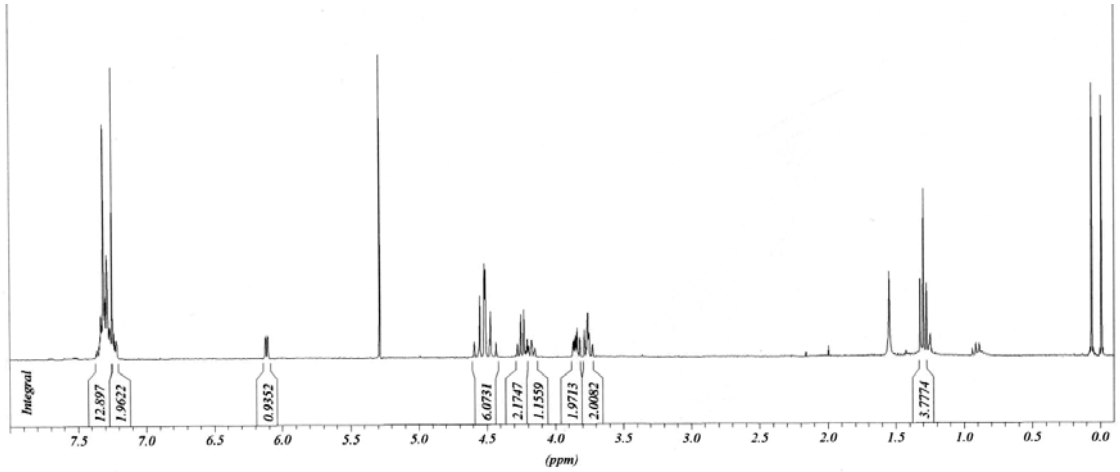

OBn
OBn
OBn
EtO2C
O
H

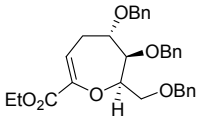
30


Integral
16.428
0.8443
5.9805
1.0552
1.8697
1.0000
1.8339
1.1638
2.8769
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

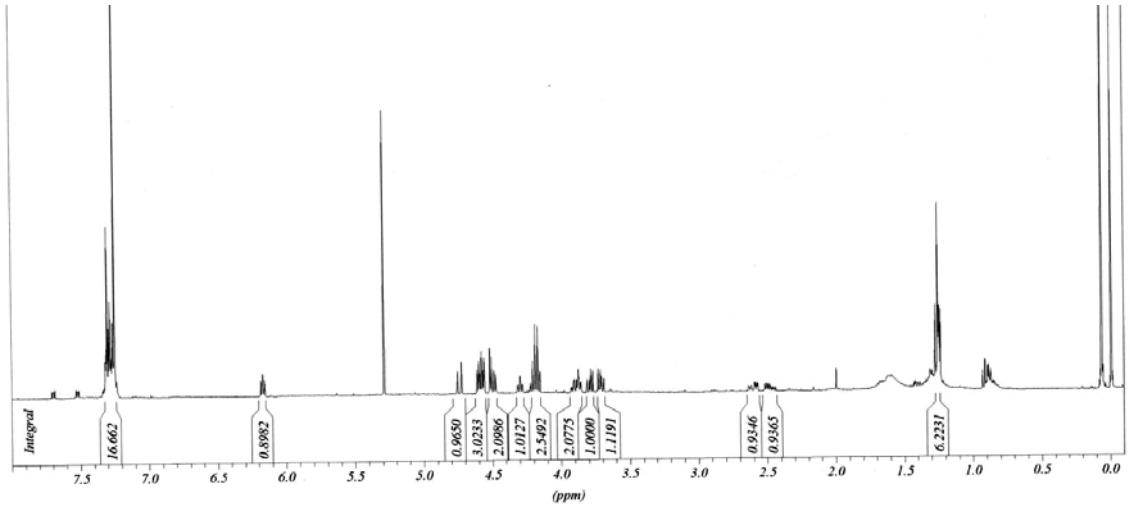

OBn
OBn
OBn
EtO2C
O
H

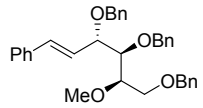
32


Integral
12.897
1.9622
0.9352
6.0731
2.1747
1.1559
1.9713
2.0082
3.7774
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

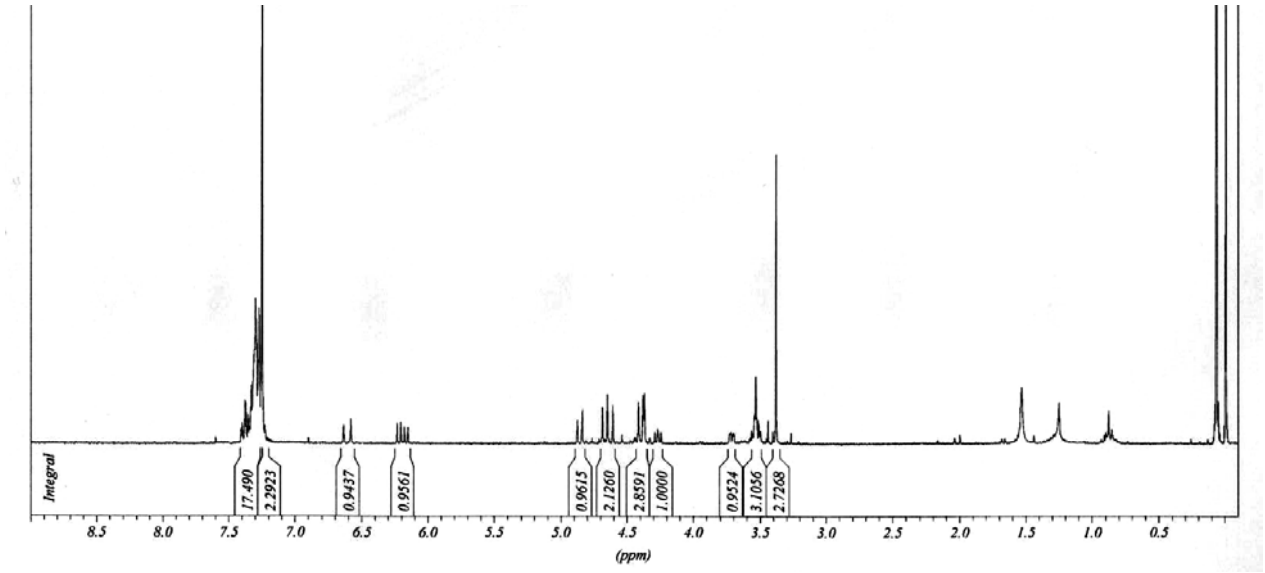

OBn
OBn
OBn
EtO2C
O
H

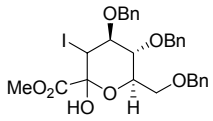
33


Integral
16.662
0.8982
0.9650
3.0233
2.0986
1.0127
2.5492
2.0775
1.0000
1.1191
0.9346
0.9365
6.2231
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


OBn
Ph
OBn
MeO
OBn

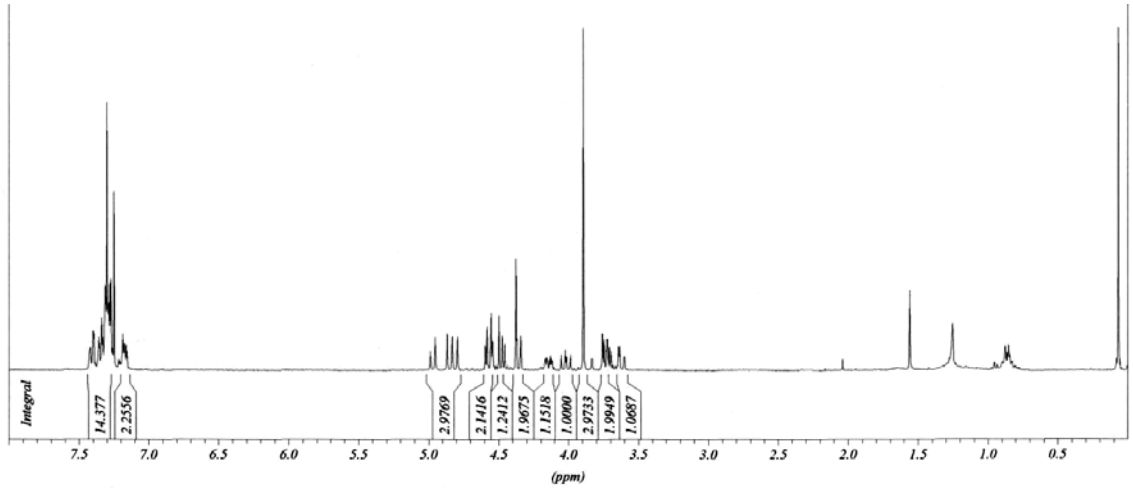
36


Integral
17.490
2.2923
0.9437
0.9561
0.9615
2.1260
2.8591
1.0000
0.9524
3.1056
2.7268
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

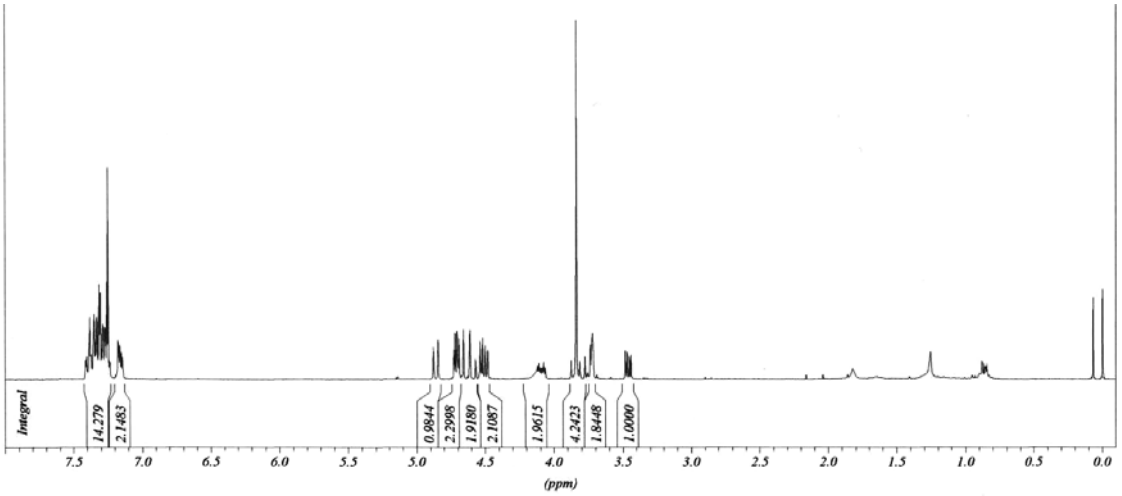


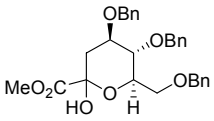
38

first diastereoisomer

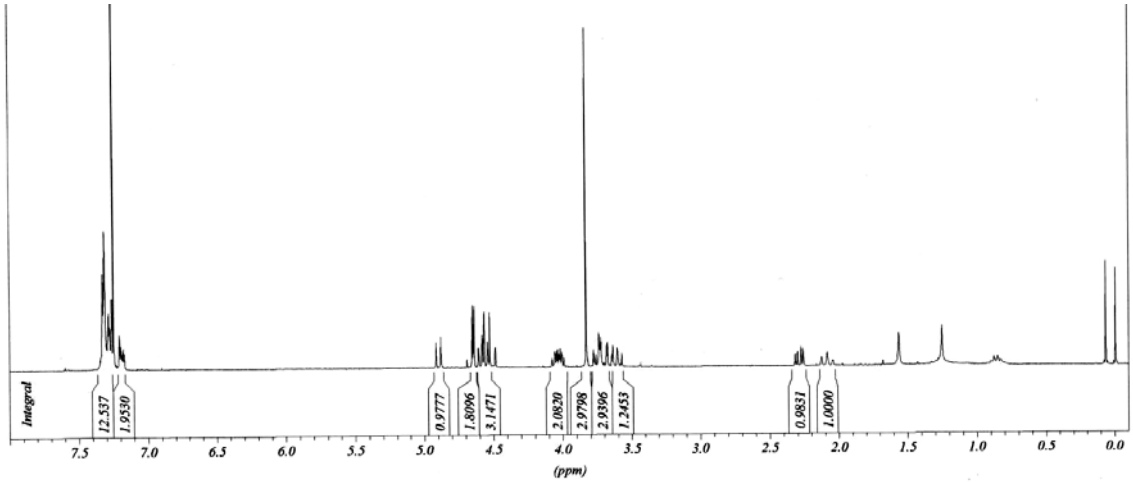


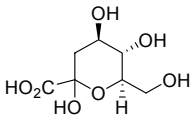
second diastereoisomer:



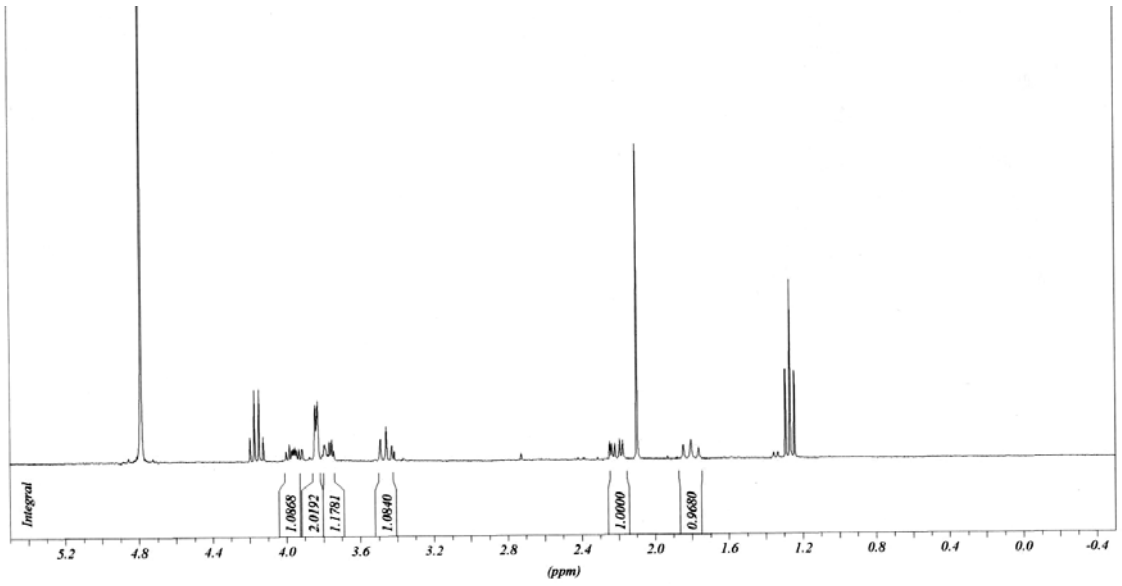

OBn
OBn
OBn
MeO2C
HO
O
H

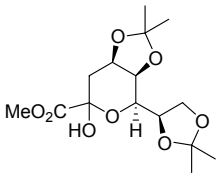
39


Integral
12.537
1.9530
0.9777
1.8096
3.1471
2.0820
2.9798
2.9396
1.2453
0.9831
1.0000
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

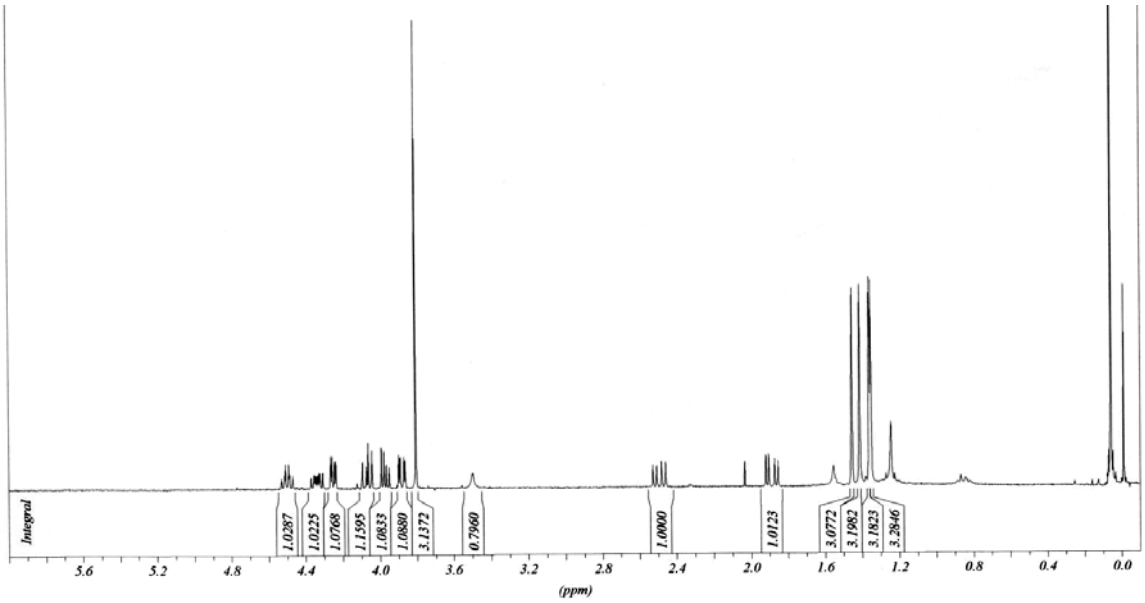

OH
OH
OH
HO2C
HO
O
H

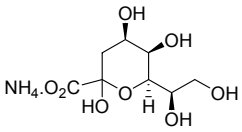
1


Integral
1.0868
2.0192
1.1781
1.0840
1.0000
0.9680
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
-0.4
(ppm)

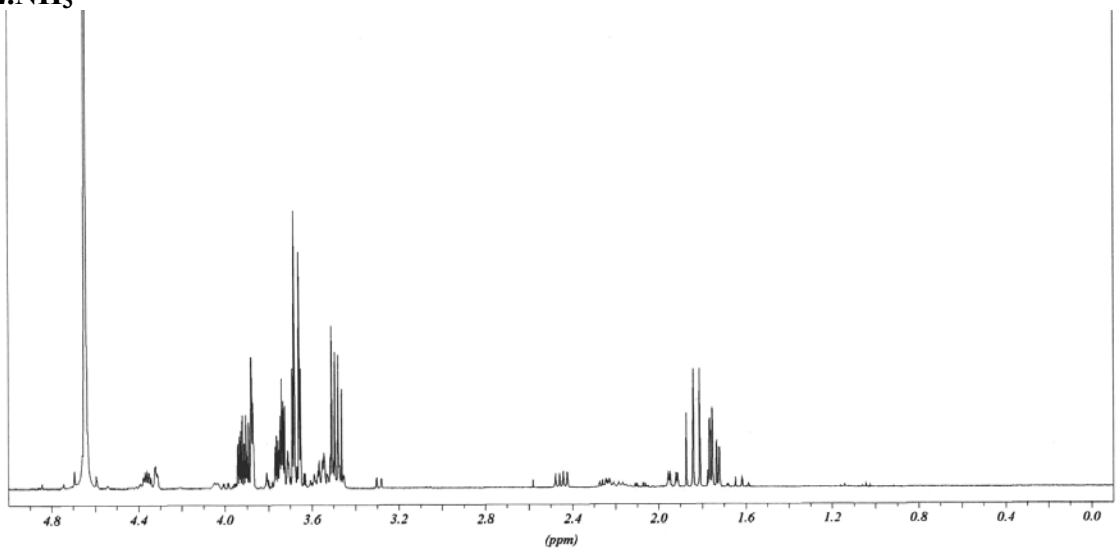


41


Integral
1.0287
1.0225
1.0768
1.1595
1.0833
1.0880
3.1372
0.7960
1.0000
1.0123
3.0772
3.1982
3.1823
3.2846
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
(ppm)



2.NH_3


4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
(ppm)