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ELECTRONIC SUPPLEMENTARY INFORMATION

A quantitative structure-reactivity relationship in *N*-acetyl oxazolidines: an electrostatic interaction controls rotamer population

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Figure S1. Hammett plot for compounds **1-10**

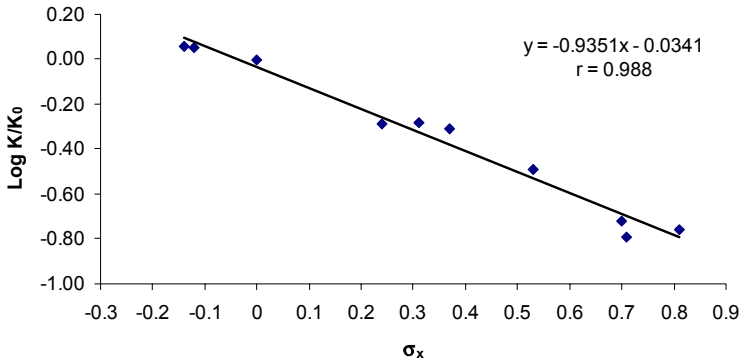


Figure S2. Hammett plot for compounds **13-22**

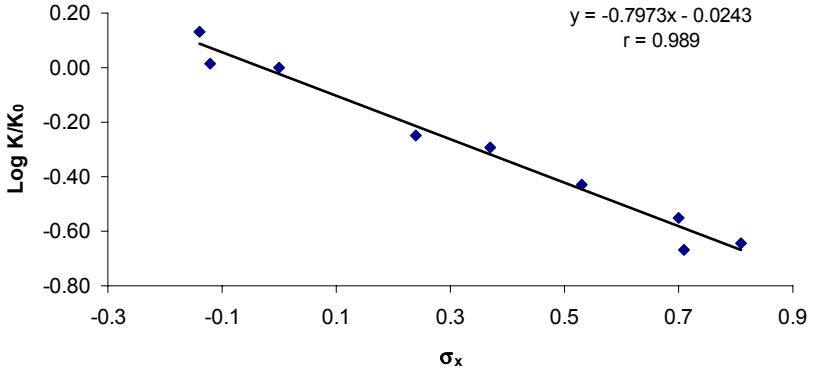


Figure S3. Hammett plot for compounds **25-34**

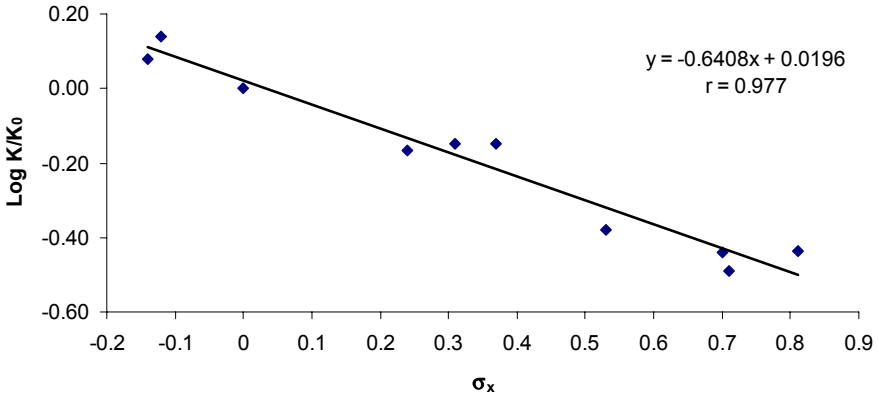


Figure S4. Hammett plot for theoretical calculation.

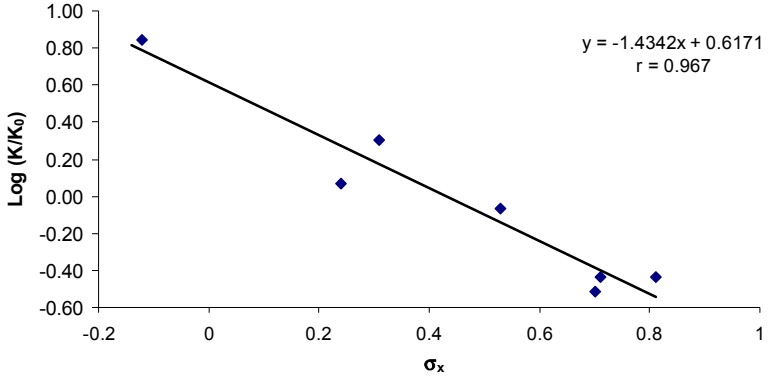


Figure S5. Hammett plot for d_1 versus σ_x

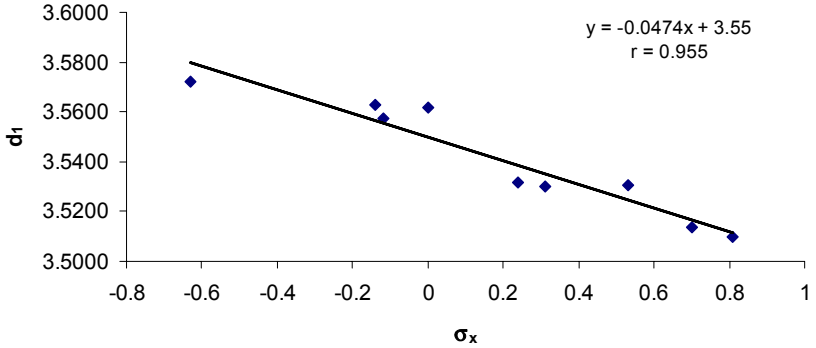


Figure S6. Hammett plot for d_2 versus σ_x

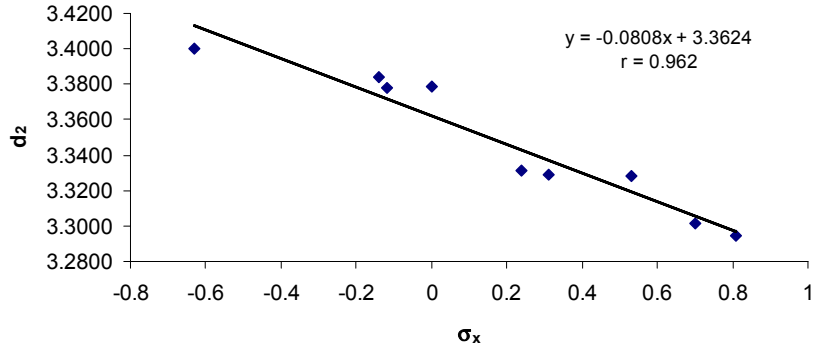


Table S1. Electronic parameters calculated for compounds **1**, **3**, **4**, **7**, and **9**.

Comp.	X	q_O [a]	q_{C1} [a]	F[b] ($x10^{10}$)	E[c] ($x10^{20}$)	σ_x [d]
1	4-NO_2	-0.503	0.133	-1.281	-4.447	0.81
3	4-CN	-0.503	0.129	-1.256	-4.335	0.70
4	4-CF_3	-0.504	0.126	-1.205	-4.201	0.53
7	4-Cl	-0.505	0.119	-1.157	-4.005	0.24
9	4-MeO	-0.507	0.120	-1.165	-4.044	-0.12

[a]In atomic units. [b]In Newtons. [c]In Joules. [d]Reference 11.

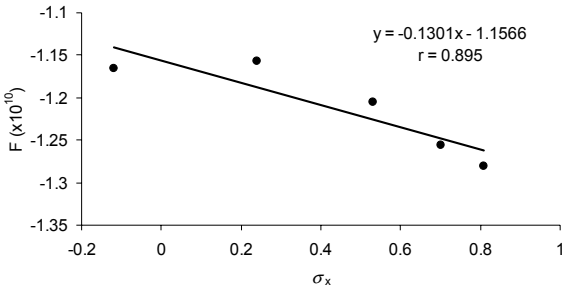


Fig. S7

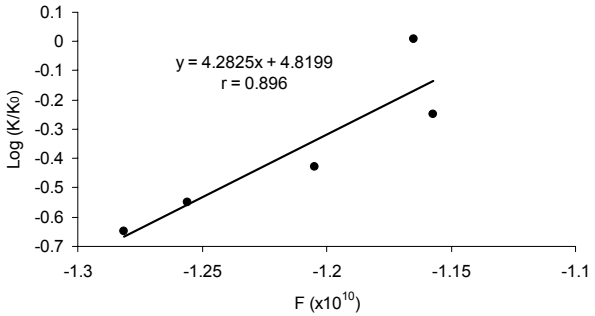


Fig. S8

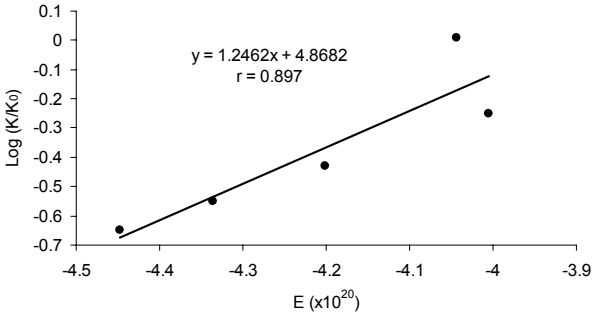


Fig. S9

Experimental

1-(4-Cyanobenzylidene)amino-1-deoxy-D-glucitol (3a)

Method A (77%); mp 164-165ºC; $[\alpha]_D^{25}$ +3; $[\alpha]_{578}^{25}$ +5; $[\alpha]_{546}^{25}$ +7 (*c* 0.5, pyridine); IR (KBr) ν_{max}/cm^{-1} 3500-3000 (OH), 1650 (C=N, arom), 1101, 1038, 1014 (C-O). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (1H, s, CH=N), 7.92 (4H, s, H-arom), 4.73 (1H, d, $J_{C2,OH}$ = 4.4 Hz, OH-2), 4.51 (2H, m, OH), 4.36 (2H, m, OH), 3.88 (1H, s, H-2), 3.85 (1H, s, H-1), 3.71 (1H, t, $J_{2,3} = J_{3,4}$ = 4.4 Hz, H-3), 3.59 (2H, m, H-6´, H-1´), 3.51 (2H, m, H-5, H-4), 3.41 (1H, dd, $J_{6,OH}$ = 5.2 Hz, $J_{6,6'}$ = 11.2 Hz, H-6´). ^{13}C NMR (100 MHz, DMSO-d_6): 161.1 (C=N), 140.6, 133.1, 128.9, 119.1, 113.1 (C-arom), 72.7 (C-2), 72.3 (C-4), 72.0 (C-5), 70.4 (C-3), 64.1 (C-6), 64.0 (C-1). Anal. calcd. for $C_{14}H_{18}N_2O_5$ (294.30): C, 57.13; H, 6.16; N, 9.52. Found: C, 57.40; H, 6.20; N, 9.46.

1-Deoxy-1-(4-trifluoromethylbenzylidene)amino-D-glucitol (4a)

Method A (74%); mp 152-153ºC; $[\alpha]_D^{22}$ +7; $[\alpha]_{578}^{22}$ +9; $[\alpha]_{546}^{22}$ 11 (*c* 0.5, pyridine); IR (KBr) ν_{max}/cm^{-1} 3500-3100 (OH), 1649 (C=N), 1582 (arom), 1131, 1113, 1074 (C-O). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.41 (1H, s, CH=N), 7.95 (2H, d, *J* = 8.0 Hz, H-arom), 7.81 (2H, d, *J* = 8.4 Hz, H-arom), 4.73 (1H, d, $J_{C2,OH}$ = 4.8 Hz, OH-2), 4.52 (2H, d, *J* = 4.4 Hz, OH), 4.36 (2H, m, OH), 3.86 (2H, m, H-2, H-1), 3.71 (1H, t, $J_{2,3} = J_{3,4}$ = 4.8 Hz, H-3), 3.57 (2H, m, H-6´, H-1´), 3.52 (2H, m, H-5, H-4), 3.41 (1H, dd, $J_{6,OH}$ = 5.4 Hz, $J_{6,6'}$ = 10.8 Hz, H-6´). ^{13}C NMR (100 MHz, DMSO-d_6): 161.2 (C=N), 142.9, 140.3, 130.8, 128.9, 126.0 (C-arom), 123.2 (CF_3), 72.8 (C-2), 72.4 (C-4), 72.0 (C-5), 70.4 (C-3), 64.0 (C-6), 63.9 (C-1). Anal. calcd. for $C_{14}H_{18}F_3NO_5$ (337.29): C, 49.85; H, 5.38; N, 4.15. Found: C, 49.60; H, 5.36; N, 4.08.

(2*R*,5*S*)-3-Acetyl-2-(4-cyanophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (3*E*,*Z*)

(92%). Recrystallized from ethanol, mp 151-152ºC; $[\alpha]_D^{23}$ -29; $[\alpha]_{578}^{23}$ -31; $[\alpha]_{546}^{23}$ -36; $[\alpha]_{436}^{23}$ -70 (*c* 0.5, chloroform); IR (KBr) ν_{max}/cm^{-1} 1744 (C=O), 1663 (C=O, amide), 1214 (C-O-C, ester), 1083, 1033 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (4H, m, H-arom), 6.29 (1H, s, H-2$_Z$), 6.04 (1H, s, H-2$_E$), 5.40 (4H, m, H-1´$_E$, H-2´$_E$, H-1´$_Z$, H-2´$_Z$), 5.16 (1H, m, H-3'$_Z$), 5.12 (1H, m, H-3'$_E$), 4.31 (1H, dd, $J_{4a,5}$ = 5.0 Hz, $J_{4b,5}$ = 10.2 Hz, H-5$_Z$), 4.27 (1H, dd, $J_{3',4''}$ = 2.4 Hz, $J_{4',4''}$ = 9.6 Hz, H-4´$_Z$), 4.20 (1H, dd, $J_{3',4''}$ = 4.0 Hz, $J_{4',4''}$ = 12.6 Hz, H-4´´$_Z$), 4.33-4.13 (4H, m, H-4´$_E$, H-4´´$_E$, H-5$_E$, H-4$_{a,E}$), 3.97 (1H, dd, $J_{4a,5}$ = 5.8 Hz, $J_{4a,4b}$ = 10.2 Hz, H-4$_{a,Z}$), 3.36 (1H, t, $J_{4b,4a}$=$J_{4b,5}$ = 10.2 Hz, H-4$_{b,Z}$), 3.22 (1H, t, $J_{4b,4a}$=$J_{4b,5}$ = 9.6 Hz, H-4$_{b,E}$), 2.16-2.00 (9X3H, s, CH_3), 1.81 (3H, s, CH_3, AcN *E* isomer). ^{13}C NMR (100 MHz, $CDCl_3$): 170.5,

170.2, 169.8 (C=O), 168.4 (N-*C*=O), 143.7 (C-arom), 132.8 (2C, C-arom, *E*), 132.1 (2C, C-arom, *Z*), 127.8 (2C, C-arom, *Z*), 127.4 (2C, C-arom, *E*), 118.6 (C-arom), 112.6 (C-arom), 89.3 (C-2_E), 88.3 (C-2_Z), 77.3 (C-5_E), 77.2 (C-5_Z), 69.1 (C-$2'_E$), 69.0 (C-$2'_Z$), 68.8 (C-$1'_E$), 68.7 (C-$1'_Z$), 67.9 (C-$3'_Z$ and C-$3'_E$), 61.5 (C-$4'_Z$ and C-$4'_E$), 47.6 (C-4_Z), 46.5 (C-4_E), 23.2 (CH_3, Ac-N *Z* isomer), 22.8 (CH_3, Ac-N *E* isomer), 20.9, 20.8, 20.7, 20.6 (CH_3, acetates). Anal. calcd. for $C_{24}H_{28}N_2O_{10}$ (504.49): C, 57.14; H, 5.59; N, 5.55. Found: C, 57.08; H, 5.68; N, 5.38.

(2*R*,5*S*)-3-Acetyl-2-(4-trifluoromethylphenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (4*E*,*Z*)

(50%); Recrystallized from ethanol, mp 159-160ºC; $[\alpha]_D^{24}$ -15; $[\alpha]_{578}^{24}$ -17; $[\alpha]_{546}^{24}$ -19; $[\alpha]_{436}^{24}$ -40; (*c* 0.5, chloroform); IR (KBr) ν_{max}/cm^{-1} 1750 (C=O), 1655 (C=O, amide), 1228 (C-O-C, ester), 1110, 1066, 1030 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (1H, d, J = 8.0 Hz, H-arom), 7.62 (2H, m, H-arom), 7.48 (1H, m, J = 7.6 Hz, H-arom), 6.30 (1H, s, H-2_Z), 6.04 (1H, s, H-2_E), 5.43 (1H, m, H-$2'_E$), 5.42 (1H, m, H-$2'_Z$), 5.40 (1H, m, H-$1'_Z$), 5.31 (1H, m, H-$1'_E$), 5.15 (1H, m, H-$3'_E$), 5.09 (1H, m, H-$3'_E$), 4.40-4.16 (7H, m, H-5_Z, H-5_E, H-$4_{a,E}$, H-$4'_Z$, H-$4'_E$, H-$4''_Z$, H-$4''_E$), 3.95 (1H, dd, $J_{4a,4b}$ = 10.2 Hz, $J_{4a,5}$ = 5.8 Hz, H-$4_{a,Z}$), 3.37 (1H, t, $J_{4b,4a}$=$J_{4b,5}$ = 10.2 Hz, H-$4_{b,Z}$), 3.23 (1H, t, $J_{4b,4a}$=$J_{4b,5}$ = 10.2 Hz, H-$4_{b,E}$), 2.10, 2.09, 2.07, 2.00 (9x3H, s, CH_3), 1.79 (3H, s, CH_3, AcN *E* isomer). ^{13}C NMR (100 MHz, $CDCl_3$): 170.6, 170.3, 170.2, 169.8 (C=O), 168.3 (N-*C*=O, *Z*), 168.0 (N-*C*=O, *E*), 142.6 (C-arom, *Z*), 142.1 (C-arom, *E*), 130.8, 127.4, 126.0, 125.2 (C-arom, *Z* and *E*), 89.5 (C-2_E), 88.5 (C-2_Z), 77.3 (C-5_Z and C-5_E), 69.1 (C-$2'_E$), 69.0 (C-$2'_Z$), 68.6 (C-$1'_Z$), 68.5 (C-$1'_E$), 68.1 (C-$3'_E$), 68.0 (C-$3'_Z$), 61.5 (C-$4'_Z$ and C-$4'_E$), 47.6 (C-4_Z), 46.5 (C-4_E), 23.3 (CH_3, Ac-N *Z* isomer), 22.8 (CH_3, Ac-N *E* isomer), 20.9, 20.8, 20.7, 20.6 (CH_3, acetates). Anal. calcd. for $C_{24}H_{28}NO_{10}$ (547.48): C, 52.65; H, 5.15; N, 2.56. Found: C, 52.52; H, 5.30; N, 2.62.

(2*R*,5*S*)-3-Acetyl-2-(4-cyanophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (27*E*,*Z*)

(90%); Recrystallized from ethanol, mp 171-172ºC; $[\alpha]_D^{22}$ -20; $[\alpha]_{578}^{22}$ -21; $[\alpha]_{546}^{22}$ -25; $[\alpha]_{436}^{22}$ -50; (*c* 0.5, pyridine); IR (KBr) ν_{max}/cm^{-1} 3400-3200 (OH), 1636 (C=O, arom), 1208 (C-N), 1115, 1075 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (2H, d, J = 8.0 Hz, H-arom, *E*), 7.83 (2H, d, J = 8.0 Hz, H-arom, *Z*), 7.67 (2H, d, J = 8.0 Hz, H-arom, *E*), 7.62 (2H, d, J = 8.0 Hz, H-arom, *Z*), 6.22 (1H, s, H-2_E), 6.04 (1H, s, H-2_Z), 4.83 (1H, d, $J_{OH,1}$ = 6.8 Hz, OH-1_Z), 4.76 (1H, d, $J_{OH,1}$ = 6.8 Hz, OH-1_E), 4.57 (1H, d, J = 7.2 Hz, OH, *E*), 4.53 (1H, d, J = 5.6 Hz, OH, *Z*), 4.51 (1H, d, J = 7.6 Hz, OH, *Z*), 4.48 (1H, d, J = 6.0 Hz, OH, *E*), 4.39 (1H, t, J = 5.6 Hz, OH-4_Z), 4.36 (1H, m, OH-4_E), 4.26 (1H, dt, $J_{4a,5}$ = 10.0 Hz, $J_{5,1'}$=$J_{4b,5}$ = 6.8 Hz, H-5_Z), 4.15 (2H, m, H-5_E and H-$4_{a,Z}$), 3.96 (1H, dd, $J_{4a,5}$ = 5.6 Hz, $J_{4a,4b}$ = 9.6 Hz, H-$4_{a,E}$), 3.81 (1H, t, $J_{1',5}$ = 6.8 Hz, $J_{1',2'}$ = 0 Hz, H-$1'_Z$), 3.76 (1H, t, $J_{1',5}$ = 6.0 Hz, $J_{1',2'}$ = 0 Hz, H-$1'_E$), 3.61 (2H, m, H-$4'_Z$ and H-$4'_E$), 3.51 (2H, m, H-$3'_Z$ and H-$3'_E$), 3.44 (4H, m, $J_{4',4''}$ = 10.8 Hz, $J_{4,OH}$ = 5.2 Hz, H-$4''_Z$ and H-$4''_E$, H-$2'_Z$, H-$2'_E$), 3.25 (1H, t, $J_{4a,4b}$=$J_{4b,5}$ = 8.0 Hz, H-$4_{b,Z}$), 3.19 (1H, t, $J_{4a,4b}$=$J_{4b,5}$ = 12.0 Hz, H-$4_{b,E}$), 2.02 (3H, s, CH_3, *Z*), 1.63 (3H, s, CH_3, *E*). ^{13}C NMR (100 MHz, $CDCl_3$): 168.1 (C=O, *Z*), 167.5 (C=O, *E*), 145.6, 133.3, 132.6, 128.9, 128.7, 119.2, 112.4, 111.6 (C-arom), 88.8 (C-2_E), 88.6 (C-2_Z), 81.3 (C-5_Z), 80.7 (C-5_E), 71.7, 71.6, 71.3, 71.1, 70.9 (C-$1'_Z$ and C-$1'_E$, C-$2'_Z$ and C-$2'_E$, C-$3'_Z$ and C-$3'_E$), 63.8 (C-$4'_Z$), 63.7 (C-$4'_E$), 48.3 (C-4_E), 47.1 (C-4_Z), 23.5 (CH_3, *Z*), 23.0 (CH_3, *E*). Anal. calcd. for $C_{16}H_{20}N_2O_6$ (336.34): C, 57.14; H, 5.99; N, 8.33. Found: C, 57.11; H, 6.04; N, 8.56.

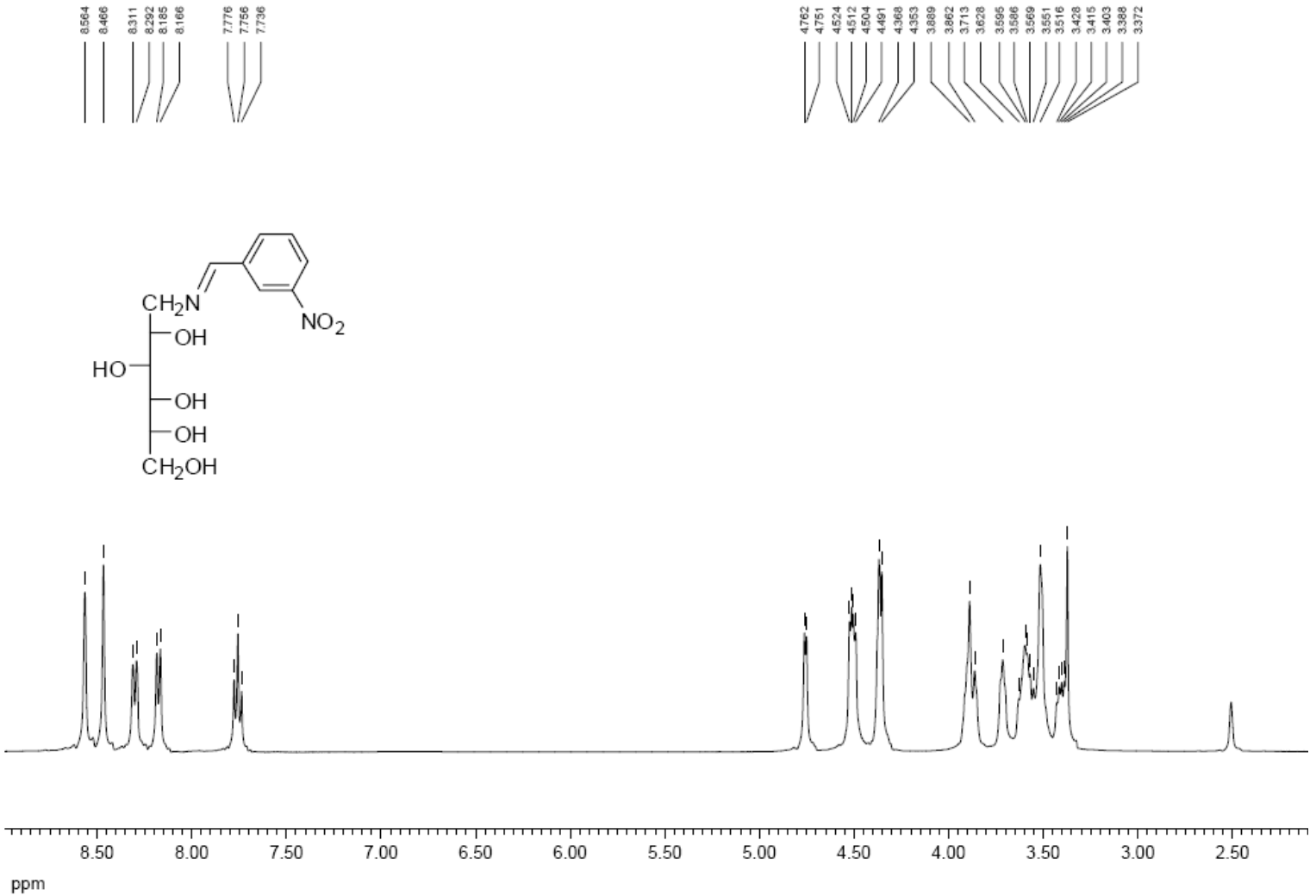
(2*R*,5*S*)-3-Acetyl-2-(4-trifluoromethylphenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (28*E*,*Z*)

(88%); Recrystallized from ethanol, mp 170-171ºC; $[\alpha]_D^{22}$ -19; $[\alpha]_{578}^{22}$ -21; $[\alpha]_{546}^{22}$ -25; $[\alpha]_{436}^{22}$ -48.2 (*c* 0.5, pyridine); IR (KBr) ν_{max}/cm^{-1} 3600-3300 (OH), 1662 (C=O), 1619 (arom), 1211 (C-N), 1109, 1067, 1050 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (2H, d, J = 8.0 Hz, H-arom, *E*), 7.72 (2H, d, J = 8.4 Hz, H-arom, *Z*), 7.69 (2H, d, H-arom, *E*), 7.64 (2H, d, J = 8.0 Hz, H-arom, *Z*), 6.23 (1H, s, H-2_E), 6.05 (1H, s, H-2_Z), 4.81 (1H, d, $J_{OH,1}$ = 6.4 Hz, OH-1_Z), 4.74 (1H, d, $J_{OH,1}$ = 6.8 Hz, OH-1_E), 4.57 (1H, d, J = 7.6 Hz, OH, *E*), 4.54 (1H, d, J = 5.6 Hz, OH, *Z*), 4.51 (1H, d, J = 7.6 Hz, OH, *Z*), 4.48 (1H, d, J = 5.6 Hz, OH, *E*), 4.39 (1H, t, J = 5.6 Hz, OH-4_Z), 4.37 (1H, m, OH-4_E), 4.27 (1H, m, $J_{4a,5}$ = 10.0 Hz, $J_{5,1'}$=$J_{4b,5}$ = 6.4 Hz, H-5_Z), 4.14 (2H, m, H-5_E and H-$4_{a,E}$), 3.97 (1H, dd, $J_{4a,5}$ = 5.6 Hz, $J_{4a,4b}$ = 9.6 Hz, H-$4_{a,Z}$), 3.82 (1H, t, $J_{1',5}$ = 7.2 Hz, $J_{1',2'}$ = 0 Hz, H-1′$_Z$), 3.77 (1H, t, $J_{1',5}$ = 6.8 Hz, $J_{1',2'}$ = 0 Hz, H-1′$_E$), 3.61 (2H, m, H-4′$_Z$ and H-4′$_E$), 3.52 (2H, m, H-3′$_Z$ and H-3′$_E$), 3.44 (4H, m, $J_{4',4''}$ = 10.8 Hz, $J_{4'',OH}$ = 5.2 Hz, H-4′′$_Z$ and H-4′′$_E$, H-2′$_Z$, H-2′$_E$), 3.25 (1H, t, $J_{4b,4a}$=$J_{4b,5}$ = 8.0 Hz, H-$4_{b,Z}$), 3.19 (1H, t, $J_{4a,4b}$=$J_{4b,5}$ = 12.0 Hz, H-$4_{b,E}$), 2.02 (3H, s, CH_3, *Z*), 1.64 (3H, s, CH_3, *E*). ^{13}C NMR (100 MHz, $CDCl_3$): 168.1 (C=O, *Z*), 167.5 (C=O, *E*), 144.9, 129.5, 128.8, 128.5, 126.2, 126.1, 125.4, 123.3 (C-arom), 88.9 (C-2_E), 88.7 (C-2_Z), 81.2 (C-5_Z), 80.6 (C-5_E), 71.7, 71.6, 71.3, 71.1, 70.9 (C-1′$_Z$ and C-1′$_E$, C-2′$_Z$ and C-2′$_E$, C-3′$_Z$ and C-3′$_E$), 63.8 (C-4′$_Z$), 63.7 (C-4′$_E$), 48.3 (C-4_Z), 47.2 (C-4_E), 23.5 (CH_3, *Z*), 23.0 (CH_3, *E*). Anal. calcd. for $C_{16}H_{20}F_3NO_6$ (379.33): C, 50.66; H, 5.31; N, 3.69. Found: C, 50.45; H, 5.36; N, 3.57.

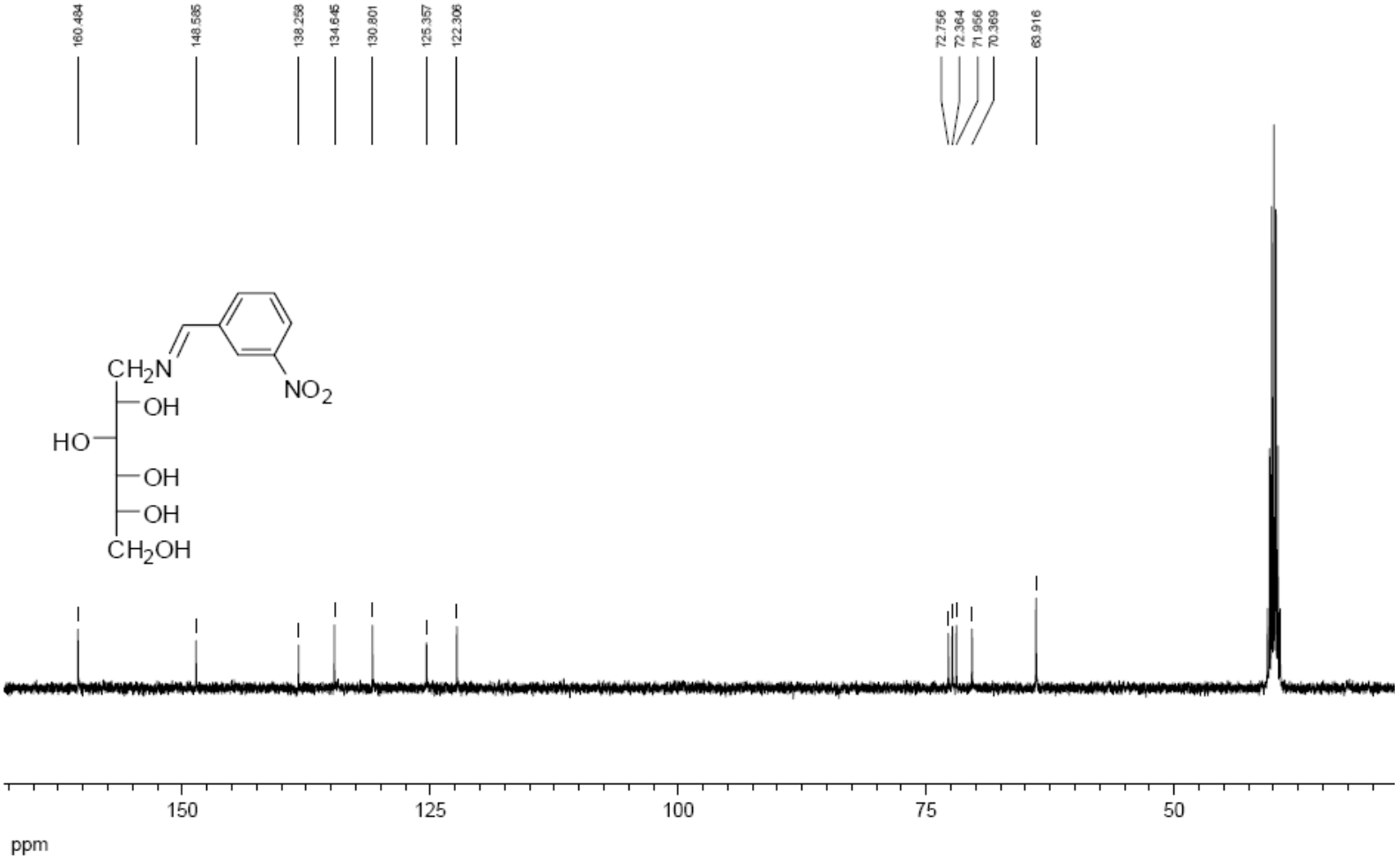
(2*R*,5*S*)-3-Acetyl-2-(4-dimethylaminophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (35*E*,*Z*)

(70%); Recrystallized from ethanol, mp 183-184ºC; $[\alpha]_D^{22}$ -22; $[\alpha]_{578}^{22}$ -28; $[\alpha]_{546}^{22}$ -28 (*c* 0.5, pyridine); IR (KBr) ν_{max}/cm^{-1} 3500-2900 (OH), 1615 (C=O), 1530 (arom), 1200 (C-N), 1099, 1077, 1037 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (4H, t, J = 9.2 Hz, H-arom), 6.72 (2H, d, J = 8.4 Hz), 6.66 (2H, d, J = 8.4 Hz, H-arom), 5.95 (1H, s, H-2_E), 5.88 (1H, s, H-2_Z), 4.75 (1H, d, $J_{OH,1}$ = 6.4 Hz, OH-1_Z), 4.70 (1H, d, $J_{OH,1}$ = 6.8, Hz OH-1_E), 4.53 (2H, d, OH), 4.48 (2H, m, OH), 4.37 (2H, c, $J_{OH,4}$ = 5.2 Hz, OH-4_Z and OH-4_E), 4.11 (1H, dt, $J_{4a,5}$ = 10.0 Hz, $J_{5,1'}$=$J_{4b,5}$ = 6.0 Hz, H-5_Z), 4.06 (2H, m, H-5_E and H-$4_{a,Z}$), 3.90 (1H, dd, $J_{4a,5}$ = 5.4 Hz, $J_{4a,4b}$ = 9.4 Hz, H-$4_{a,E}$), 3.80 (2H, c, $J_{1',5}$ = 7.6 Hz, $J_{1',2'}$ = 0 Hz, H-1′$_Z$ and H-1′$_E$), 3.60 (2H, m, H-4′$_Z$ and H-4′$_E$), 3.49 (2H, m, H-3′$_Z$ and H-3′$_E$), 3.44 (2H, dd, $J_{4',4''}$ = 8.0 Hz, $J_{4'',OH}$ = 3.2 Hz, H-4′′$_Z$ and H-4′′$_E$), 3.23 (2H, t, $J_{2',OH}$=$J_{2',3'}$ = 7.6 Hz, H-2′$_Z$ and H-2′$_E$), 3.13 (2H, t, H-$4_{b,E}$ and H-$4_{b,Z}$), 2.91 (3H, s, CH_3-N, *E*), 2.88 (3H, s, CH_3-N, *Z*), 1.98 (3H, s, CH_3, *Z*), 1.58 (3H, s, CH_3, *E*). ^{13}C NMR (100 MHz, $CDCl_3$): 167.5, (C=O), 151.3, 150.9, 128.7, 128.4, 128.2, 127.1, 112.3, 112.1 (C-arom), 90.1 (C-2_E), 89.5 (C-2_Z), 80.3 (C-5_Z), 79.66 (C-5_E), 71.7, 71.6, 71.3, 71.2, 71.0 (C-1′$_Z$ and C-1′$_E$, C-2′$_Z$ and C-2′$_E$, C-3′$_Z$ and C-3′$_E$), 63.8 (C-4′$_Z$ and C-4′$_E$), 48.4 (C-4_E), 47.4 (C-4_Z), 40.7 (CH_3-N, *Z*), 40.5 (CH_3-N, *E*), 23.7 (CH_3, *Z*), 22.9 (CH_3, *E*). Anal. calcd. for $C_{17}H_{26}N_2O_6$ (354.40): C, 57.61; H, 7.39; N, 7.90. Found: C, 57.46; H, 7.45; N, 7.78.

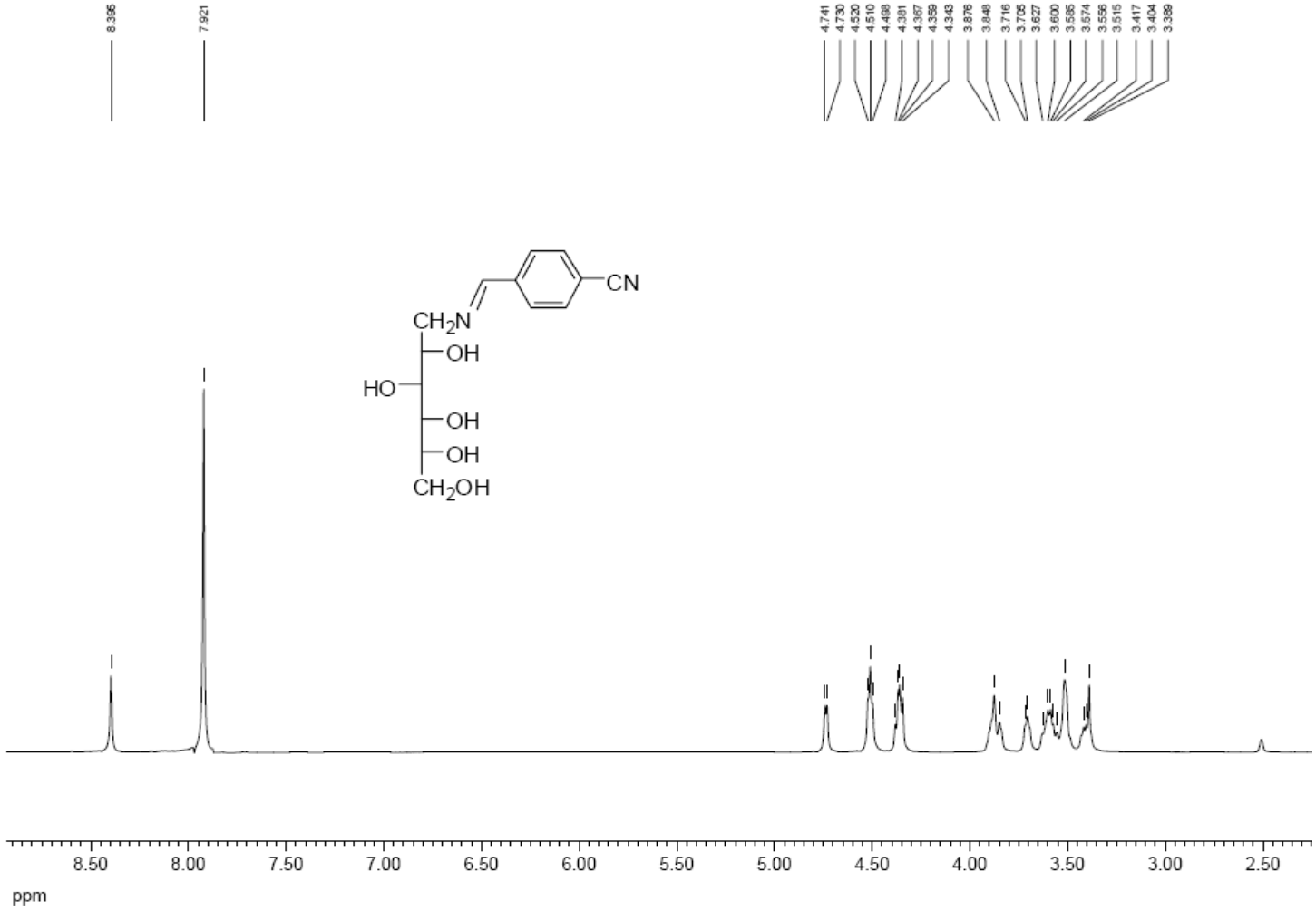
^{1}H-NMR Spectrum for 1-deoxy-1-(3-nitrobenzylidene)amino-D-glucitol (**2a**)



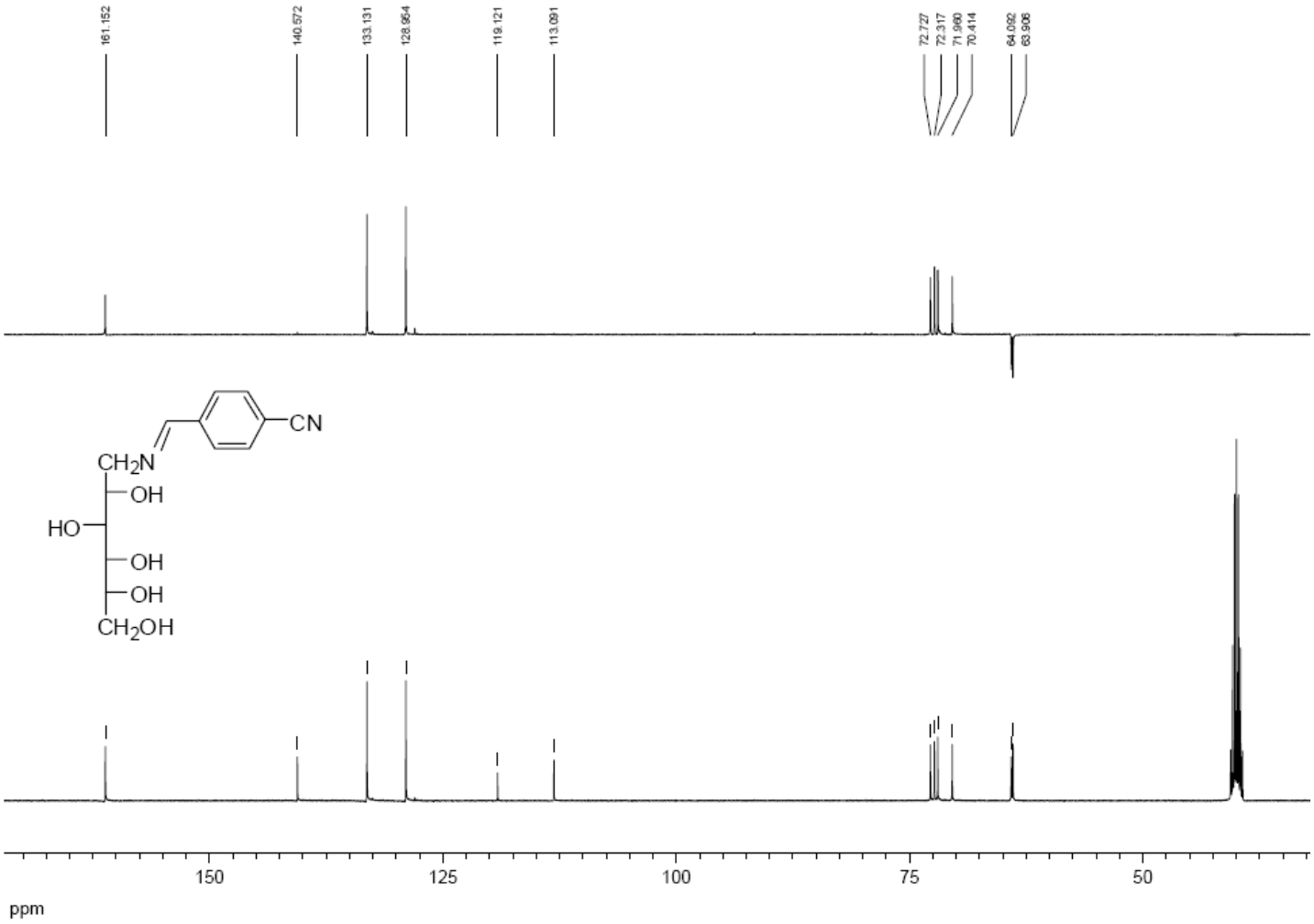
^{13}C-NMR Spectrum for 1-deoxy-1-(3-nitrobenzylidene)amino-D-glucitol (**2a**)



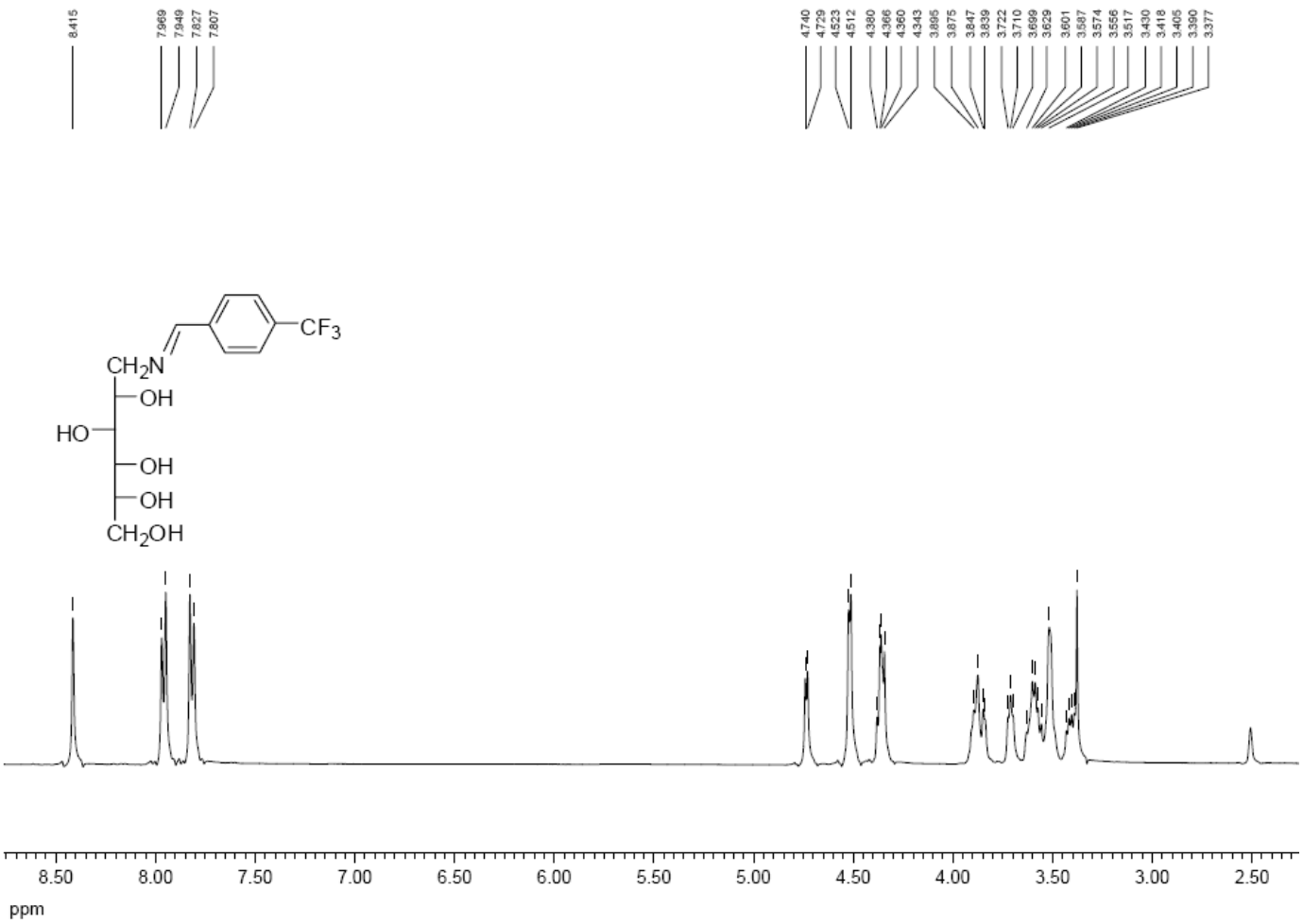
^{1}H-NMR Spectrum for 1-deoxy-1-(4-cyanobenzylidene)amino-D-glucitol (**3a**)



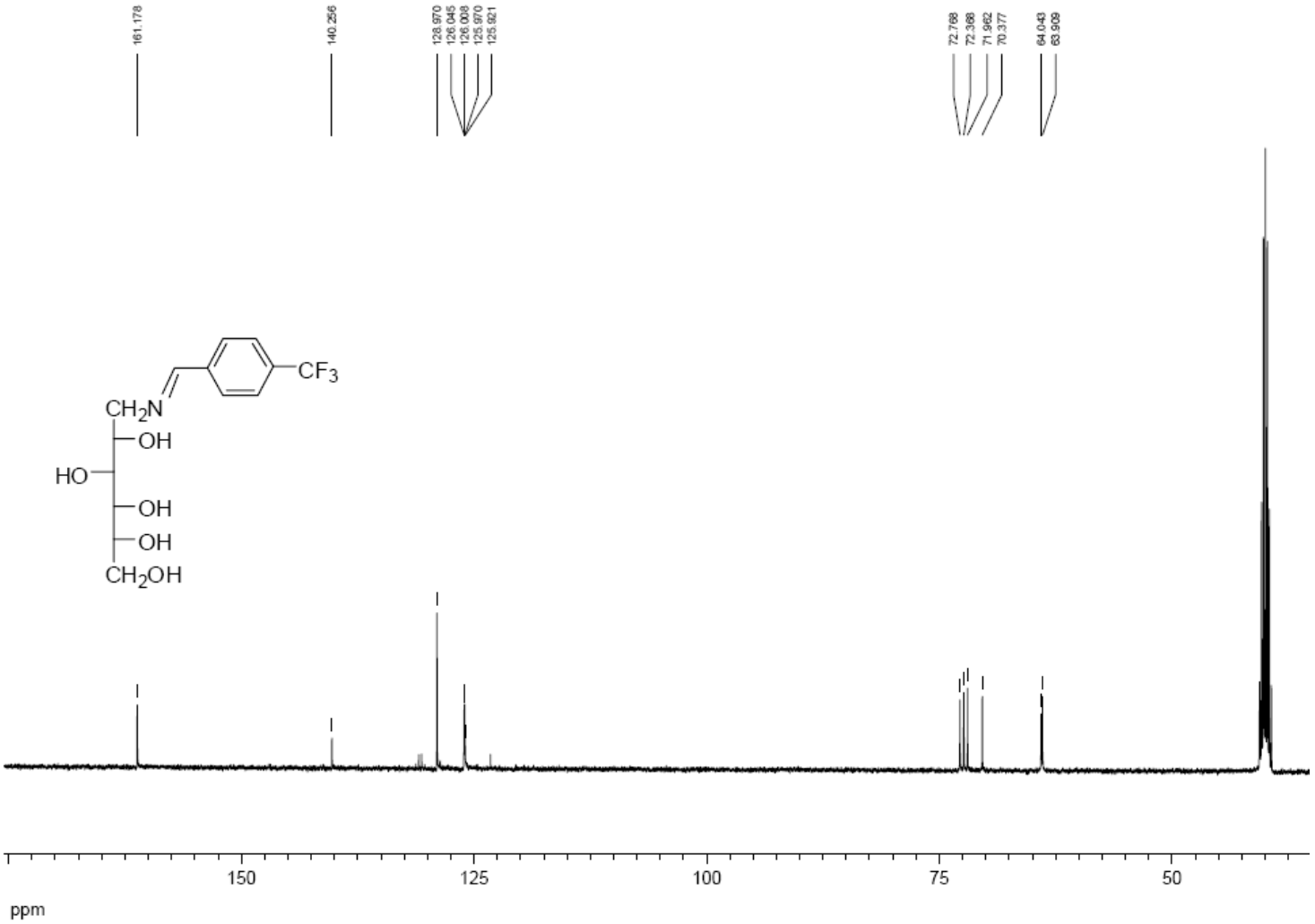
^{13}C-NMR Spectrum for 1-deoxy-1-(4-cyanobenzylidene)amino-D-glucitol (**3a**)



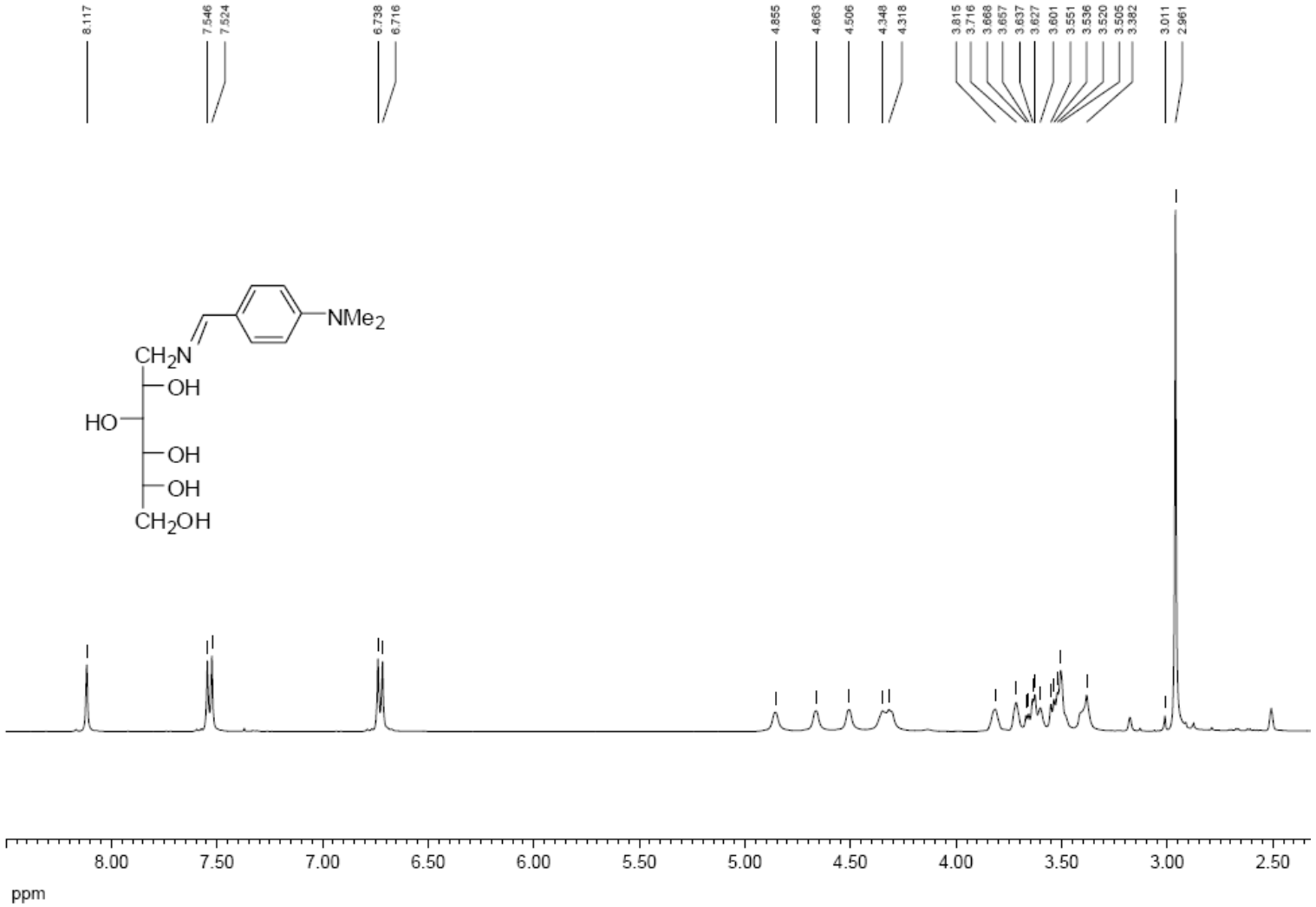
^{1}H-NMR Spectrum for 1-deoxy-1-(4-trifluoromethylbenzylidene)amino-D-glucitol (**4a**)



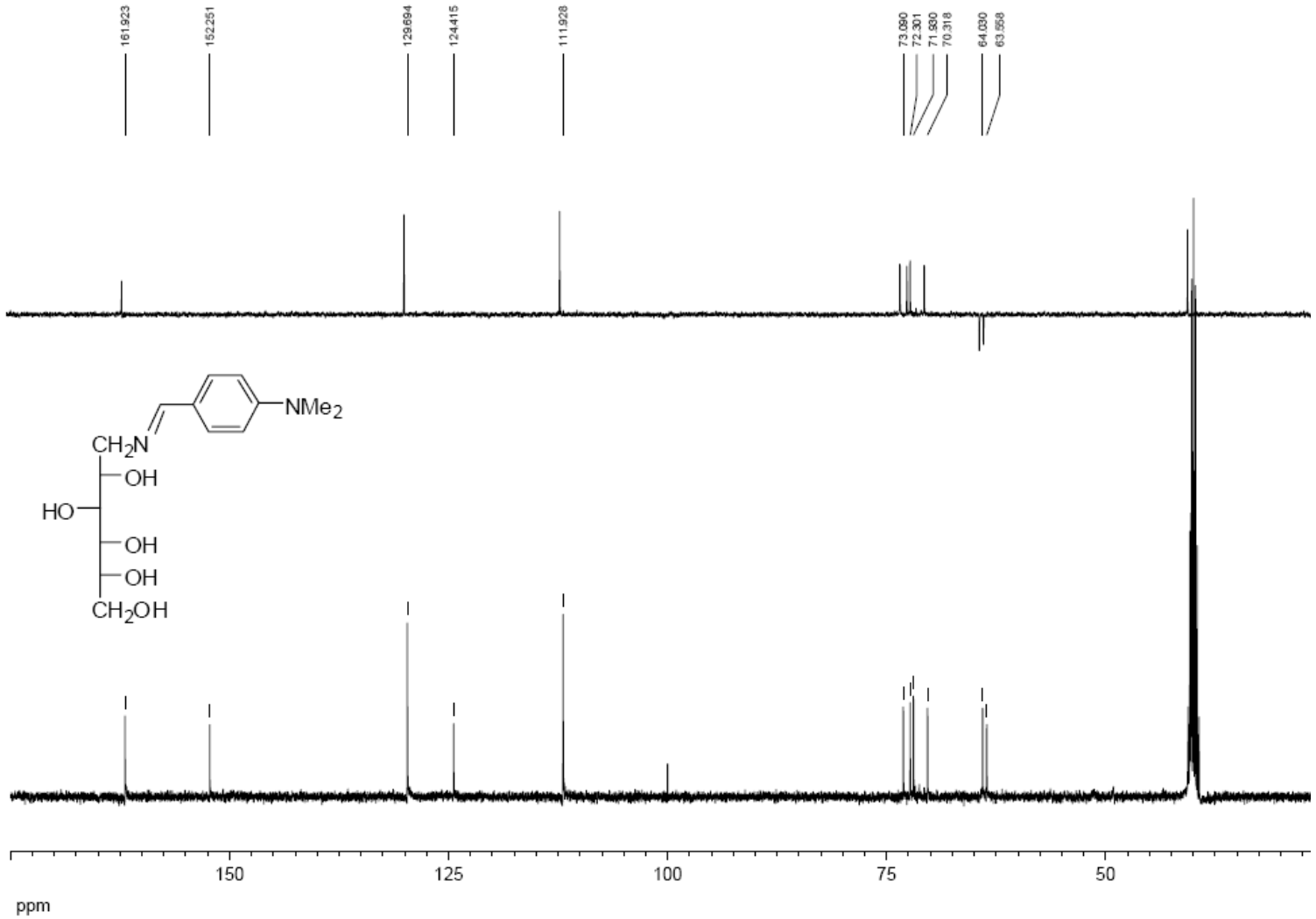
^{13}C-NMR Spectrum for 1-deoxy-1-(4-trifluoromethylbenzylidene)amino-D-glucitol (**4a**)



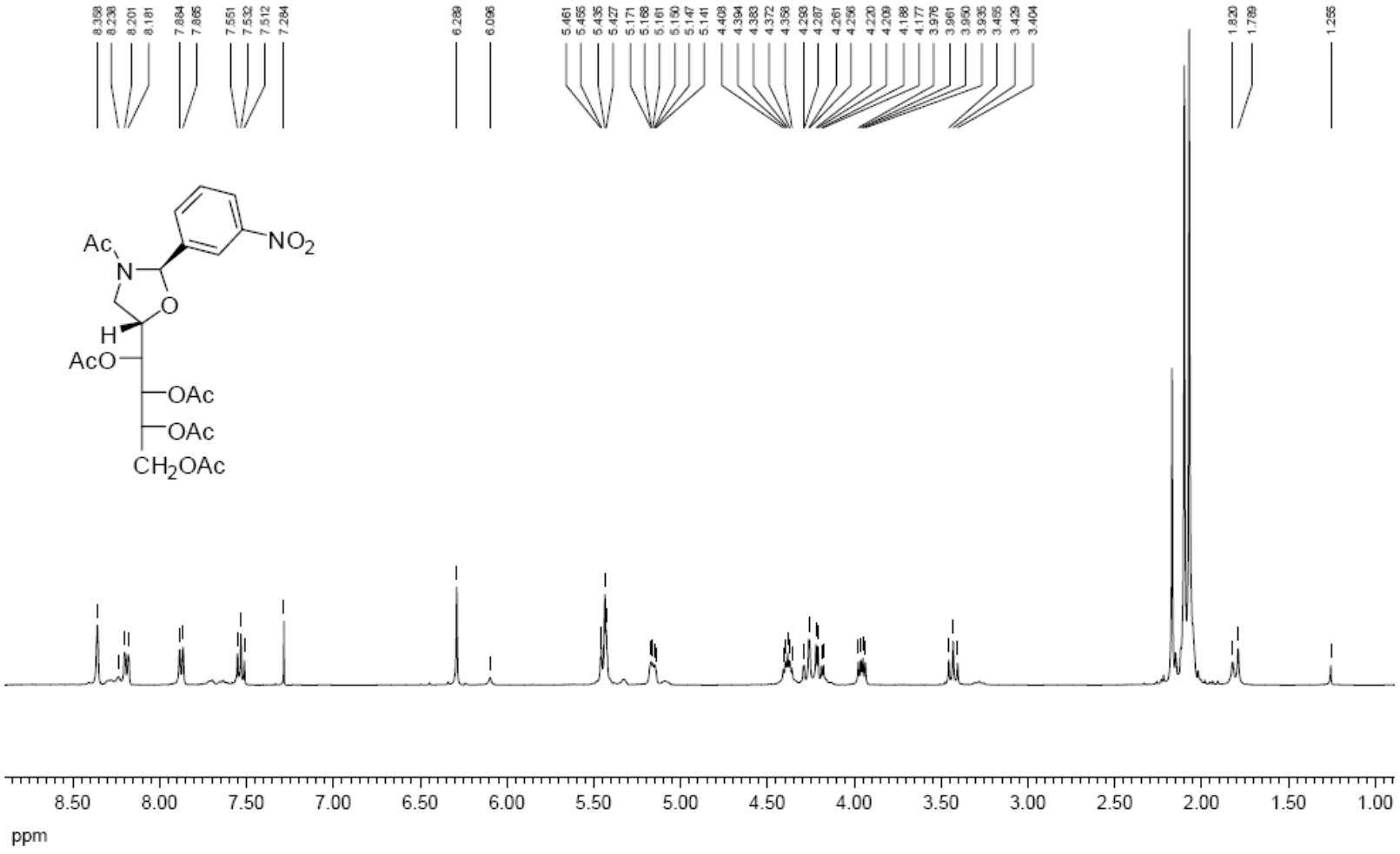
^{1}H-NMR Spectrum for 1-(4-dimethylaminobenzylidene)amino-1-deoxy-1-D-glucitol (**37**)



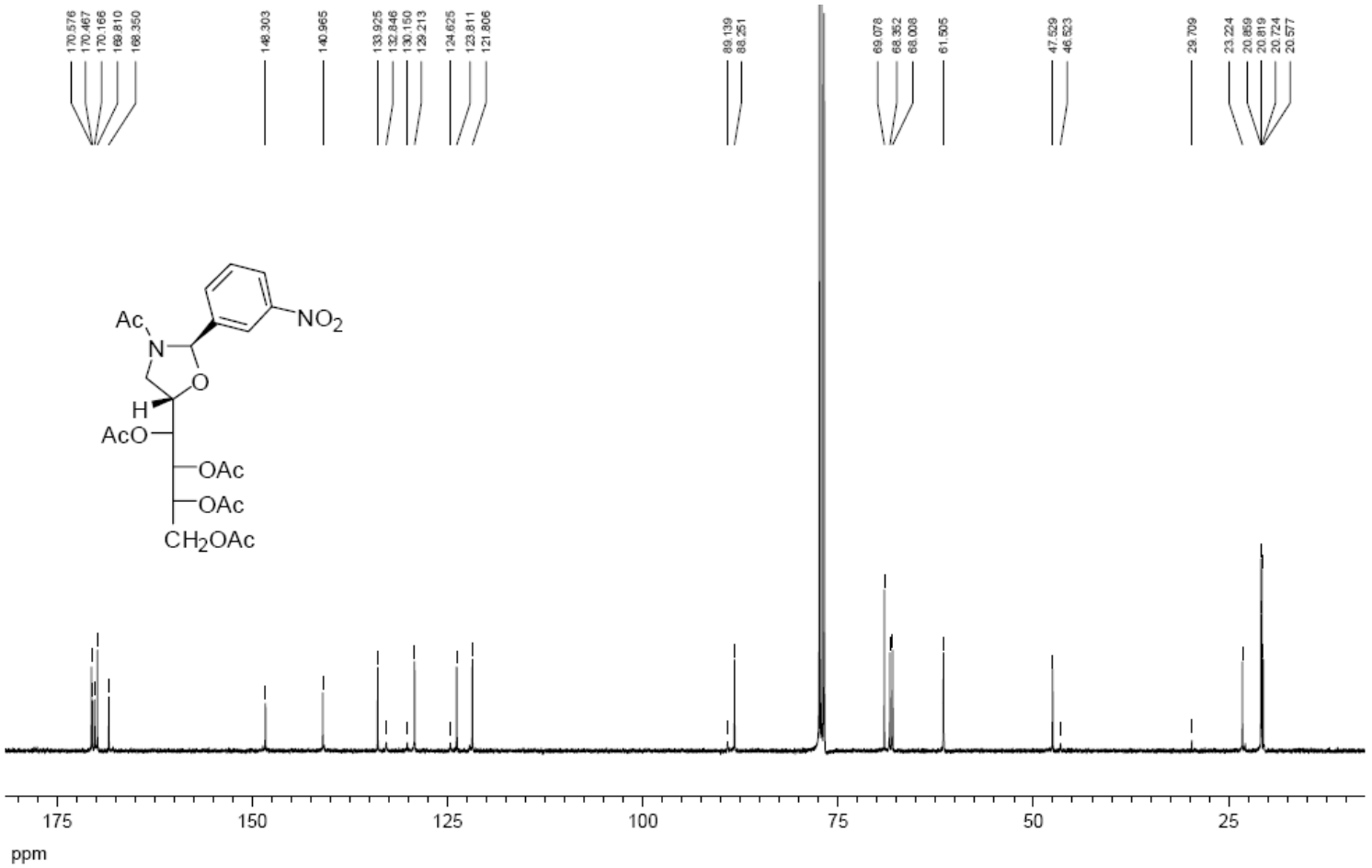
^{13}C-NMR Spectrum for 1-(4-dimethylaminobenzylidene)amino-1-deoxy-1-D-glucitol (**37**)



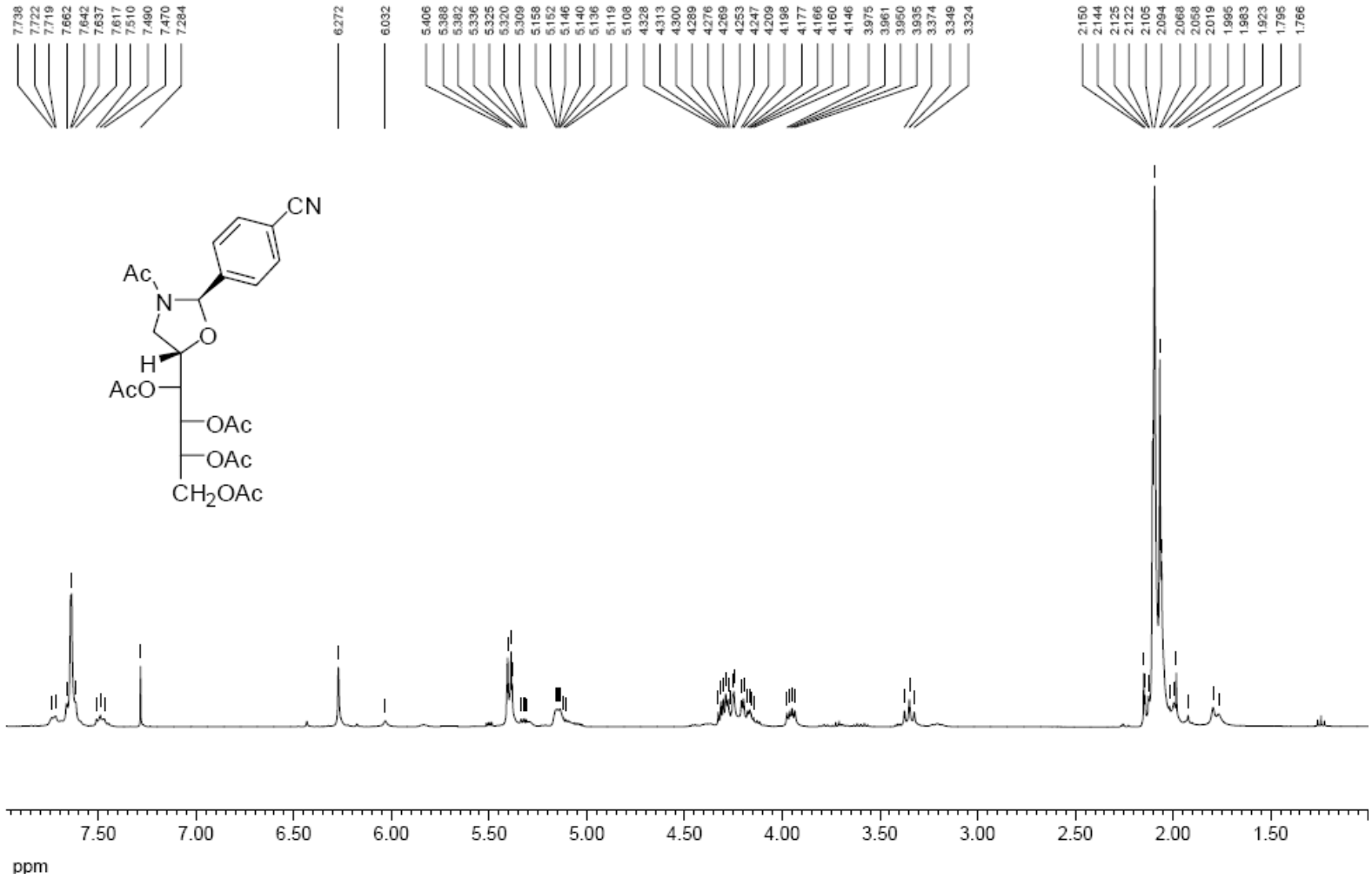
^{1}H-NMR Spectrum for (2*R*, 5*S*)-3-acetyl-2-(3-nitrophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**2*E*,*Z***)



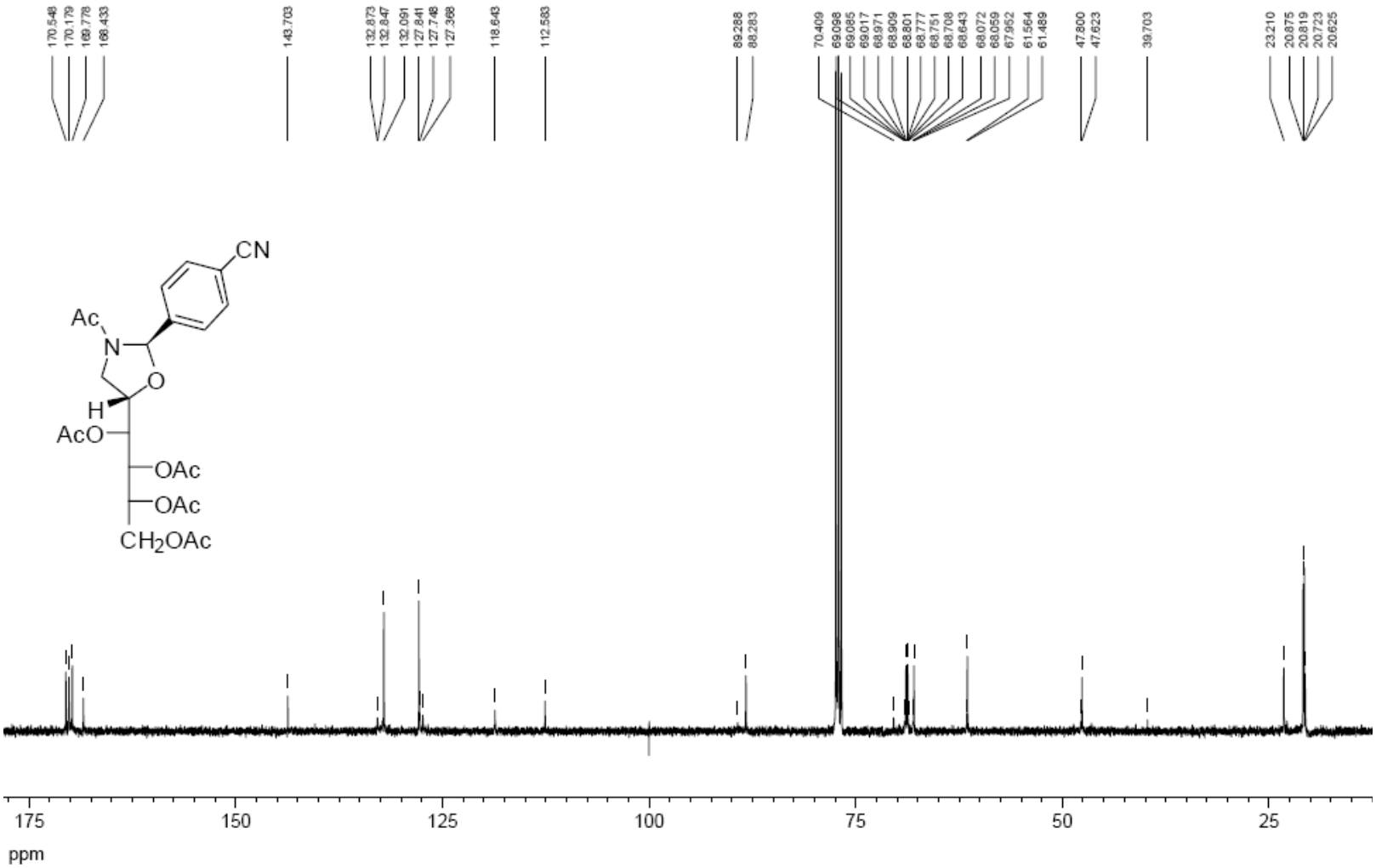
^{13}C-NMR Spectrum for (2*R*, 5*S*)-3-acetyl-2-(3-nitrophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**2*E*,*Z***)



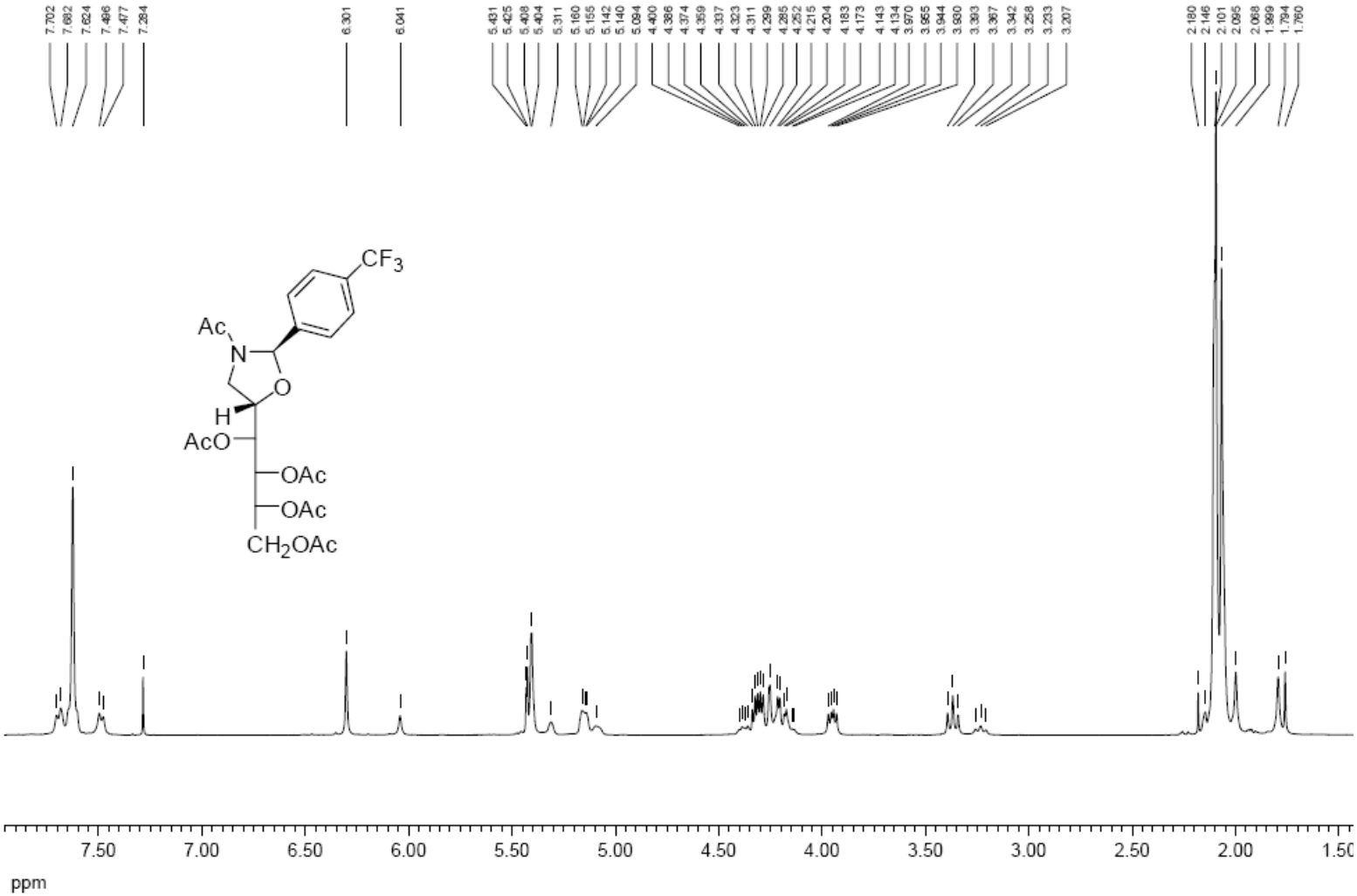
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-cyanophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**3*E*,*Z***)



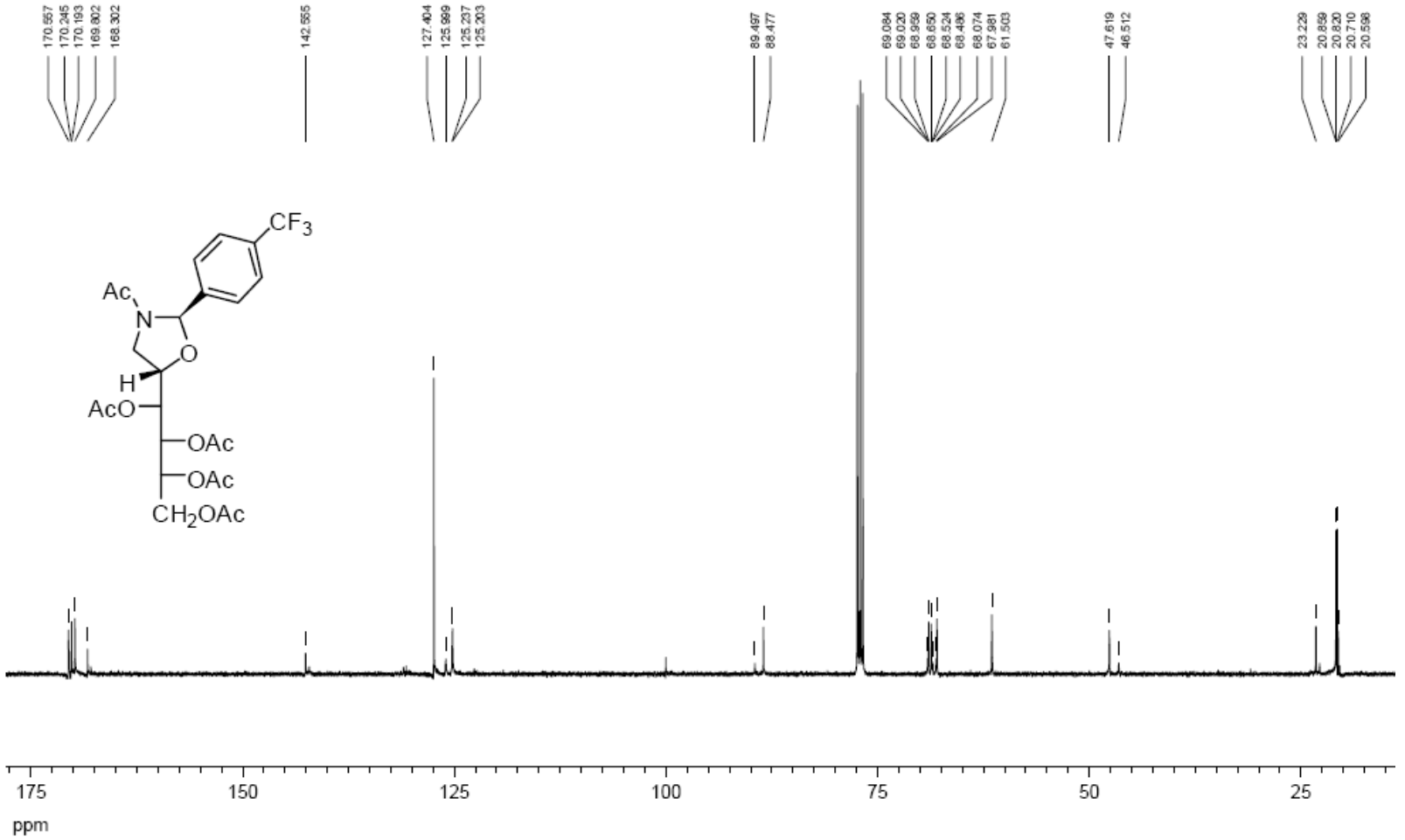
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-cyanophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**3*E*,*Z***)



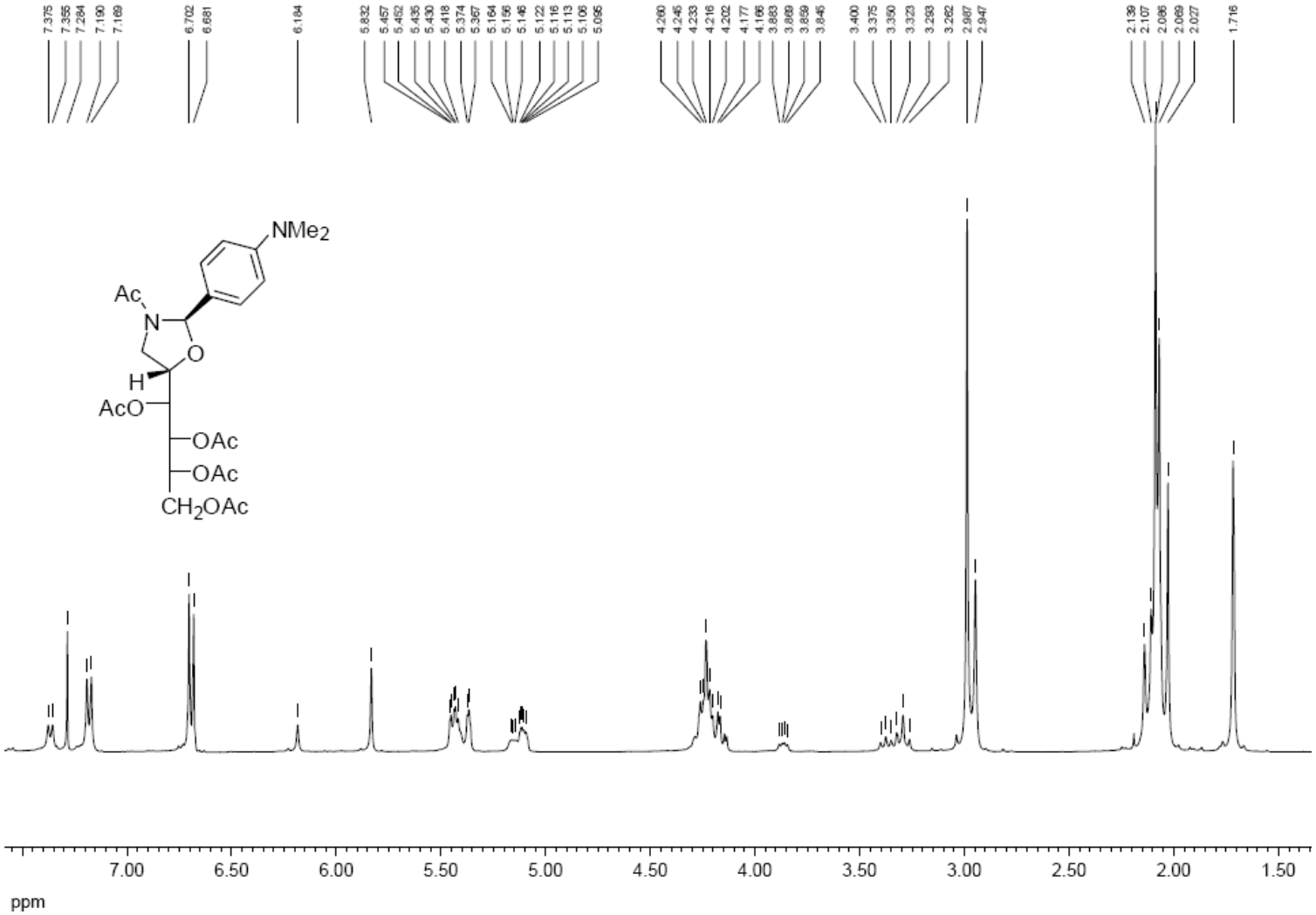
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-trifluoromethylphenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**4*E*,*Z***)



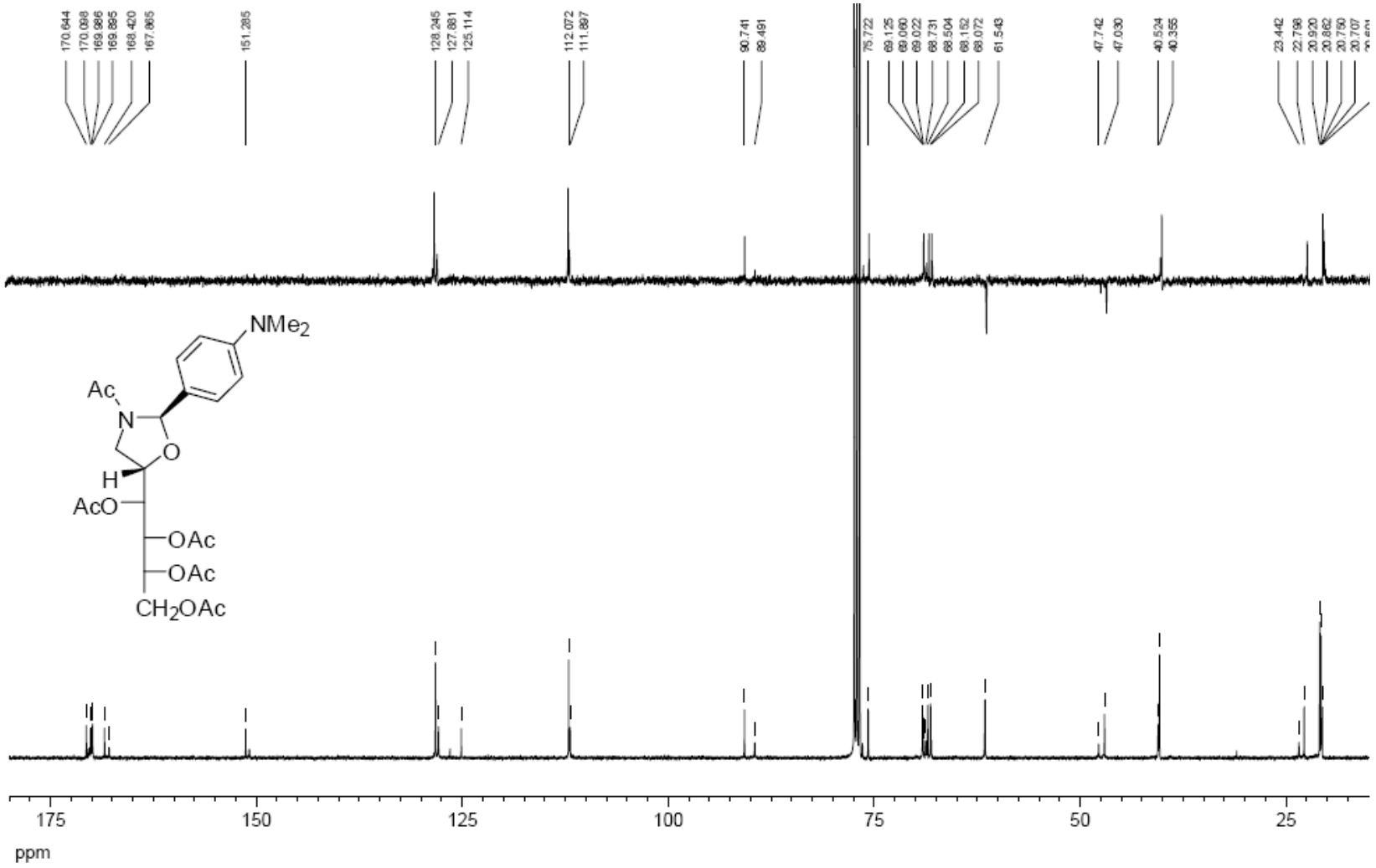
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-trifluoromethylphenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**4*E*,*Z***)



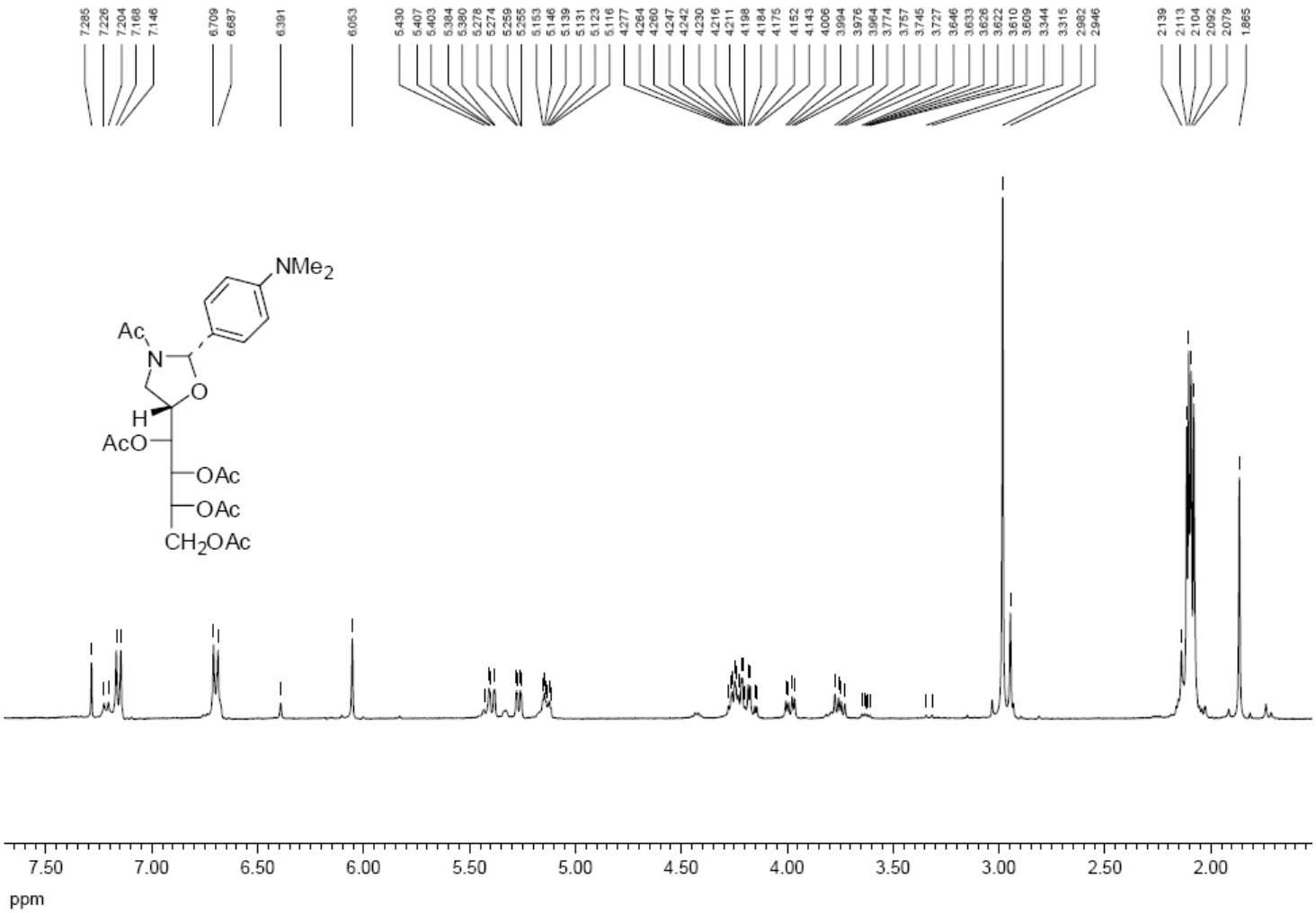
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**11*E*,*Z***)



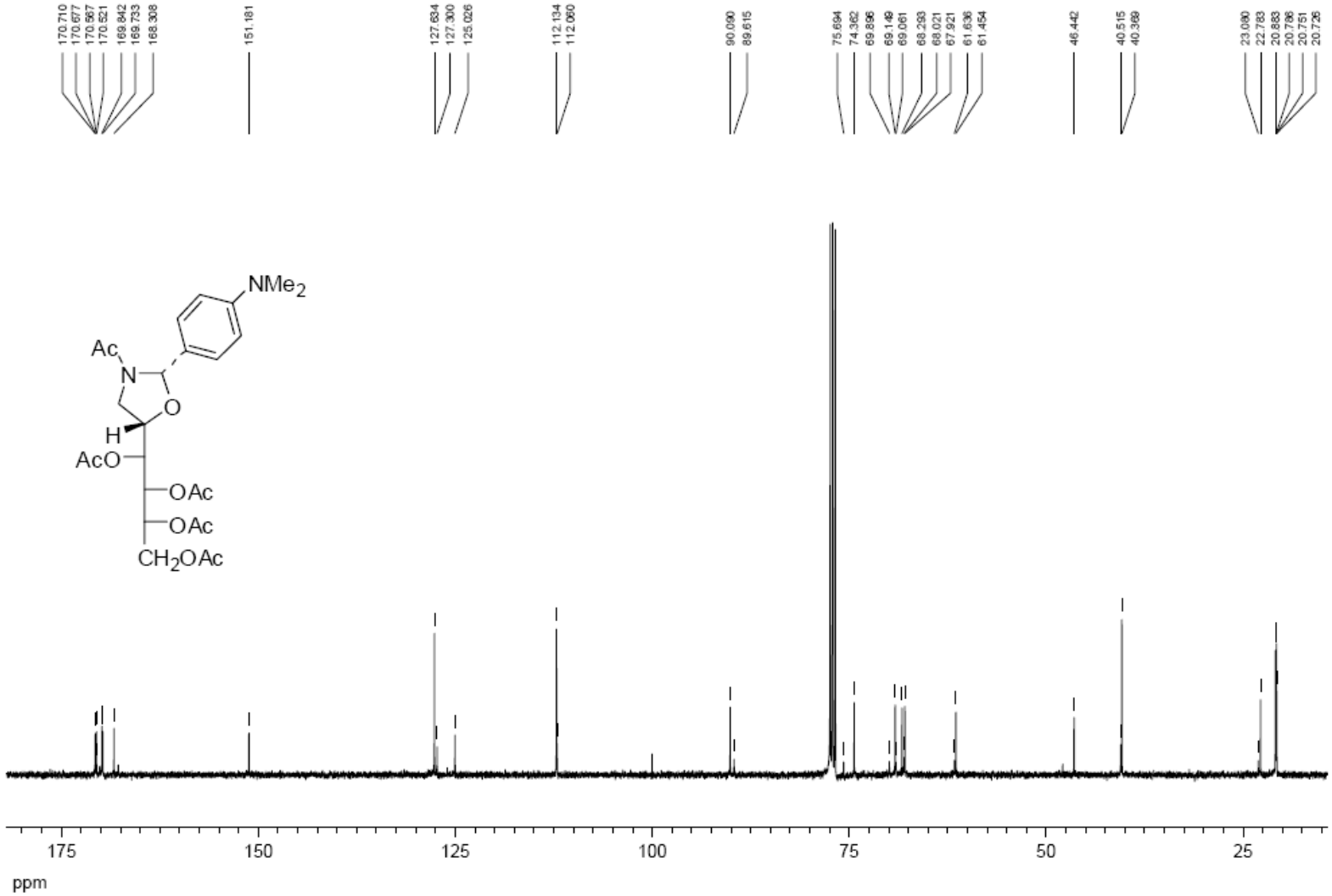
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**11*E*,*Z***)



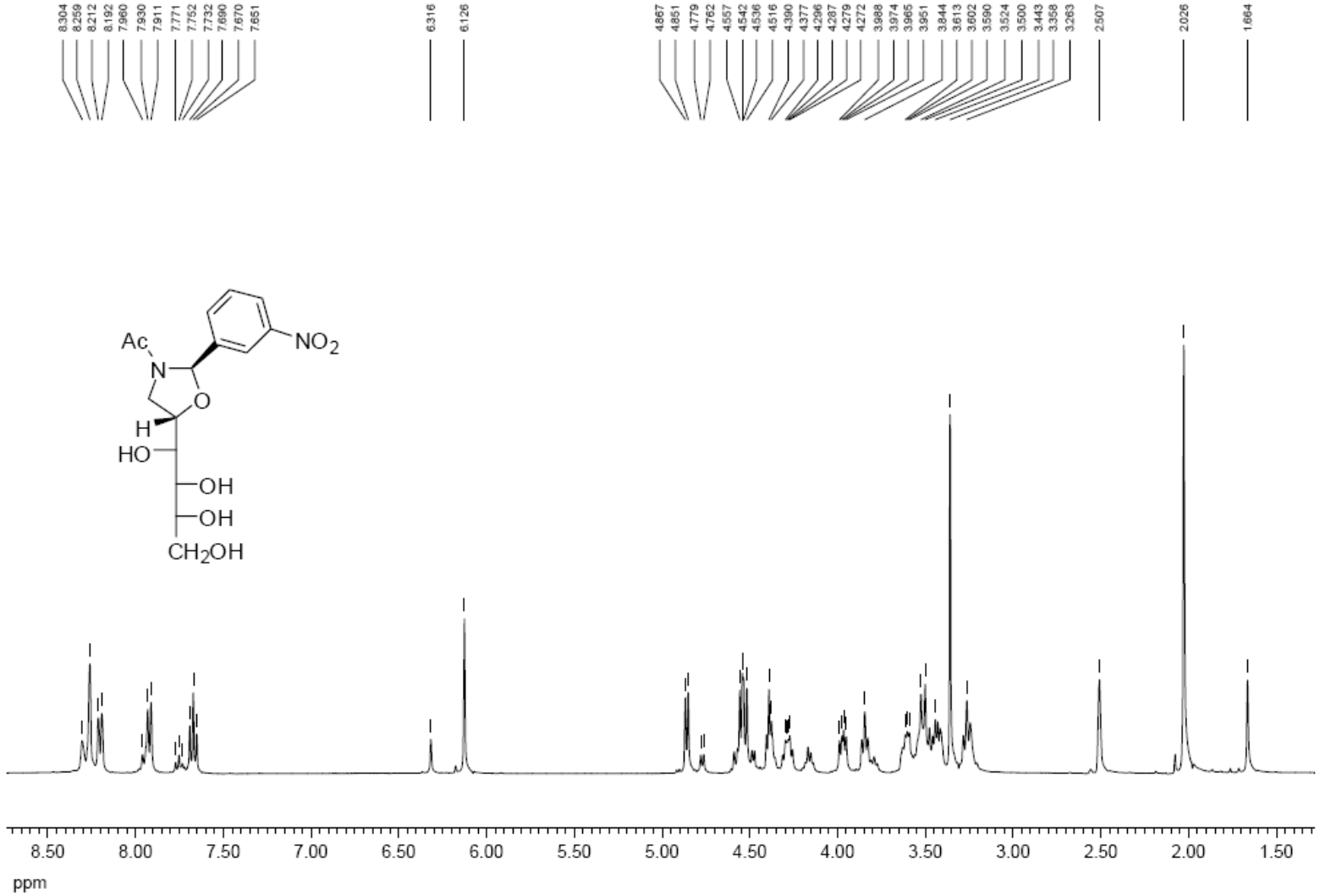
^{1}H-NMR Spectrum for (2*S*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**23*E*,*Z***)



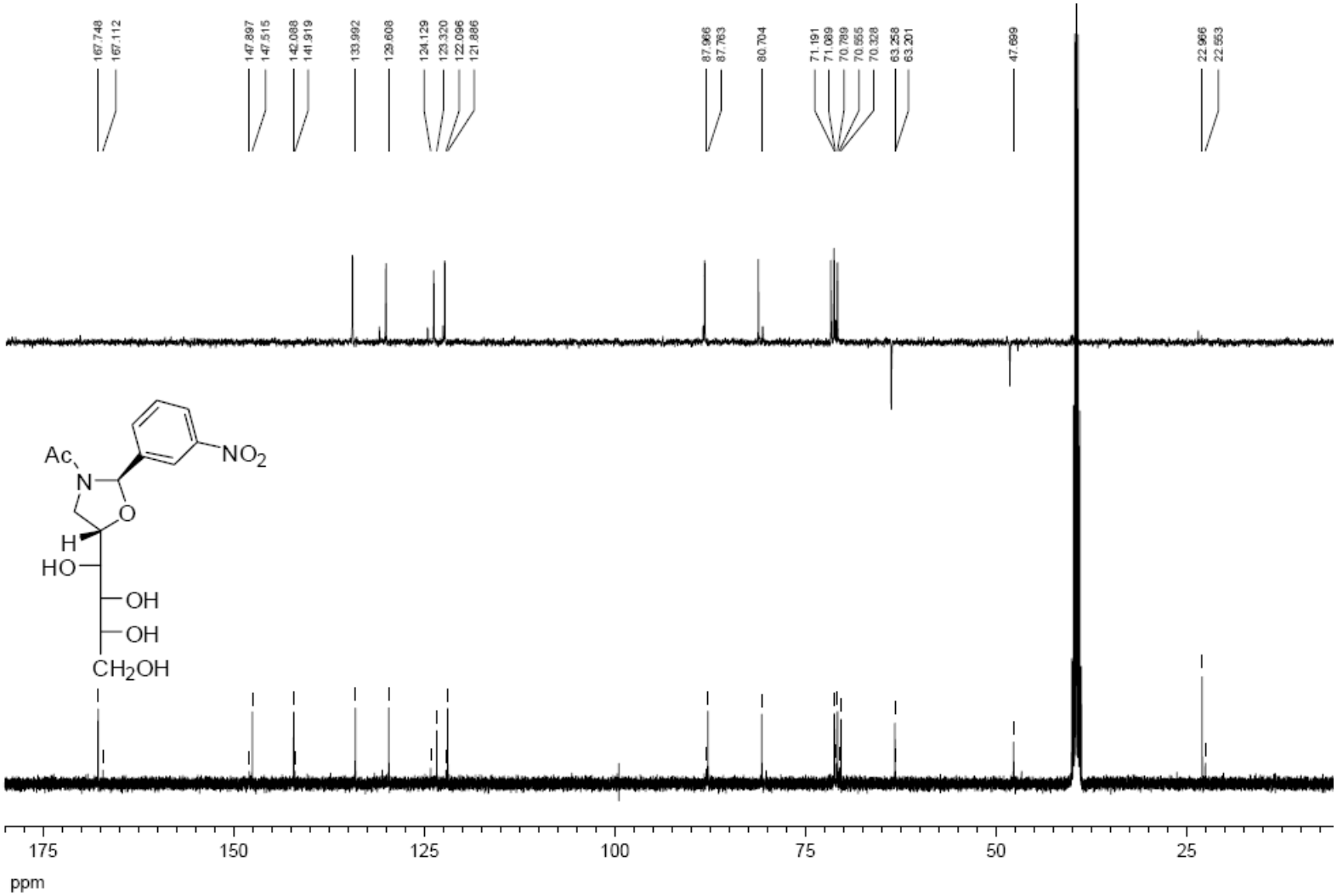
^{13}C-NMR Spectrum for (2*S*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**23*E*,*Z***)



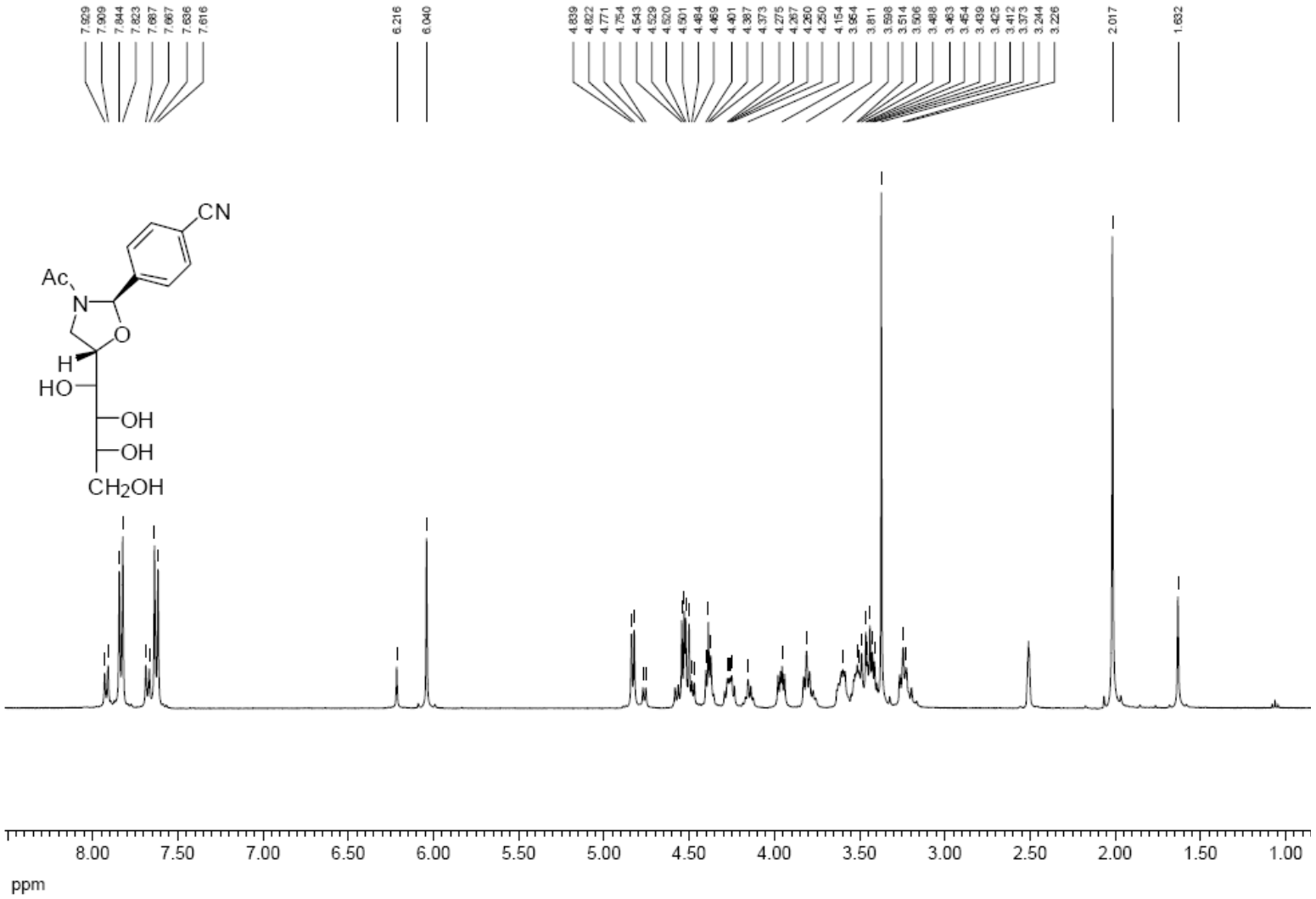
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(3-nitrophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**26*E,Z***)



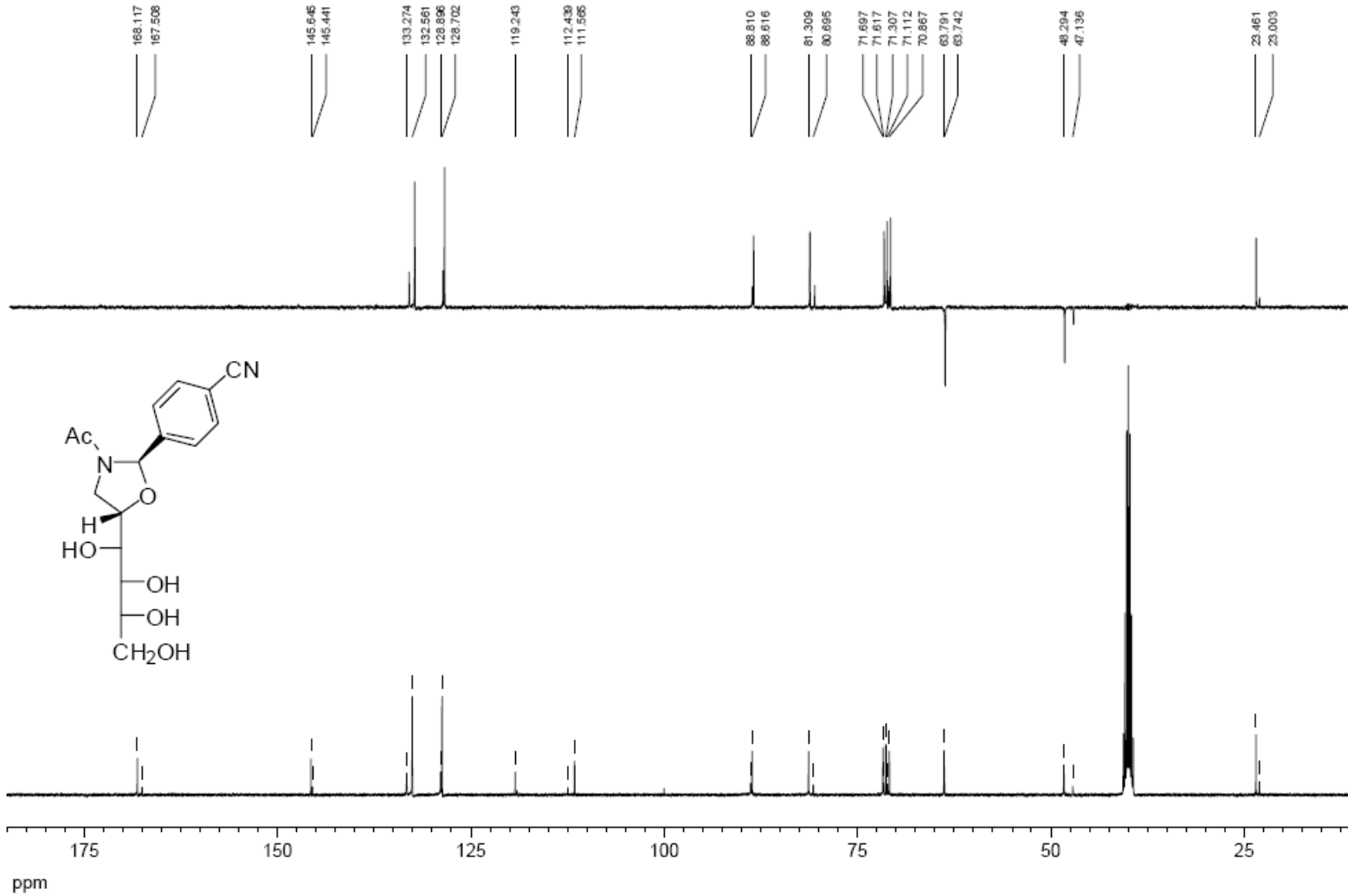
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(3-nitrophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**26*E,Z***)



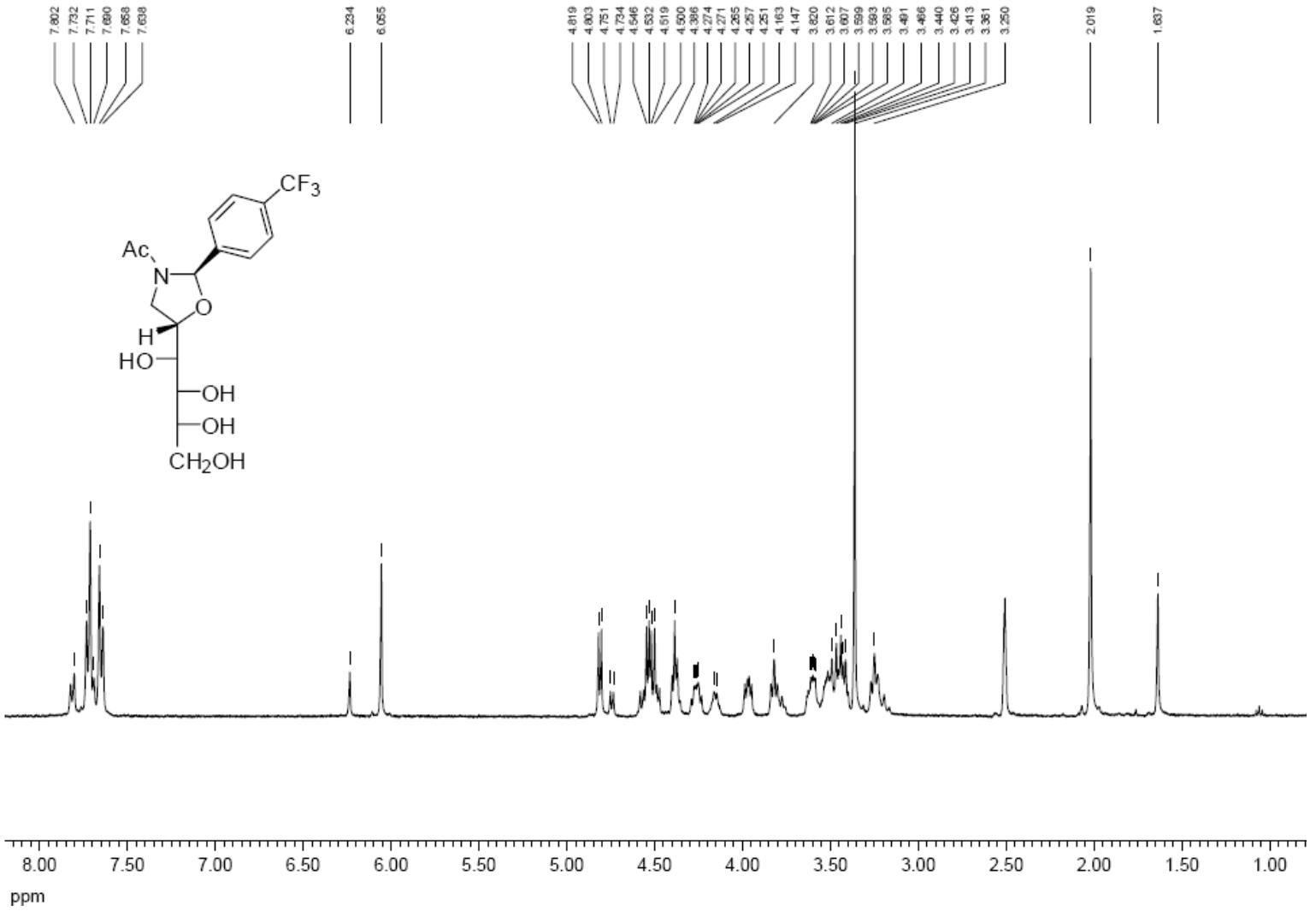
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-cyanophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**27E,Z**)



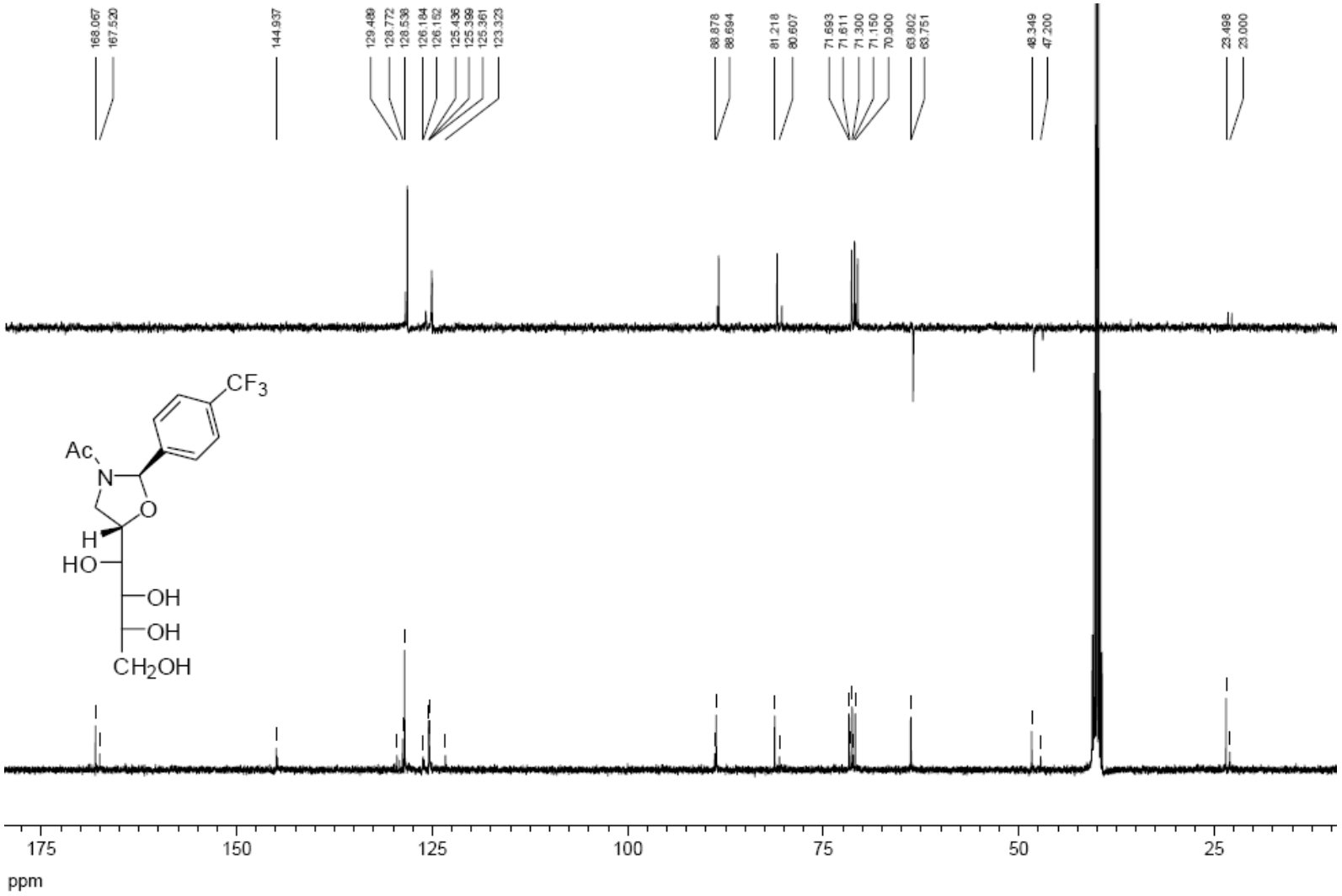
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-cyanophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**27*E,Z***)



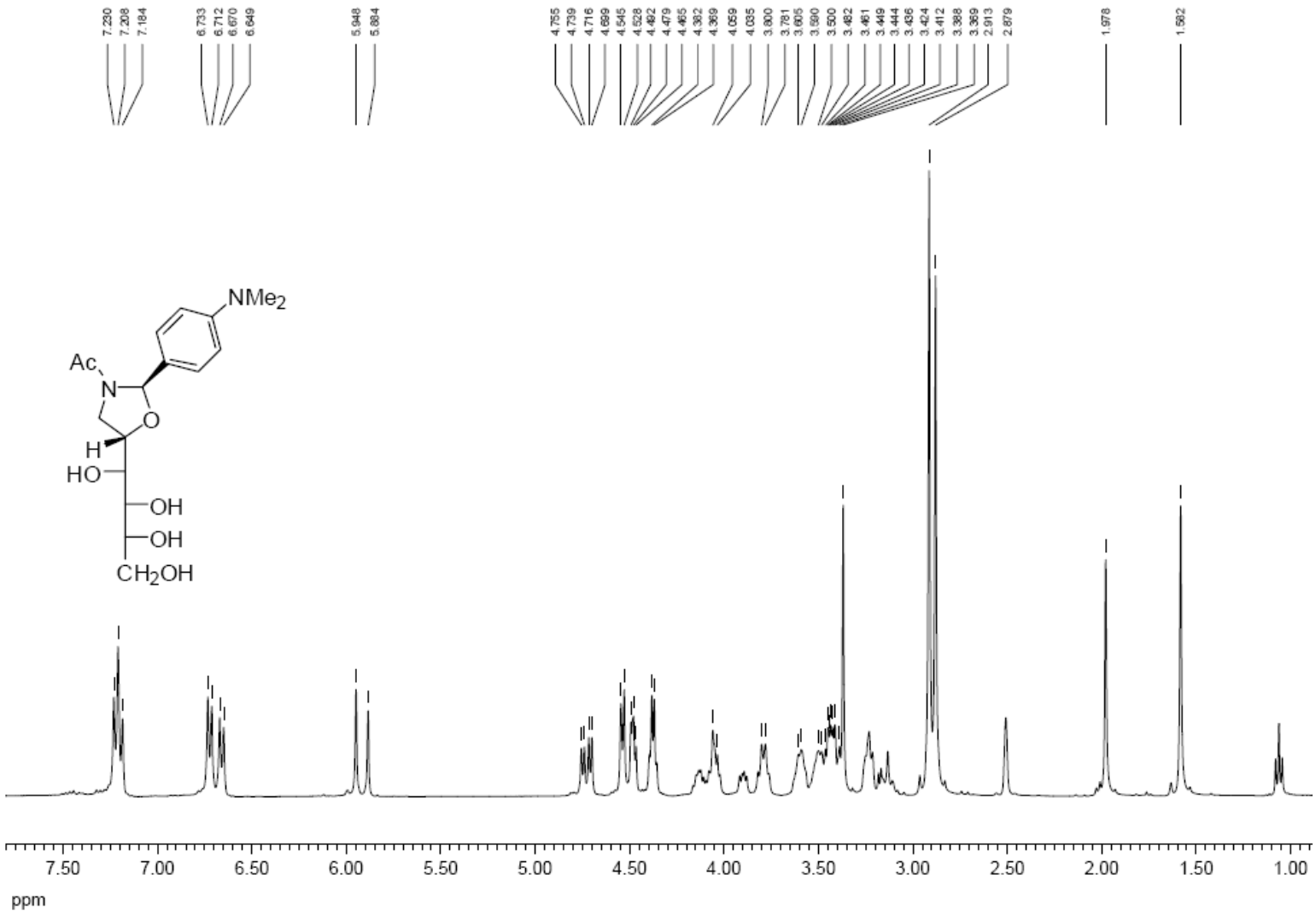
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-trifluoromethylphenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**28*E,Z***)



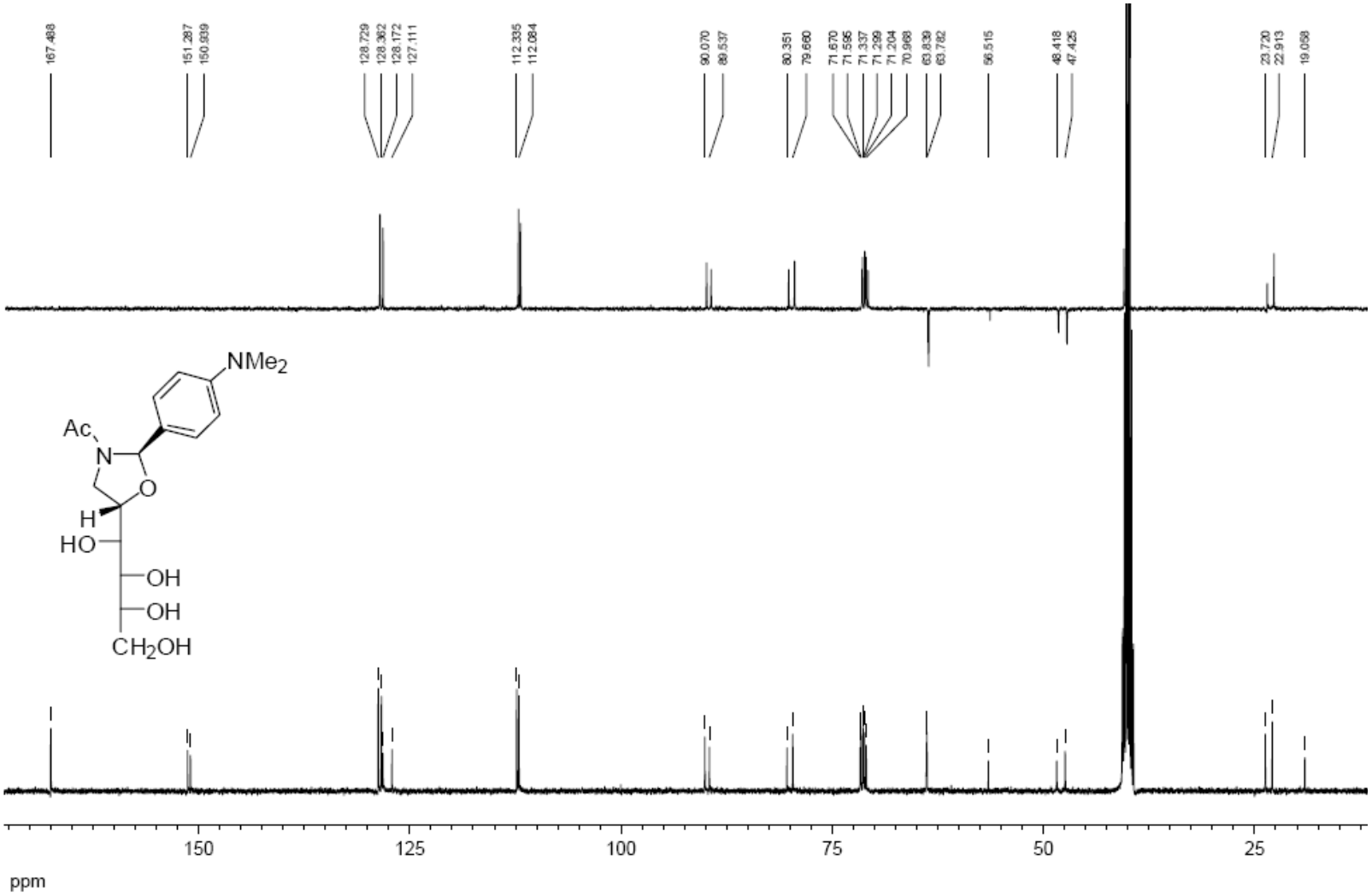
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-trifluoromethylphenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**28*E,Z***)



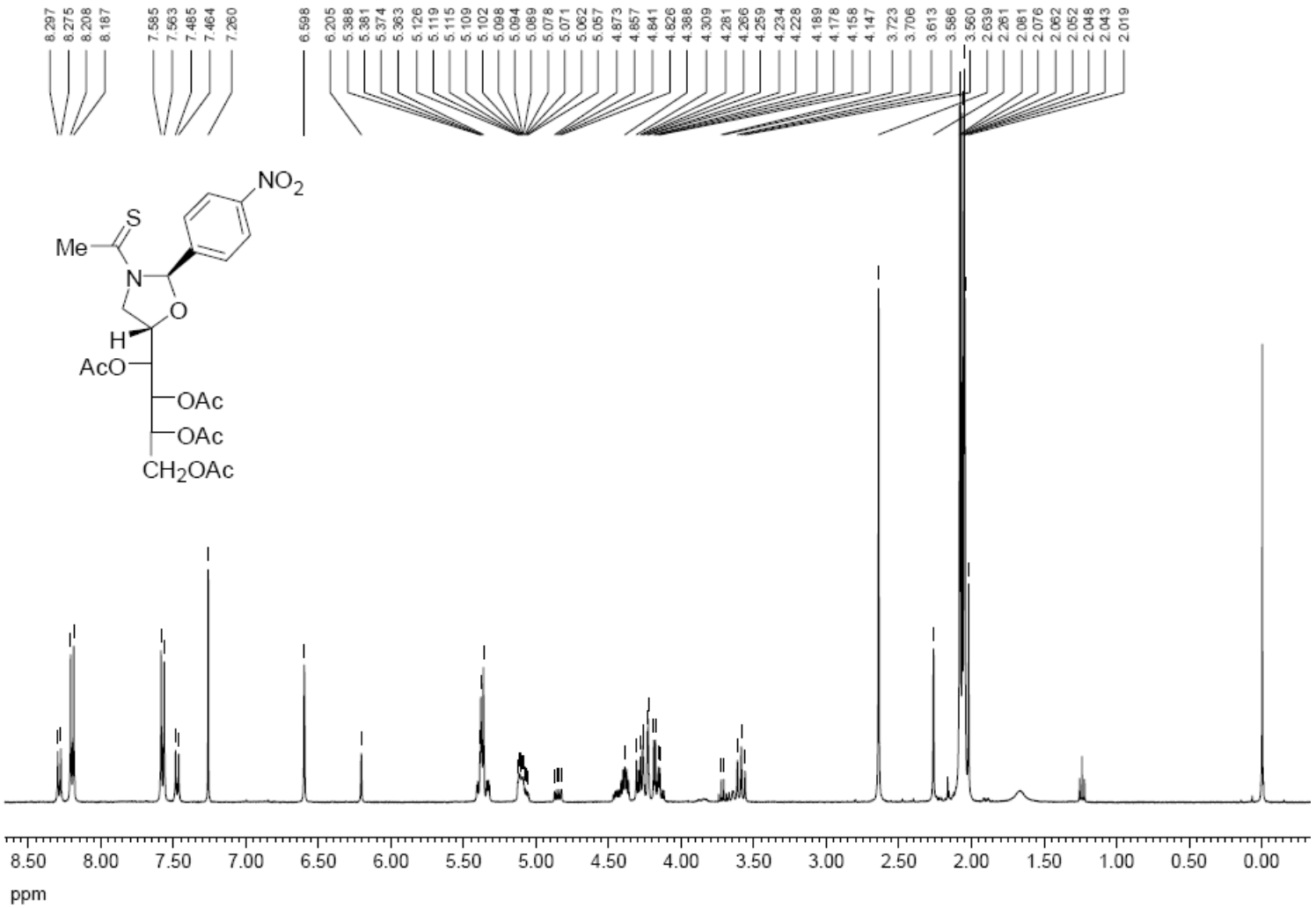
^{1}H-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**35*E,Z***)



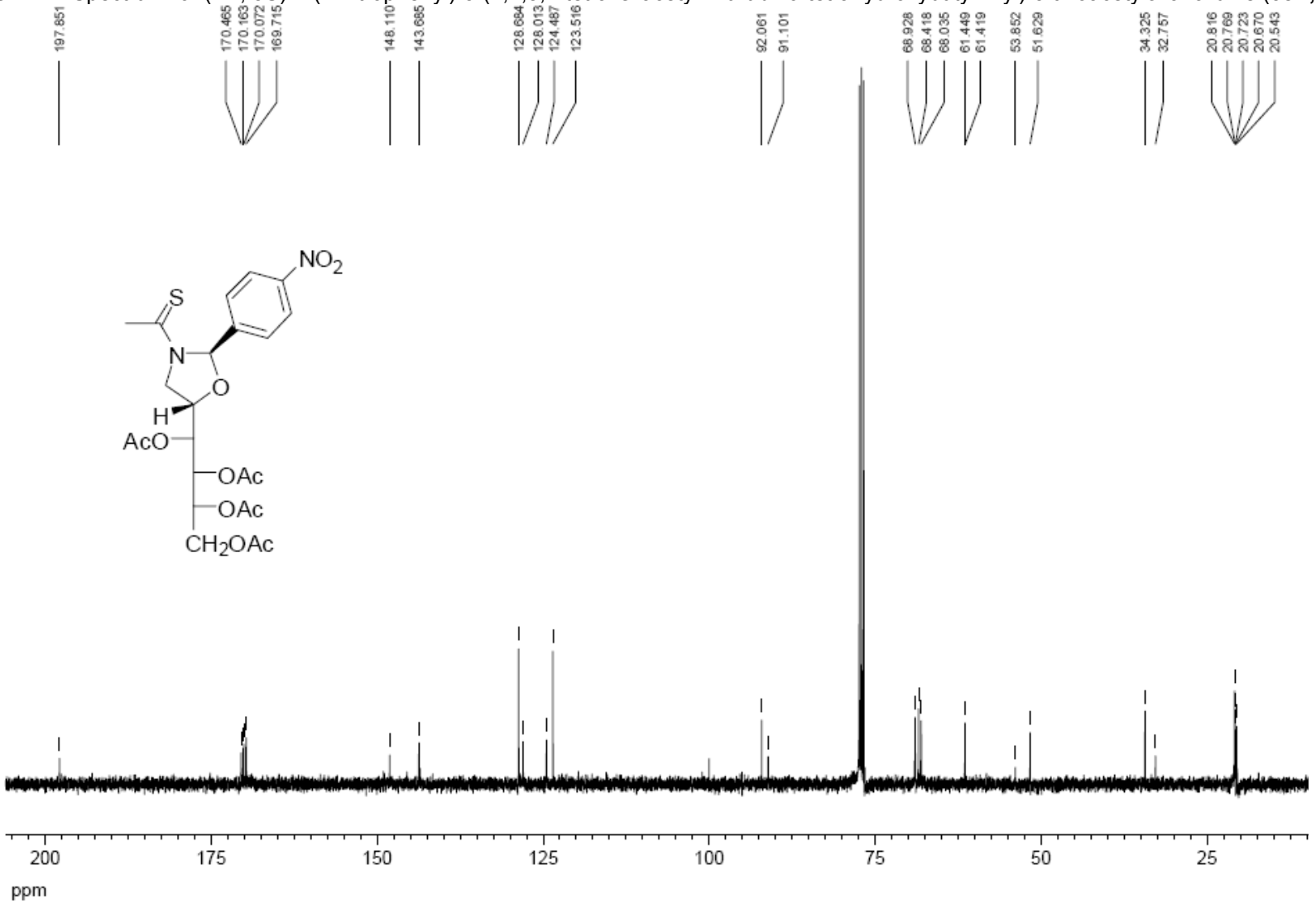
^{13}C-NMR Spectrum for (2*R*,5*S*)-3-acetyl-2-(4-dimethylaminophenyl)-5-(D-*arabino*-tetrahydroxybutyl-1-yl)oxazolidine (**35*E,Z***)



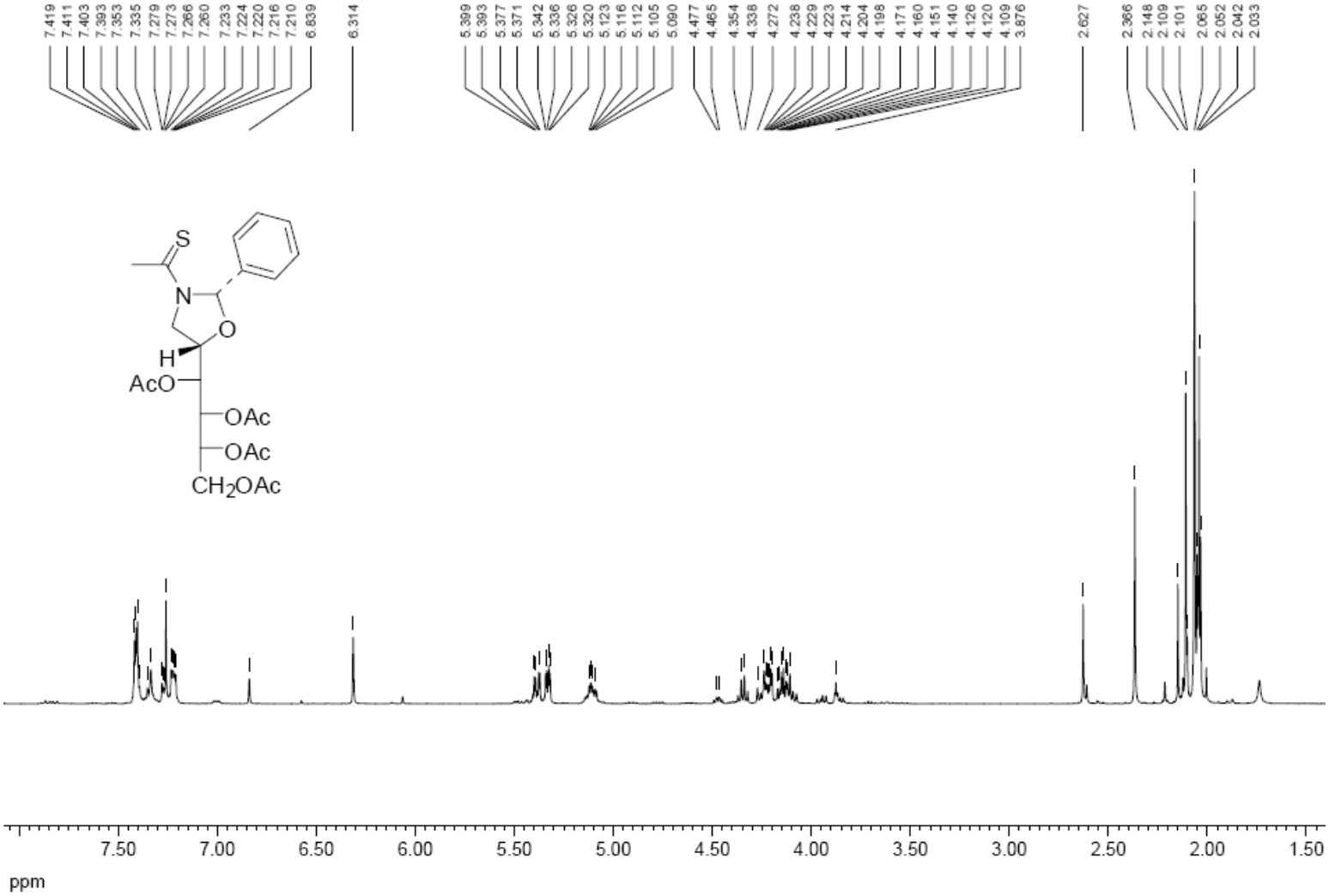
^{1}H-NMR Spectrum for (2*R*, 5*S*)-2-(4-nitrophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)-3-thioacetyloxazolidine (**38*E,Z***)



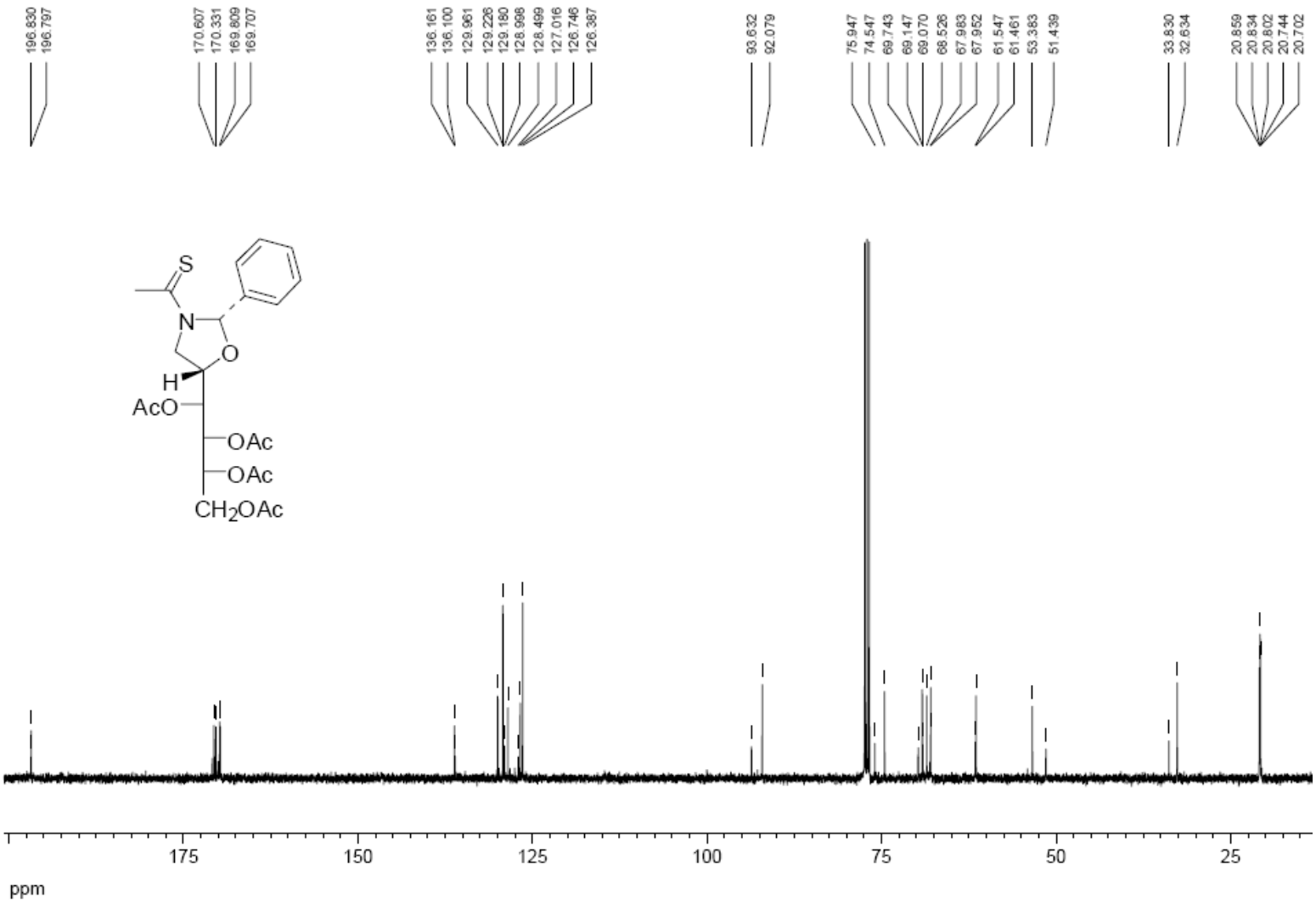
^{13}C-NMR Spectrum for (2*R*, 5*S*)-2-(4-nitrophenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)-3-thioacetyloxazolidine (**38*E*,*Z***)



^{1}H-NMR Spectrum for (2*S*, 5*S*)-2-(phenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)-3-thioacetyloxazolidine (**40*E,Z***)



^{13}C-NMR Spectrum for (2*S*, 5*S*)-2-(phenyl)-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetrahydroxybutyl-1-yl)-3-thioacetyloxazolidine (**40*E,Z***)



THEORETICAL CALCULATIONS

Cartesians coordinates for compound **1Z**

E= -1904.989685 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.283601	-0.192534	1.498851
2	6	0	2.136643	-1.266642	1.140929
3	7	0	1.316322	-2.079374	0.233538
4	6	0	0.265467	-1.256574	-0.359954
5	6	0	0.436360	0.097112	0.385863
6	6	0	3.446618	-0.797378	0.511172
7	6	0	3.764315	0.562664	0.422044
8	6	0	4.970697	0.970342	-0.145103
9	6	0	5.855612	0.000301	-0.607065
10	6	0	5.570906	-1.362205	-0.513436
11	6	0	4.361611	-1.756141	0.048542
12	7	0	7.129633	0.424369	-1.208041
13	8	0	7.894049	-0.453578	-1.608527
14	6	0	-0.881579	0.645952	0.955564
15	8	0	-0.716208	1.655231	1.962859
16	6	0	0.070256	2.739098	1.743119
17	8	0	0.688429	2.940311	0.718846
18	6	0	1.323260	-3.453850	0.323797
19	8	0	2.175805	-4.034082	0.989585
20	6	0	-1.911241	1.097180	-0.138107
21	8	0	-2.150718	2.501487	-0.091591

22	6	0	-1.708817	3.413632	-1.033114
23	8	0	-2.043303	4.557209	-0.878188
24	6	0	0.251207	-4.190445	-0.457509
25	6	0	-3.287267	0.433605	0.092587
26	8	0	-3.068359	-0.979945	-0.034517
27	6	0	-3.504125	-1.931621	0.867519
28	8	0	-3.078393	-3.049701	0.718249
29	6	0	0.052885	3.648352	2.944157
30	6	0	-4.330265	0.870916	-0.937462
31	8	0	-5.573864	0.239667	-0.634644
32	6	0	-6.077977	-0.828197	-1.334657
33	8	0	-6.999658	-1.428212	-0.842710
34	6	0	-0.859508	2.922722	-2.183506
35	6	0	-4.472129	-1.522826	1.952371
36	6	0	-5.468362	-1.171917	-2.677868
37	8	0	7.356423	1.632567	-1.277499
38	1	0	-5.462001	-0.310448	-3.354454
39	1	0	-4.438406	-1.525538	-2.561941
40	1	0	-0.719861	-1.701642	-0.199742
41	1	0	-6.068493	-1.969264	-3.116215
42	1	0	6.291530	-2.084949	-0.875759
43	1	0	-0.943786	4.091480	3.046312
44	1	0	5.232271	2.017904	-0.229845
45	1	0	0.261519	3.082565	3.856701
46	1	0	4.122096	-2.810819	0.143811
47	1	0	2.347841	-1.851943	2.040239
48	1	0	3.068685	1.305237	0.797743
49	1	0	0.409525	-1.125589	-1.439786
50	1	0	0.916773	0.832469	-0.262487
51	1	0	-3.643146	0.690060	1.094055
52	1	0	-1.323019	-0.173626	1.526846
53	1	0	-1.550330	0.791672	-1.124981
54	1	0	-4.493340	1.947748	-0.860968
55	1	0	-3.986630	0.632979	-1.948236
56	1	0	0.458100	-5.258843	-0.386366

57	1	0	0.249259	-3.891609	-1.512135
58	1	0	-0.749342	-3.990759	-0.054976
59	1	0	-4.007180	-0.823613	2.657096
60	1	0	-4.756913	-2.424768	2.494275
61	1	0	-5.361882	-1.045120	1.532355
62	1	0	-0.620270	3.786909	-2.803376
63	1	0	-1.383599	2.182441	-2.798248
64	1	0	0.068899	2.480281	-1.812580
65	1	0	0.790160	4.439998	2.809151

Cartesians coordinates for compound **1E**

E= -1904.987392 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.332463	0.767055	1.307437
2	6	0	-2.295760	1.642451	0.739687
3	7	0	-1.598471	2.260558	-0.386441
4	6	0	-0.410357	1.475753	-0.731048
5	6	0	-0.544867	0.264412	0.214309
6	6	0	-3.567825	0.881431	0.354823
7	6	0	-4.129311	0.953365	-0.923695
8	6	0	-5.298984	0.256602	-1.226184
9	6	0	-5.894593	-0.511724	-0.231179
10	6	0	-5.354989	-0.606946	1.051647
11	6	0	-4.189100	0.094074	1.336014
12	6	0	0.791721	-0.191911	0.808204
13	8	0	0.680594	-1.156237	1.869078

14	6	0	-0.044856	-2.297054	1.711162
15	8	0	-0.677305	-2.579775	0.718082
16	7	0	-7.132422	-1.247172	-0.541586
17	8	0	-7.583359	-1.149801	-1.682168
18	6	0	-1.693144	3.571110	-0.810024
19	8	0	-0.903664	4.014250	-1.631307
20	6	0	1.878211	-0.633004	-0.221864
21	8	0	2.022654	-2.051756	-0.283920
22	6	0	1.540679	-2.858952	-1.293744
23	8	0	1.845199	-4.021306	-1.255887
24	6	0	0.685336	-2.239594	-2.375296
25	6	0	-2.812984	4.407349	-0.211710
26	6	0	0.062565	-3.152710	2.947927
27	6	0	3.265021	-0.100883	0.209327
28	8	0	3.159524	1.324343	0.172123
29	6	0	3.747695	2.179334	1.088803
30	8	0	3.636524	3.357912	0.879776
31	6	0	4.449968	1.585571	2.288775
32	6	0	4.374077	-0.555947	-0.736016
33	8	0	5.605423	-0.097884	-0.170263
34	6	0	6.812144	-0.281793	-0.793776
35	8	0	7.804417	0.090840	-0.222547
36	6	0	6.805488	-0.933924	-2.159756
37	8	0	-7.640863	-1.913157	0.359297
38	1	0	-1.080461	-0.556081	-0.266761
39	1	0	4.798874	2.413765	2.905896
40	1	0	-5.847987	-1.221027	1.795024
41	1	0	-5.748233	0.299204	-2.210732
42	1	0	-0.417792	1.185362	-1.786440
43	1	0	1.179681	0.688320	1.324696
44	1	0	-2.917233	5.310639	-0.813987
45	1	0	0.494779	2.067663	-0.549273
46	1	0	1.224252	-1.468571	-2.937227
47	1	0	7.838222	-1.026704	-2.495647
48	1	0	1.647013	-0.212584	-1.205187

49	1	0	-3.769094	3.874916	-0.181346
50	1	0	-2.559382	4.704653	0.813676
51	1	0	0.396703	-3.036053	-3.061351
52	1	0	6.245978	-0.328918	-2.882193
53	1	0	-3.745814	0.022726	2.324689
54	1	0	-3.647417	1.551931	-1.689576
55	1	0	3.479759	-0.465078	1.218431
56	1	0	-2.535689	2.383209	1.509974
57	1	0	6.343743	-1.926940	-2.129876
58	1	0	5.300996	0.974441	1.976805
59	1	0	4.367056	-1.646636	-0.813901
60	1	0	4.211359	-0.112317	-1.725872
61	1	0	-0.661535	-3.965642	2.887953
62	1	0	1.073039	-3.572353	3.007089
63	1	0	-0.215606	-1.793011	-1.946314
64	1	0	-0.103353	-2.555737	3.849068
65	1	0	3.774137	0.959180	2.882642

Cartesians coordinates for compound **2Z**

E= -1904.989246 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.319280	0.428077	-1.478062
2	6	0	-2.344786	-0.514659	-1.208761
3	7	0	-1.671775	-1.549640	-0.418404
4	6	0	-0.496920	-0.984471	0.240161
5	6	0	-0.435671	0.451687	-0.356229

6	6	0	-3.539507	0.110959	-0.490040
7	6	0	-3.651313	1.497051	-0.337088
8	6	0	-4.761431	2.055316	0.304451
9	6	0	-5.777667	1.239830	0.791609
10	6	0	-5.653488	-0.139034	0.621094
11	6	0	-4.558492	-0.719471	-0.010740
12	7	0	-6.722753	-1.014219	1.135281
13	8	0	-6.580311	-2.228963	1.008281
14	6	0	0.957148	0.828494	-0.885731
15	8	0	0.969508	1.948818	-1.783529
16	6	0	0.374823	3.120854	-1.447221
17	8	0	-0.212586	3.317030	-0.403982
18	6	0	-1.905521	-2.884558	-0.674932
19	8	0	-2.841836	-3.227259	-1.389167
20	6	0	2.042829	0.987869	0.234548
21	8	0	2.508620	2.331820	0.333531
22	6	0	2.209667	3.201952	1.365832
23	8	0	2.718820	4.289551	1.322846
24	6	0	-0.972706	-3.877734	-0.007913
25	6	0	3.292442	0.136800	-0.081839
26	8	0	2.842711	-1.226611	-0.097751
27	6	0	3.124389	-2.139201	-1.096987
28	8	0	2.521813	-3.182457	-1.059167
29	6	0	0.562251	4.134791	-2.545785
30	6	0	4.388021	0.290629	0.975753
31	8	0	5.505261	-0.520108	0.614179
32	6	0	5.787405	-1.730686	1.197821
33	8	0	6.597369	-2.434468	0.650137
34	6	0	1.290326	2.735421	2.471897
35	6	0	4.153731	-1.782297	-2.142915
36	6	0	5.090567	-2.094651	2.492255
37	8	0	-7.694594	-0.475347	1.666125
38	1	0	5.233502	-1.326199	3.259829
39	1	0	4.015100	-2.227773	2.334873
40	1	0	0.398543	-1.570367	0.017251

41	1	0	5.516473	-3.035214	2.841569
42	1	0	1.618097	4.423838	-2.590471
43	1	0	-4.831613	3.132621	0.422012
44	1	0	0.291766	3.707005	-3.515293
45	1	0	-4.512048	-1.795103	-0.136743
46	1	0	-2.666492	-0.952066	-2.157588
47	1	0	-2.864382	2.139918	-0.717465
48	1	0	-0.616597	-0.946890	1.330317
49	1	0	-0.786230	1.184254	0.373749
50	1	0	3.689231	0.432948	-1.056712
51	1	0	1.257368	0.009298	-1.542807
52	1	0	1.632766	0.642150	1.188522
53	1	0	4.739040	1.324299	0.992299
54	1	0	3.998701	0.031861	1.964848
55	1	0	-1.354721	-4.880216	-0.203765
56	1	0	-0.924472	-3.714441	1.074867
57	1	0	0.048250	-3.798988	-0.400785
58	1	0	3.810124	-0.952262	-2.771297
59	1	0	4.297853	-2.659459	-2.773800
60	1	0	5.103559	-1.494445	-1.683512
61	1	0	1.191977	3.557076	3.181479
62	1	0	1.687485	1.860478	2.998444
63	1	0	0.303404	2.488291	2.071408
64	1	0	-0.045194	5.014854	-2.333418
65	1	0	-6.650320	1.641545	1.291074

Cartesians coordinates for compound **2E**

E= -1904.986958 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.411652	0.557784	1.469220
2	6	0	-2.600205	1.140599	0.961662
3	7	0	-2.170348	1.830321	-0.250687
4	6	0	-1.017743	1.110585	-0.798716
5	6	0	-0.659759	0.105969	0.332810
6	6	0	-3.681482	0.086361	0.702201
7	6	0	-4.684032	0.316492	-0.240980
8	6	0	-5.684455	-0.637392	-0.410582
9	6	0	-5.716838	-1.822349	0.321077
10	6	0	-4.705360	-2.048123	1.251889
11	6	0	-3.696753	-1.101595	1.445598
12	7	0	-6.739676	-0.385349	-1.407877
13	8	0	-6.688248	0.669110	-2.040526
14	6	0	0.821520	0.156494	0.725491
15	8	0	1.142565	-0.428500	2.004628
16	6	0	0.589968	-1.596581	2.443917
17	8	0	-0.255303	-2.230963	1.858817
18	6	0	-2.311713	3.181597	-0.526607
19	8	0	-1.641140	3.710597	-1.399842
20	6	0	1.800164	-0.390334	-0.336564
21	8	0	1.827500	-1.820939	-0.309582
22	6	0	1.340026	-2.647486	-1.294291
23	8	0	1.507956	-3.830605	-1.160406
24	6	0	0.647325	-2.027253	-2.490940
25	6	0	-3.342695	3.950345	0.284418
26	6	0	1.190898	-1.968463	3.778337
27	6	0	3.243389	0.070438	-0.030219
28	8	0	3.237625	1.495616	-0.132341
29	6	0	3.905042	2.334164	0.742599
30	8	0	3.921957	3.505147	0.471339
31	6	0	4.528041	1.733369	1.982787
32	6	0	4.264026	-0.493720	-1.015040

33	8	0	5.548630	-0.113892	-0.511656
34	6	0	6.707478	-0.346762	-1.205175
35	8	0	7.749037	-0.044282	-0.682520
36	6	0	6.590653	-0.958540	-2.585027
37	8	0	-7.610019	-1.243666	-1.546901
38	1	0	-0.969040	-0.908736	0.077079
39	1	0	4.939071	2.552864	2.572662
40	1	0	-4.698017	-2.969564	1.826016
41	1	0	-1.274805	0.597761	-1.731771
42	1	0	1.064930	1.212273	0.868315
43	1	0	-3.518988	4.901625	-0.218879
44	1	0	-0.227226	1.835675	-1.017744
45	1	0	1.323899	-1.382035	-3.062790
46	1	0	7.597610	-1.118859	-2.970143
47	1	0	1.514181	-0.005752	-1.320869
48	1	0	-4.290860	3.413123	0.386904
49	1	0	-2.961216	4.159548	1.291673
50	1	0	0.312578	-2.841544	-3.133595
51	1	0	6.050033	-0.290377	-3.265114
52	1	0	-2.897980	-1.293283	2.153954
53	1	0	-4.693415	1.208853	-0.854351
54	1	0	3.502466	-0.263243	0.976618
55	1	0	-2.949057	1.855009	1.712006
56	1	0	6.055109	-1.913887	-2.561063
57	1	0	5.329359	1.038499	1.715474
58	1	0	4.178901	-1.583626	-1.061334
59	1	0	4.089744	-0.064085	-2.008725
60	1	0	0.669079	-2.838769	4.177141
61	1	0	2.252569	-2.207121	3.652525
62	1	0	-0.218393	-1.426595	-2.196665
63	1	0	1.120340	-1.130234	4.478017
64	1	0	3.785020	1.194537	2.581831
65	1	0	-6.511985	-2.537029	0.149067

Cartesians coordinates for compound **3Z**

E= -1792.734337 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.595062	-0.163591	1.418195
2	6	0	2.452275	-1.226527	1.035582
3	7	0	1.612760	-2.054423	0.159378
4	6	0	0.532119	-1.248059	-0.402271
5	6	0	0.713838	0.112263	0.328870
6	6	0	3.732475	-0.739763	0.359965
7	6	0	4.031808	0.623078	0.263691
8	6	0	5.211580	1.044995	-0.345724
9	6	0	6.114368	0.099542	-0.855306
10	6	0	5.824010	-1.271913	-0.743087
11	6	0	4.641985	-1.683986	-0.139490
12	6	0	7.328685	0.530185	-1.485262
13	7	0	8.312832	0.880302	-1.997749
14	6	0	-0.591690	0.655239	0.931613
15	8	0	-0.406260	1.670918	1.929168
16	6	0	0.367664	2.758163	1.684354
17	8	0	0.958096	2.958823	0.643674
18	6	0	1.640271	-3.427946	0.254397
19	8	0	2.522479	-3.995394	0.892155
20	6	0	-1.652240	1.094287	-0.137081
21	8	0	-1.901618	2.496999	-0.089301

22	6	0	-1.489201	3.409466	-1.043617
23	8	0	-1.827705	4.551218	-0.883554
24	6	0	0.551781	-4.181290	-0.487712
25	6	0	-3.017231	0.421377	0.128805
26	8	0	-2.791155	-0.991134	0.003473
27	6	0	-3.198144	-1.941097	0.920695
28	8	0	-2.767389	-3.056706	0.767673
29	6	0	0.376114	3.672422	2.881770
30	6	0	-4.086570	0.846107	-0.879269
31	8	0	-5.317906	0.205711	-0.547112
32	6	0	-5.826837	-0.870040	-1.231498
33	8	0	-6.733728	-1.474898	-0.718479
34	6	0	-0.665288	2.921329	-2.213481
35	6	0	-4.143890	-1.533319	2.025475
36	6	0	-5.240905	-1.215889	-2.584746
37	1	0	-5.256139	-0.358279	-3.266088
38	1	0	-4.205592	-1.559310	-2.487550
39	1	0	-0.441829	-1.702882	-0.204549
40	1	0	-5.842295	-2.021181	-3.006537
41	1	0	6.528187	-2.002440	-1.128424
42	1	0	-0.620102	4.110420	3.007694
43	1	0	5.439010	2.103208	-0.426345
44	1	0	0.611392	3.111702	3.790948
45	1	0	4.419613	-2.742147	-0.039672
46	1	0	2.700695	-1.805344	1.929456
47	1	0	3.341592	1.356701	0.666450
48	1	0	0.636330	-1.122767	-1.487371
49	1	0	1.169610	0.846330	-0.338583
50	1	0	-3.351957	0.680255	1.136897
51	1	0	-1.012435	-0.163898	1.518902
52	1	0	-1.313155	0.788324	-1.131548
53	1	0	-4.256896	1.921827	-0.802979
54	1	0	-3.763437	0.607456	-1.896613
55	1	0	0.772371	-5.246931	-0.416211
56	1	0	0.513543	-3.889779	-1.543722

57	1	0	-0.437947	-3.989542	-0.055666
58	1	0	-3.668349	-0.825886	2.714744
59	1	0	-4.408615	-2.434059	2.579408
60	1	0	-5.047001	-1.065506	1.623145
61	1	0	-0.447640	3.785523	-2.841241
62	1	0	-1.199095	2.175780	-2.813306
63	1	0	0.275018	2.486295	-1.864449
64	1	0	1.105116	4.467661	2.724649

Cartesians coordinates for compound **3E**

E= -1792.731878 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.641832	0.675680	1.280382
2	6	0	-2.632648	1.512316	0.700964
3	7	0	-1.943892	2.161907	-0.413001
4	6	0	-0.732260	1.412797	-0.754591
5	6	0	-0.829782	0.199401	0.194056
6	6	0	-3.866104	0.702572	0.291821
7	6	0	-4.435034	0.791732	-0.981659
8	6	0	-5.570827	0.051664	-1.305466
9	6	0	-6.150470	-0.793434	-0.347885
10	6	0	-5.579208	-0.891330	0.933511
11	6	0	-4.447914	-0.147332	1.243521
12	6	0	0.519579	-0.206150	0.795659
13	8	0	0.440026	-1.165313	1.864304
14	6	0	-0.251680	-2.328507	1.718256

15	8	0	-0.878944	-2.638730	0.730256
16	6	0	-7.320832	-1.555738	-0.674083
17	7	0	-8.271110	-2.172597	-0.937805
18	6	0	-2.069389	3.473714	-0.822980
19	8	0	-1.284862	3.947127	-1.632286
20	6	0	1.622530	-0.619329	-0.227470
21	8	0	1.801927	-2.034363	-0.289720
22	6	0	1.341151	-2.853399	-1.299646
23	8	0	1.672327	-4.008409	-1.260135
24	6	0	0.475145	-2.254886	-2.384470
25	6	0	-3.216576	4.273691	-0.226377
26	6	0	-0.114316	-3.169581	2.962239
27	6	0	2.993485	-0.054446	0.212577
28	8	0	2.855413	1.367971	0.173344
29	6	0	3.420592	2.236333	1.091935
30	8	0	3.290498	3.412109	0.878277
31	6	0	4.122513	1.658607	2.299868
32	6	0	4.119450	-0.483925	-0.724834
33	8	0	5.335795	0.003441	-0.150942
34	6	0	6.550535	-0.151175	-0.766631
35	8	0	7.529825	0.246133	-0.189623
36	6	0	6.568445	-0.804821	-2.131818
37	1	0	-1.332428	-0.641264	-0.287518
38	1	0	4.449825	2.494505	2.918434
39	1	0	-6.025474	-1.550745	1.670773
40	1	0	-6.009136	0.122254	-2.295718
41	1	0	-0.728844	1.119222	-1.809221
42	1	0	0.876812	0.690906	1.305421
43	1	0	-3.341039	5.178821	-0.822061
44	1	0	0.153752	2.032939	-0.573192
45	1	0	0.997886	-1.471562	-2.944655
46	1	0	7.605296	-0.873512	-2.460767
47	1	0	1.387021	-0.203549	-1.211814
48	1	0	-4.157990	3.715157	-0.207446
49	1	0	-2.978722	4.569429	0.803204

50	1	0	0.207753	-3.058189	-3.071152
51	1	0	5.999579	-0.214041	-2.858717
52	1	0	-3.998599	-0.233880	2.228290
53	1	0	-3.983097	1.437160	-1.727782
54	1	0	3.209751	-0.412799	1.223411
55	1	0	-2.912084	2.240810	1.469438
56	1	0	6.130063	-1.808391	-2.103531
57	1	0	4.988019	1.063516	1.996947
58	1	0	4.138862	-1.574489	-0.802189
59	1	0	3.953074	-0.044626	-1.716003
60	1	0	-0.810483	-4.007090	2.910072
61	1	0	0.909839	-3.554117	3.024313
62	1	0	-0.437692	-1.829074	-1.959608
63	1	0	-0.299828	-2.570779	3.858376
64	1	0	3.453190	1.020414	2.888495

Cartesians coordinates for compound **4Z**

E= -2037.525349 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.978848	-0.220826	1.583413
2	6	0	1.824727	-1.309199	1.245079
3	7	0	1.014276	-2.100591	0.311018
4	6	0	0.026000	-1.243186	-0.335602
5	6	0	0.177073	0.094881	0.445007
6	6	0	3.158723	-0.859849	0.654275

7	6	0	3.516655	0.490573	0.606595
8	6	0	4.748098	0.874579	0.074766
9	6	0	5.634946	-0.092403	-0.400536
10	6	0	5.289499	-1.446430	-0.338837
11	6	0	4.058874	-1.827706	0.187008
12	6	0	6.936044	0.323246	-1.029805
13	9	0	6.802262	0.534760	-2.362087
14	6	0	-1.160243	0.635207	0.976145
15	8	0	-1.032514	1.628783	2.004792
16	6	0	-0.237558	2.715079	1.832454
17	8	0	0.412437	2.937646	0.832952
18	6	0	0.979695	-3.474255	0.393654
19	8	0	1.784909	-4.082459	1.092642
20	6	0	-2.155439	1.100970	-0.141892
21	8	0	-2.382802	2.507775	-0.098340
22	6	0	-1.897813	3.418644	-1.018705
23	8	0	-2.231645	4.564165	-0.875861
24	6	0	-0.076820	-4.177604	-0.438873
25	6	0	-3.544295	0.452519	0.052349
26	8	0	-3.340775	-0.962851	-0.079945
27	6	0	-3.817574	-1.914925	0.800444
28	8	0	-3.420026	-3.042021	0.642809
29	6	0	-0.290118	3.597585	3.052712
30	6	0	-4.558099	0.909975	-0.998063
31	8	0	-5.817125	0.293350	-0.729362
32	6	0	-6.315691	-0.767110	-1.444216
33	8	0	-7.262026	-1.351841	-0.981418
34	6	0	-1.005524	2.924533	-2.134705
35	6	0	-4.791267	-1.494462	1.875864
36	6	0	-5.668998	-1.122713	-2.766859
37	9	0	7.410908	1.473103	-0.500139
38	9	0	7.893926	-0.618764	-0.879867
39	1	0	-5.631880	-0.263683	-3.445610
40	1	0	-4.647295	-1.487577	-2.617915
41	1	0	-0.977790	-1.667636	-0.250064

42	1	0	-6.264775	-1.914420	-3.221073
43	1	0	5.987163	-2.198268	-0.693052
44	1	0	-1.289782	4.037537	3.137698
45	1	0	5.021396	1.924216	0.039940
46	1	0	-0.105652	3.011493	3.957646
47	1	0	3.793911	-2.878751	0.252625
48	1	0	1.994902	-1.902966	2.147160
49	1	0	2.834524	1.242706	0.988875
50	1	0	0.245704	-1.096120	-1.400723
51	1	0	0.685079	0.840568	-0.169401
52	1	0	-3.919315	0.706685	1.047379
53	1	0	-1.618464	-0.194666	1.518838
54	1	0	-1.773290	0.794388	-1.120401
55	1	0	-4.709527	1.988116	-0.917241
56	1	0	-4.194231	0.675192	-2.002478
57	1	0	0.101206	-5.251300	-0.368732
58	1	0	-0.027754	-3.870808	-1.490091
59	1	0	-1.088188	-3.957740	-0.075823
60	1	0	-4.318379	-0.817906	2.597235
61	1	0	-5.108854	-2.395671	2.400463
62	1	0	-5.661310	-0.987309	1.449187
63	1	0	-0.736572	3.788110	-2.743172
64	1	0	-1.508513	2.188010	-2.771205
65	1	0	-0.095448	2.476154	-1.727263
66	1	0	0.449721	4.392415	2.955913

Cartesians coordinates for compound **4E**

E= -2037.523857 HF

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-1.024470	0.865803	1.305821
2	6	0	-1.981900	1.749268	0.736540
3	7	0	-1.288173	2.329240	-0.413159
4	6	0	-0.121799	1.515501	-0.759772
5	6	0	-0.265290	0.326213	0.211613
6	6	0	-3.276225	1.011446	0.388852
7	6	0	-3.837945	1.033464	-0.889330
8	6	0	-5.029570	0.354745	-1.152260
9	6	0	-5.665046	-0.354458	-0.134017
10	6	0	-5.106134	-0.388027	1.148724
11	6	0	-3.920683	0.291305	1.404802
12	6	0	1.072007	-0.141856	0.794691
13	8	0	0.960131	-1.088200	1.872326
14	6	0	0.212067	-2.218307	1.743615
15	8	0	-0.433334	-2.510852	0.762127
16	6	0	-6.979394	-1.042255	-0.389687
17	9	0	-7.152947	-1.334218	-1.696834
18	6	0	-1.379462	3.623106	-0.881075
19	8	0	-0.600127	4.031603	-1.730657
20	6	0	2.143485	-0.613390	-0.235478
21	8	0	2.243952	-2.035876	-0.305716
22	6	0	1.727218	-2.824704	-1.311854
23	8	0	2.004575	-3.994373	-1.286253
24	6	0	0.868101	-2.179073	-2.374830
25	6	0	-2.482738	4.488212	-0.293303
26	6	0	0.312368	-3.048043	2.998886
27	6	0	3.546054	-0.130012	0.202319
28	8	0	3.493864	1.298039	0.159526
29	6	0	4.112237	2.131634	1.075387
30	8	0	4.065615	3.312233	0.853589
31	6	0	4.764318	1.515472	2.292644
32	6	0	4.644549	-0.627393	-0.733897
33	8	0	5.887148	-0.209078	-0.161126

34	6	0	7.089932	-0.429185	-0.779665
35	8	0	8.091587	-0.093879	-0.201484
36	6	0	7.068482	-1.070531	-2.150708
37	9	0	-7.081527	-2.197953	0.303808
38	9	0	-8.025674	-0.268889	-0.015014
39	1	0	-0.824104	-0.492851	-0.244777
40	1	0	5.138283	2.331670	2.911079
41	1	0	-5.595042	-0.951852	1.936649
42	1	0	-5.457327	0.370930	-2.149015
43	1	0	-0.150804	1.205024	-1.809160
44	1	0	1.478356	0.740914	1.292641
45	1	0	-2.582324	5.377262	-0.917190
46	1	0	0.797904	2.092449	-0.603154
47	1	0	1.410333	-1.408465	-2.934002
48	1	0	8.099362	-1.199005	-2.480493
49	1	0	1.929203	-0.179355	-1.216751
50	1	0	-3.443799	3.966573	-0.241138
51	1	0	-2.216592	4.807249	0.722325
52	1	0	0.558272	-2.962300	-3.066841
53	1	0	6.537024	-0.439113	-2.871768
54	1	0	-3.479310	0.253281	2.396685
55	1	0	-3.341375	1.578035	-1.686007
56	1	0	3.741230	-0.498127	1.213843
57	1	0	-2.188162	2.510783	1.496326
58	1	0	6.569596	-2.045684	-2.132332
59	1	0	5.593684	0.865662	2.000845
60	1	0	4.601179	-1.717505	-0.806996
61	1	0	4.503737	-0.182983	-1.726684
62	1	0	-0.413121	-3.860599	2.952570
63	1	0	1.321895	-3.467049	3.074708
64	1	0	-0.020143	-1.724860	-1.927602
65	1	0	0.141022	-2.430884	3.885452
66	1	0	4.050241	0.923492	2.876860

Cartesians coordinates for compound **6Z**

E= -1928.321962 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.035891	-0.207227	1.428763
2	6	0	1.864907	-1.298168	1.055883
3	7	0	1.001351	-2.103434	0.183040
4	6	0	-0.020391	-1.254930	-0.421325
5	6	0	0.173368	0.093710	0.331941
6	6	0	3.158540	-0.850807	0.380501
7	6	0	3.506785	0.500399	0.293584
8	6	0	4.700298	0.886981	-0.320258
9	6	0	5.554580	-0.086475	-0.832010
10	6	0	5.224509	-1.440338	-0.748326
11	6	0	4.030477	-1.818497	-0.139103
12	8	0	6.707780	0.299760	-1.509183
13	6	0	7.924443	0.436661	-0.873518
14	6	0	7.967204	0.149786	0.612006
15	6	0	-1.133283	0.644273	0.925485
16	8	0	-0.950538	1.646423	1.937660
17	6	0	-0.159232	2.726428	1.717427
18	8	0	0.446185	2.935163	0.687353
19	6	0	0.979551	-3.475590	0.279019
20	8	0	1.829331	-4.073735	0.933230
21	6	0	-2.178088	1.106552	-0.147732

22	8	0	-2.396730	2.514835	-0.104020
23	6	0	-1.951471	3.417039	-1.052816
24	8	0	-2.270690	4.565542	-0.900710
25	6	0	-0.121373	-4.192144	-0.481878
26	6	0	-3.559384	0.466441	0.113937
27	8	0	-3.368291	-0.950844	-0.015486
28	6	0	-3.809765	-1.893339	0.893341
29	8	0	-3.422723	-3.023146	0.729257
30	6	0	-0.153542	3.623049	2.928562
31	6	0	-4.616213	0.920726	-0.894631
32	8	0	-5.863476	0.307413	-0.570046
33	6	0	-6.394276	-0.753414	-1.260963
34	8	0	-7.321482	-1.335012	-0.757385
35	6	0	-1.117777	2.910713	-2.207847
36	6	0	-4.736098	-1.459827	2.005005
37	6	0	-5.804960	-1.112848	-2.609256
38	8	0	8.872401	0.773947	-1.532294
39	1	0	-5.795793	-0.255341	-3.290879
40	1	0	-4.778328	-1.478956	-2.503630
41	1	0	-1.018281	-1.677042	-0.276642
42	1	0	-6.420825	-1.904586	-3.035780
43	1	0	5.898075	-2.181290	-1.168584
44	1	0	-1.146455	4.069100	3.052119
45	1	0	4.968094	1.935305	-0.412305
46	1	0	0.067751	3.046532	3.831386
47	1	0	3.770653	-2.869788	-0.056619
48	1	0	2.087244	-1.879450	1.954619
49	1	0	2.843360	1.255433	0.702583
50	1	0	0.141967	-1.122390	-1.498608
51	1	0	0.646974	0.830114	-0.320014
52	1	0	-3.888803	0.730196	1.122461
53	1	0	-1.569090	-0.177908	1.497451
54	1	0	-1.842635	0.790896	-1.140433
55	1	0	-4.762028	1.999604	-0.813058
56	1	0	-4.295630	0.680358	-1.912352

57	1	0	0.059490	-5.264707	-0.402269
58	1	0	-0.128320	-3.904564	-1.539687
59	1	0	-1.111911	-3.963867	-0.070049
60	1	0	-4.233073	-0.774112	2.696649
61	1	0	-5.030209	-2.354527	2.553872
62	1	0	-5.624043	-0.958245	1.609646
63	1	0	-0.872441	3.769160	-2.833300
64	1	0	-1.656078	2.174686	-2.815396
65	1	0	-0.192320	2.457609	-1.842627
66	1	0	0.584771	4.413153	2.790039
67	1	0	7.284354	0.806714	1.160107
68	1	0	7.661058	-0.879718	0.823280
69	1	0	8.988891	0.308460	0.957460

Cartesians coordinates for compound **6E**

E= -1928.321271 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.046578	0.711533	1.293185
2	6	0	-2.030821	1.564412	0.722072
3	7	0	-1.341559	2.190832	-0.406544
4	6	0	-0.144165	1.422991	-0.752588
5	6	0	-0.254462	0.215956	0.202131
6	6	0	-3.287410	0.782477	0.336872
7	6	0	-3.834811	0.816184	-0.948294
8	6	0	-4.990106	0.091916	-1.251208
9	6	0	-5.601937	-0.668078	-0.257485

10	6	0	-5.061584	-0.726438	1.029391
11	6	0	-3.911059	0.000611	1.319818
12	6	0	1.093475	-0.208377	0.794365
13	8	0	1.007291	-1.169398	1.861201
14	6	0	0.304279	-2.325402	1.713278
15	8	0	-0.320221	-2.631477	0.722392
16	8	0	-6.708336	-1.447031	-0.572395
17	6	0	-8.003222	-0.986134	-0.428206
18	6	0	-8.182016	0.426744	0.083652
19	6	0	-1.470036	3.489329	-0.849948
20	8	0	-0.695609	3.941641	-1.681771
21	6	0	2.189343	-0.629000	-0.233175
22	8	0	2.357545	-2.045189	-0.302192
23	6	0	1.883971	-2.856914	-1.311928
24	8	0	2.215113	-4.012437	-1.284186
25	6	0	1.002927	-2.251196	-2.380274
26	6	0	-2.608250	4.306202	-0.258653
27	6	0	0.425245	-3.165249	2.959990
28	6	0	3.566931	-0.079497	0.206102
29	8	0	3.445026	1.344620	0.171653
30	6	0	4.020196	2.202655	1.092988
31	8	0	3.906923	3.380870	0.882576
32	6	0	4.711981	1.612427	2.300930
33	6	0	4.686984	-0.517558	-0.734267
34	8	0	5.909287	-0.044190	-0.160630
35	6	0	7.120875	-0.208166	-0.779410
36	8	0	8.105651	0.176248	-0.202778
37	6	0	7.129432	-0.855139	-2.147935
38	8	0	-8.902501	-1.728882	-0.717168
39	1	0	-0.776061	-0.617522	-0.271830
40	1	0	5.048261	2.442319	2.922773
41	1	0	-5.537219	-1.350360	1.779936
42	1	0	-5.410077	0.099760	-2.252409
43	1	0	-0.152476	1.125346	-1.806101
44	1	0	1.462252	0.683224	1.305500

45	1	0	-2.736959	5.198446	-0.872650
46	1	0	0.752968	2.029758	-0.579601
47	1	0	1.514269	-1.458802	-2.938113
48	1	0	8.164943	-0.933548	-2.478934
49	1	0	1.955838	-0.207074	-1.215326
50	1	0	-3.549681	3.748953	-0.217645
51	1	0	-2.358751	4.622911	0.761893
52	1	0	0.731209	-3.048386	-3.072374
53	1	0	6.565945	-0.254398	-2.870847
54	1	0	-3.478878	-0.052039	2.315211
55	1	0	-3.352304	1.404003	-1.722757
56	1	0	3.780982	-0.443369	1.215403
57	1	0	-2.276507	2.304842	1.490826
58	1	0	6.679910	-1.853876	-2.124141
59	1	0	5.570852	1.007587	1.998329
60	1	0	4.695341	-1.607967	-0.814802
61	1	0	4.523719	-0.073598	-1.723841
62	1	0	-0.272711	-4.000774	2.900742
63	1	0	1.447613	-3.551964	3.035828
64	1	0	0.093456	-1.835728	-1.938282
65	1	0	0.229835	-2.564235	3.852603
66	1	0	4.033301	0.980839	2.885920
67	1	0	-7.736557	0.545240	1.076632
68	1	0	-7.694137	1.150017	-0.577589
69	1	0	-9.250750	0.635559	0.133067

Cartesians coordinates for compound **7Z**

E= -2160.094282 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.491393	-0.144062	1.441323
2	6	0	2.344570	-1.219260	1.076725
3	7	0	1.504173	-2.041384	0.196308
4	6	0	0.471625	-1.213186	-0.417157
5	6	0	0.630106	0.138303	0.338839
6	6	0	3.635666	-0.748130	0.413840
7	6	0	3.954919	0.609002	0.319238
8	6	0	5.147937	1.020036	-0.279915
9	6	0	6.026361	0.058991	-0.772621
10	6	0	5.735568	-1.302238	-0.672405
11	6	0	4.539924	-1.699489	-0.078200
12	17	0	7.532169	0.568032	-1.530105
13	6	0	-0.692744	0.657042	0.924844
14	8	0	-0.540165	1.666316	1.934965
15	6	0	0.226963	2.764113	1.716214
16	8	0	0.828124	2.987339	0.686760
17	6	0	1.506536	-3.413718	0.293337
18	8	0	2.360252	-3.996357	0.956005
19	6	0	-1.746284	1.087949	-0.152407
20	8	0	-1.997457	2.491197	-0.119470
21	6	0	-1.568785	3.396493	-1.072522
22	8	0	-1.916968	4.538072	-0.931906
23	6	0	0.425384	-4.150493	-0.476918
24	6	0	-3.112914	0.418362	0.113259
25	8	0	-2.890230	-0.995207	-0.007119
26	6	0	-3.308506	-1.941332	0.908897
27	8	0	-2.900055	-3.064132	0.749036
28	6	0	0.213038	3.658595	2.928869
29	6	0	-4.180006	0.841660	-0.897804
30	8	0	-5.413911	0.205317	-0.566123
31	6	0	-5.921729	-0.874449	-1.244679
32	8	0	-6.837231	-1.469244	-0.735072

33	6	0	-0.716259	2.901697	-2.218903
34	6	0	-4.237963	-1.519964	2.022654
35	6	0	-5.323474	-1.237775	-2.588001
36	1	0	-5.331540	-0.388548	-3.279930
37	1	0	-4.289493	-1.580774	-2.476786
38	1	0	-0.518915	-1.655602	-0.282372
39	1	0	-5.922084	-2.047382	-3.005456
40	1	0	6.436684	-2.038066	-1.051983
41	1	0	-0.792609	4.071802	3.062644
42	1	0	5.392018	2.074199	-0.358779
43	1	0	0.461142	3.087381	3.828176
44	1	0	4.308179	-2.756392	0.017124
45	1	0	2.569832	-1.795890	1.977685
46	1	0	3.272351	1.353530	0.715989
47	1	0	0.641397	-1.076127	-1.492788
48	1	0	1.091235	0.886009	-0.309067
49	1	0	-3.448433	0.681311	1.119970
50	1	0	-1.108559	-0.175138	1.497276
51	1	0	-1.403407	0.772934	-1.142745
52	1	0	-4.348486	1.917843	-0.825142
53	1	0	-3.855817	0.599317	-1.913937
54	1	0	0.627972	-5.219323	-0.399308
55	1	0	0.418561	-3.859803	-1.533858
56	1	0	-0.572025	-3.944358	-0.069796
57	1	0	-3.745570	-0.820009	2.707661
58	1	0	-4.511228	-2.417118	2.578241
59	1	0	-5.137868	-1.038960	1.628697
60	1	0	-0.487527	3.761244	-2.849117
61	1	0	-1.233608	2.148950	-2.824171
62	1	0	0.217296	2.473005	-1.845006
63	1	0	0.924795	4.471935	2.786112

Cartesians coordinates for compound **7E**

E= -2160.093091 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.524853	0.702623	1.276459
2	6	0	-2.516259	1.547353	0.704583
3	7	0	-1.831236	2.179624	-0.423500
4	6	0	-0.624918	1.424770	-0.766019
5	6	0	-0.726791	0.215406	0.186347
6	6	0	-3.765536	0.754873	0.319446
7	6	0	-4.310227	0.778317	-0.966331
8	6	0	-5.461548	0.047779	-1.270409
9	6	0	-6.065765	-0.712096	-0.272708
10	6	0	-5.537686	-0.754919	1.019225
11	6	0	-4.391041	-0.020035	1.305737
12	6	0	0.623390	-0.197918	0.781041
13	8	0	0.543341	-1.163334	1.844748
14	6	0	-0.151041	-2.324024	1.692999
15	8	0	-0.770397	-2.633642	0.700028
16	17	0	-7.516228	-1.632894	-0.642601
17	6	0	-1.972301	3.476340	-0.868806
18	8	0	-1.199003	3.935433	-1.698161
19	6	0	1.727812	-0.604523	-0.242022
20	8	0	1.900025	-2.019653	-0.326111
21	6	0	1.431839	-2.821851	-1.345347

22	8	0	1.765368	-3.976996	-1.328693
23	6	0	0.553294	-2.207275	-2.410774
24	6	0	-3.121899	4.280964	-0.283398
25	6	0	-0.028269	-3.164056	2.939539
26	6	0	3.100563	-0.057697	0.215427
27	8	0	2.978041	1.366558	0.192838
28	6	0	3.546279	2.215700	1.126621
29	8	0	3.443165	3.395831	0.922048
30	6	0	4.217550	1.613767	2.340418
31	6	0	4.230495	-0.485639	-0.717766
32	8	0	5.446265	-0.016440	-0.126798
33	6	0	6.664587	-0.175342	-0.733319
34	8	0	7.643019	0.204186	-0.142772
35	6	0	6.688295	-0.811260	-2.106890
36	1	0	-1.240328	-0.621802	-0.289851
37	1	0	4.546389	2.437622	2.974153
38	1	0	-6.018228	-1.356503	1.783274
39	1	0	-5.881628	0.067655	-2.270348
40	1	0	-0.625831	1.129165	-1.820149
41	1	0	0.981731	0.695802	1.295997
42	1	0	-3.254677	5.173579	-0.895963
43	1	0	0.265612	2.039969	-0.588190
44	1	0	1.063780	-1.406251	-2.956911
45	1	0	7.727413	-0.887289	-2.426974
46	1	0	1.501735	-0.171456	-1.221035
47	1	0	-4.058437	3.715033	-0.250507
48	1	0	-2.882784	4.597158	0.739804
49	1	0	0.288048	-2.997424	-3.113382
50	1	0	6.132924	-0.204590	-2.831126
51	1	0	-3.968220	-0.058331	2.305896
52	1	0	-3.832975	1.367805	-1.742869
53	1	0	3.305213	-0.430740	1.223293
54	1	0	-2.768903	2.285463	1.473290
55	1	0	6.238296	-1.809990	-2.096003
56	1	0	5.079683	1.009448	2.046085

57	1	0	4.241009	-1.575164	-0.808968
58	1	0	4.076924	-0.032072	-1.704540
59	1	0	-0.714945	-4.008411	2.874094
60	1	0	0.998458	-3.537239	3.023410
61	1	0	-0.359956	-1.800406	-1.968530
62	1	0	-0.238812	-2.566567	3.831121
63	1	0	3.528313	0.979045	2.909376

Cartesians coordinates for compound **8Z**

E= -1700.486841 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.077959	0.017578	1.187911
2	6	0	2.943678	-1.033954	0.779688
3	7	0	2.063694	-1.916886	0.004238
4	6	0	0.968996	-1.139281	-0.565317
5	6	0	1.124121	0.236281	0.150065
6	6	0	4.148064	-0.534715	-0.013283
7	6	0	4.416957	0.830732	-0.145980
8	6	0	5.536035	1.260145	-0.864655
9	6	0	6.398768	0.329995	-1.443530
10	6	0	6.140584	-1.036047	-1.298868
11	6	0	5.022258	-1.468044	-0.587919
12	6	0	-0.173382	0.707863	0.825858
13	8	0	0.007722	1.745846	1.802258
14	6	0	0.707947	2.869885	1.506098
15	8	0	1.211238	3.101863	0.427495

16	6	0	2.108668	-3.283074	0.159820
17	8	0	3.019871	-3.817203	0.785322
18	6	0	-1.326075	1.064378	-0.173374
19	8	0	-1.639014	2.455852	-0.153170
20	6	0	-1.324965	3.356262	-1.153363
21	8	0	-1.721474	4.482360	-1.013910
22	6	0	0.998158	-4.078932	-0.503700
23	6	0	-2.637225	0.346187	0.215749
24	8	0	-2.366063	-1.060182	0.114654
25	6	0	-2.682271	-1.994671	1.081614
26	8	0	-2.262049	-3.111483	0.911704
27	6	0	0.760871	3.779887	2.706398
28	6	0	-3.796208	0.697611	-0.719251
29	8	0	-4.971609	0.011997	-0.287339
30	6	0	-5.472921	-1.105160	-0.908104
31	8	0	-6.333114	-1.721108	-0.331854
32	6	0	-0.527566	2.877177	-2.345136
33	6	0	-3.522084	-1.567944	2.262750
34	6	0	-4.937204	-1.481864	-2.274212
35	1	0	-5.030329	-0.656760	-2.988836
36	1	0	-3.882249	-1.769443	-2.216631
37	1	0	0.004393	-1.611435	-0.362111
38	1	0	-5.517966	-2.332616	-2.630582
39	1	0	6.813613	-1.767304	-1.739090
40	1	0	-0.250393	4.123691	2.948636
41	1	0	5.732281	2.324367	-0.966911
42	1	0	1.146005	3.239239	3.576152
43	1	0	4.826572	-2.529141	-0.461950
44	1	0	3.270126	-1.570826	1.673968
45	1	0	3.752793	1.556090	0.313077
46	1	0	1.070277	-1.021920	-1.651925
47	1	0	1.500038	0.988327	-0.546100
48	1	0	-2.903113	0.624419	1.238896
49	1	0	-0.503609	-0.129171	1.445465
50	1	0	-1.047237	0.738659	-1.180369

51	1	0	-4.009996	1.766105	-0.652967
52	1	0	-3.536356	0.450227	-1.752506
53	1	0	1.237174	-5.137878	-0.398411
54	1	0	0.910287	-3.832629	-1.568251
55	1	0	0.025033	-3.884251	-0.036614
56	1	0	-2.988781	-0.841661	2.887109
57	1	0	-3.725223	-2.457740	2.858691
58	1	0	-4.463675	-1.115855	1.938131
59	1	0	-0.398630	3.728625	-3.013530
60	1	0	-1.036955	2.075100	-2.890722
61	1	0	0.455284	2.519012	-2.027245
62	1	0	1.395295	4.637542	2.481901
63	1	0	7.270525	0.664961	-1.999592

Cartesians coordinates for compound **8E**

E= -1700.485497 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.058419	0.358859	1.170169
2	6	0	-3.099621	1.159408	0.615107
3	7	0	-2.445879	1.852967	-0.498323
4	6	0	-1.139166	1.263454	-0.780539
5	6	0	-1.180441	-0.001949	0.094625
6	6	0	-4.303877	0.309388	0.221711
7	6	0	-4.594044	-0.025046	-1.104403
8	6	0	-5.682815	-0.848090	-1.403441
9	6	0	-6.490958	-1.341405	-0.379569

10	6	0	-6.209251	-1.007629	0.948066
11	6	0	-5.123640	-0.186428	1.244327
12	6	0	0.170884	-0.346816	0.729190
13	8	0	0.119859	-1.391991	1.717070
14	6	0	-0.465101	-2.590263	1.445373
15	8	0	-0.985448	-2.882443	0.392156
16	6	0	-2.787103	3.065888	-1.050694
17	8	0	-2.068039	3.590721	-1.891544
18	6	0	1.352107	-0.584086	-0.261286
19	8	0	1.655356	-1.969267	-0.431207
20	6	0	1.306908	-2.730123	-1.526805
21	8	0	1.737641	-3.851912	-1.573432
22	6	0	0.432910	-2.112261	-2.594536
23	6	0	-4.078200	3.699447	-0.559915
24	6	0	-0.366034	-3.494653	2.648365
25	6	0	2.649098	0.047663	0.296212
26	8	0	2.396972	1.453456	0.369610
27	6	0	2.847259	2.276672	1.386459
28	8	0	2.642670	3.455120	1.263248
29	6	0	3.525405	1.647192	2.582226
30	6	0	3.848066	-0.202654	-0.615339
31	8	0	4.991652	0.331537	0.059104
32	6	0	6.226397	0.397743	-0.530542
33	8	0	7.145833	0.810578	0.128619
34	6	0	6.340968	-0.042813	-1.974291
35	1	0	-1.602669	-0.847451	-0.452404
36	1	0	3.758550	2.447558	3.284765
37	1	0	-6.837691	-1.384926	1.750279
38	1	0	-5.899160	-1.099847	-2.438185
39	1	0	-1.032432	1.041492	-1.846946
40	1	0	0.426585	0.531413	1.325388
41	1	0	-4.315150	4.537263	-1.216848
42	1	0	-0.333576	1.953220	-0.496837
43	1	0	0.907748	-1.243704	-3.064525
44	1	0	7.388298	0.028447	-2.267621

45	1	0	1.130388	-0.105520	-1.219715
46	1	0	-4.911425	2.989652	-0.550736
47	1	0	-3.951833	4.082244	0.460786
48	1	0	0.259861	-2.872241	-3.356694
49	1	0	5.741631	0.600726	-2.628459
50	1	0	-4.903003	0.069019	2.278471
51	1	0	-3.975490	0.369652	-1.905028
52	1	0	2.849212	-0.380172	1.282927
53	1	0	-3.391273	1.862559	1.403764
54	1	0	5.993943	-1.072575	-2.112663
55	1	0	4.446627	1.140753	2.282393
56	1	0	3.969453	-1.276476	-0.783441
57	1	0	3.685225	0.307052	-1.572542
58	1	0	-0.926987	-4.409884	2.458071
59	1	0	0.684916	-3.740950	2.834619
60	1	0	-0.527084	-1.799715	-2.175515
61	1	0	-0.751358	-2.989686	3.539169
62	1	0	2.873956	0.917293	3.076572
63	1	0	-7.339257	-1.979060	-0.612954

Cartesians coordinates for compound **9Z**

E= -1814.979507 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.473833	-0.025371	1.456138
2	6	0	2.354092	-1.092740	1.123760
3	7	0	1.532355	-1.948971	0.257525

4	6	0	0.524401	-1.139962	-0.415645
5	6	0	0.625341	0.220899	0.336540
6	6	0	3.637894	-0.610001	0.459589
7	6	0	3.946160	0.752683	0.355564
8	6	0	5.133254	1.169533	-0.237210
9	6	0	6.046376	0.226984	-0.727872
10	6	0	5.755732	-1.138987	-0.615664
11	6	0	4.558379	-1.544738	-0.024010
12	8	0	7.182362	0.736654	-1.289867
13	6	0	8.153036	-0.171530	-1.784032
14	6	0	-0.726519	0.692410	0.895675
15	8	0	-0.632482	1.715512	1.899709
16	6	0	0.100572	2.837859	1.687193
17	8	0	0.701683	3.082411	0.663116
18	6	0	1.542588	-3.317239	0.386340
19	8	0	2.383509	-3.880407	1.081727
20	6	0	-1.782000	1.068826	-0.198278
21	8	0	-2.072438	2.465287	-0.204995
22	6	0	-1.649232	3.359052	-1.170324
23	8	0	-2.038433	4.491792	-1.069929
24	6	0	0.483683	-4.080534	-0.390849
25	6	0	-3.133458	0.372508	0.076477
26	8	0	-2.877784	-1.038679	-0.000867
27	6	0	-3.284226	-1.966016	0.939036
28	8	0	-2.873556	-3.090739	0.801081
29	6	0	0.052762	3.726849	2.903460
30	6	0	-4.202917	0.739172	-0.954066
31	8	0	-5.424860	0.083881	-0.613645
32	6	0	-5.891406	-1.038071	-1.251995
33	8	0	-6.804975	-1.630549	-0.736112
34	6	0	-0.751682	2.863486	-2.281492
35	6	0	-4.203785	-1.522538	2.052792
36	6	0	-5.252673	-1.449356	-2.562563
37	1	0	-5.269875	-0.635706	-3.295889
38	1	0	-4.212035	-1.754860	-2.411958

39	1	0	-0.466073	-1.594962	-0.329690
40	1	0	-5.818445	-2.295812	-2.951770
41	1	0	6.448641	-1.889664	-0.978624
42	1	0	-0.976360	4.060448	3.073541
43	1	0	5.376968	2.223793	-0.325696
44	1	0	0.373670	3.172252	3.790485
45	1	0	4.343082	-2.605143	0.074460
46	1	0	2.575640	-1.644866	2.040565
47	1	0	3.253077	1.492202	0.743923
48	1	0	0.749486	-1.007256	-1.481837
49	1	0	1.072369	0.980462	-0.307258
50	1	0	-3.482875	0.656833	1.072456
51	1	0	-1.115957	-0.152200	1.468489
52	1	0	-1.424795	0.737557	-1.178192
53	1	0	-4.398678	1.812355	-0.914200
54	1	0	-3.865295	0.475476	-1.960527
55	1	0	0.695109	-5.145431	-0.286424
56	1	0	0.494976	-3.812699	-1.453784
57	1	0	-0.523749	-3.877235	-0.007442
58	1	0	-3.708968	-0.800534	2.712665
59	1	0	-4.463260	-2.406954	2.634758
60	1	0	-5.112647	-1.059825	1.657362
61	1	0	-0.535679	3.713344	-2.929128
62	1	0	-1.228222	2.077890	-2.878464
63	1	0	0.185664	2.476644	-1.873160
64	1	0	0.697545	4.591296	2.744192
65	1	0	7.750581	-0.793888	-2.594570
66	1	0	8.967172	0.442880	-2.173215
67	1	0	8.539344	-0.823223	-0.989140

Cartesians coordinates for compound **9E**

E= -1814.979987 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.487674	0.726342	1.280446
2	6	0	-2.488242	1.572194	0.712438
3	7	0	-1.829274	2.134626	-0.470941
4	6	0	-0.594081	1.413102	-0.768030
5	6	0	-0.698847	0.218189	0.196624
6	6	0	-3.771365	0.807127	0.420918
7	6	0	-4.163094	0.435552	-0.864832
8	6	0	-5.325690	-0.310543	-1.084150
9	6	0	-6.115632	-0.695526	0.003955
10	6	0	-5.733269	-0.323597	1.303951
11	6	0	-4.578824	0.416806	1.502438
12	6	0	0.649491	-0.197431	0.793997
13	8	0	0.562435	-1.162579	1.857756
14	6	0	-0.133466	-2.321287	1.702658
15	8	0	-0.724171	-2.643720	0.696293
16	8	0	-7.267107	-1.417736	-0.087141
17	6	0	-7.705280	-1.828292	-1.373819
18	6	0	-2.087298	3.337065	-1.086380
19	8	0	-1.367354	3.740623	-1.991394
20	6	0	1.758700	-0.601055	-0.225306

21	8	0	1.944075	-2.015050	-0.305335
22	6	0	1.480736	-2.822328	-1.321710
23	8	0	1.826808	-3.974118	-1.307035
24	6	0	0.591365	-2.217543	-2.383857
25	6	0	-3.288853	4.117994	-0.580447
26	6	0	-0.059096	-3.138348	2.968321
27	6	0	3.126865	-0.041464	0.230598
28	8	0	2.994827	1.381931	0.197312
29	6	0	3.554000	2.241498	1.125939
30	8	0	3.443019	3.419637	0.912892
31	6	0	4.226849	1.653302	2.345595
32	6	0	4.260975	-0.467380	-0.698361
33	8	0	5.473158	0.016804	-0.111356
34	6	0	6.691139	-0.130886	-0.720445
35	8	0	7.667598	0.260000	-0.133780
36	6	0	6.717978	-0.769537	-2.092825
37	1	0	-1.218435	-0.621459	-0.270044
38	1	0	4.550688	2.484030	2.972905
39	1	0	-6.361577	-0.627112	2.135409
40	1	0	-8.628661	-2.386557	-1.210533
41	1	0	-5.601183	-0.578598	-2.097591
42	1	0	-0.559729	1.110963	-1.819510
43	1	0	1.005334	0.695720	1.311662
44	1	0	-3.491342	4.923454	-1.287492
45	1	0	-6.968395	-2.479948	-1.861165
46	1	0	-7.911779	-0.967194	-2.022873
47	1	0	0.280441	2.046369	-0.569979
48	1	0	1.092517	-1.413908	-2.934794
49	1	0	7.757169	-0.837188	-2.414576
50	1	0	1.530699	-0.173463	-1.206179
51	1	0	-4.177494	3.488555	-0.470648
52	1	0	-3.068943	4.562074	0.398758
53	1	0	0.329013	-3.011652	-3.083131
54	1	0	6.156172	-0.169026	-2.817246
55	1	0	-4.290516	0.693882	2.514009

56	1	0	-3.562784	0.739638	-1.717360
57	1	0	3.332866	-0.405560	1.241467
58	1	0	-2.682053	2.347252	1.462974
59	1	0	6.276408	-1.771976	-2.079244
60	1	0	5.092311	1.050828	2.057354
61	1	0	4.281008	-1.557440	-0.780572
62	1	0	4.103783	-0.023241	-1.688789
63	1	0	-0.681753	-4.026710	2.860584
64	1	0	0.978582	-3.436167	3.152788
65	1	0	-0.321938	-1.816852	-1.936445
66	1	0	-0.390686	-2.543832	3.825041
67	1	0	3.539919	1.019982	2.918894

Cartesians coordinates for compound **10Z**

E= -1739.780642 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.774346	-0.070562	1.340432
2	6	0	2.630475	-1.141063	0.960650
3	7	0	1.767887	-1.982715	0.121451
4	6	0	0.737231	-1.159614	-0.499345
5	6	0	0.884037	0.194340	0.258128
6	6	0	3.889603	-0.664253	0.245177
7	6	0	4.204560	0.691747	0.139965
8	6	0	5.376245	1.095780	-0.506119
9	6	0	6.264098	0.163211	-1.050105
10	6	0	5.945299	-1.198053	-0.922876

11	6	0	4.778214	-1.609914	-0.286880
12	6	0	7.525318	0.598813	-1.759362
13	6	0	-0.438185	0.678122	0.874598
14	8	0	-0.290398	1.692938	1.880595
15	6	0	0.447920	2.807383	1.646360
16	8	0	1.010774	3.051910	0.600672
17	6	0	1.764409	-3.352071	0.249089
18	8	0	2.622499	-3.926585	0.912860
19	6	0	-1.531448	1.075604	-0.173804
20	8	0	-1.806161	2.475215	-0.157058
21	6	0	-1.410747	3.373071	-1.130302
22	8	0	-1.780988	4.509552	-1.003763
23	6	0	0.669001	-4.100280	-0.490969
24	6	0	-2.878740	0.391355	0.147060
25	8	0	-2.642436	-1.021286	0.042614
26	6	0	-3.024369	-1.955797	0.985716
27	8	0	-2.630417	-3.082744	0.820108
28	6	0	0.460980	3.687531	2.869910
29	6	0	-3.983679	0.783550	-0.835547
30	8	0	-5.197550	0.133710	-0.458107
31	6	0	-5.705135	-0.966627	-1.102960
32	8	0	-6.605521	-1.559096	-0.564563
33	6	0	-0.565313	2.877538	-2.281693
34	6	0	-3.898828	-1.516484	2.136808
35	6	0	-5.125350	-1.354908	-2.447615
36	1	0	-5.162518	-0.524477	-3.161147
37	1	0	-4.083263	-1.675831	-2.347531
38	1	0	-0.252207	-1.606873	-0.372148
39	1	0	-5.717103	-2.185596	-2.832125
40	1	0	6.625076	-1.946237	-1.325766
41	1	0	-0.556826	4.027462	3.088383
42	1	0	5.602747	2.157141	-0.581711
43	1	0	0.816758	3.123527	3.737545
44	1	0	4.555192	-2.668338	-0.184644
45	1	0	2.889396	-1.703654	1.861200

46	1	0	3.538167	1.434846	0.566655
47	1	0	0.914651	-1.020423	-1.573632
48	1	0	1.313780	0.953561	-0.397660
49	1	0	-3.184479	0.666858	1.159742
50	1	0	-0.815169	-0.165373	1.457475
51	1	0	-1.216124	0.749107	-1.169635
52	1	0	-4.166721	1.857892	-0.772338
53	1	0	-3.687352	0.532272	-1.858009
54	1	0	0.873521	-5.167762	-0.400155
55	1	0	0.642457	-3.826526	-1.552082
56	1	0	-0.321003	-3.889501	-0.068289
57	1	0	-3.372077	-0.809624	2.788370
58	1	0	-4.148869	-2.405461	2.715932
59	1	0	-4.814797	-1.037243	1.779408
60	1	0	-0.364433	3.731377	-2.928950
61	1	0	-1.075694	2.104459	-2.866938
62	1	0	0.382452	2.474363	-1.915498
63	1	0	1.105086	4.548172	2.688731
64	1	0	8.400337	0.046283	-1.397010
65	1	0	7.458971	0.419845	-2.840649
66	1	0	7.718083	1.666459	-1.613318

Cartesians coordinates for compound **10E**

E= -1739.779314 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.775071	0.545074	1.208362

2	6	0	-2.781499	1.389865	0.652502
3	7	0	-2.107385	2.027493	-0.482621
4	6	0	-0.840515	1.361047	-0.773925
5	6	0	-0.935408	0.116904	0.127424
6	6	0	-4.033945	0.601123	0.289371
7	6	0	-4.367968	0.264268	-1.023676
8	6	0	-5.503774	-0.504192	-1.291882
9	6	0	-6.334408	-0.954096	-0.261427
10	6	0	-5.994127	-0.608030	1.056228
11	6	0	-4.865370	0.157200	1.327351
12	6	0	0.406468	-0.285237	0.748188
13	8	0	0.318993	-1.307572	1.757348
14	6	0	-0.330989	-2.479037	1.519584
15	8	0	-0.884558	-2.764626	0.481597
16	6	0	-7.566322	-1.780355	-0.547370
17	6	0	-2.387315	3.248835	-1.049792
18	8	0	-1.652105	3.719186	-1.908961
19	6	0	1.559056	-0.600493	-0.253691
20	8	0	1.788050	-2.002341	-0.402876
21	6	0	1.383167	-2.765097	-1.477175
22	8	0	1.754604	-3.908513	-1.507585
23	6	0	0.524160	-2.124146	-2.543452
24	6	0	-3.633682	3.961828	-0.552237
25	6	0	-0.256419	-3.364344	2.738542
26	6	0	2.895326	-0.029681	0.276136
27	8	0	2.719781	1.388355	0.333303
28	6	0	3.225565	2.198827	1.333867
29	8	0	3.087734	3.385237	1.195142
30	6	0	3.877115	1.548726	2.533593
31	6	0	4.067101	-0.353677	-0.647511
32	8	0	5.245836	0.123836	0.008956
33	6	0	6.472199	0.136406	-0.600905
34	8	0	7.420290	0.504485	0.044081
35	6	0	6.542786	-0.303082	-2.047880
36	1	0	-1.410675	-0.715344	-0.395995

37	1	0	4.157314	2.344191	3.224416
38	1	0	-6.625421	-0.941947	1.876924
39	1	0	-5.746886	-0.754672	-2.321867
40	1	0	-0.764428	1.112725	-1.837165
41	1	0	0.715539	0.590337	1.322743
42	1	0	-3.828830	4.804957	-1.216057
43	1	0	0.006245	2.011039	-0.517483
44	1	0	1.030761	-1.284904	-3.032978
45	1	0	7.587603	-0.281143	-2.357580
46	1	0	1.348655	-0.127229	-1.217234
47	1	0	-4.506092	3.301183	-0.526554
48	1	0	-3.474368	4.347067	0.462924
49	1	0	0.306558	-2.886898	-3.291285
50	1	0	5.965106	0.371637	-2.690065
51	1	0	-4.618784	0.408886	2.356656
52	1	0	-3.746551	0.612602	-1.843542
53	1	0	3.086791	-0.454603	1.265757
54	1	0	-3.022089	2.121569	1.432382
55	1	0	6.144171	-1.314261	-2.184302
56	1	0	4.768262	0.990276	2.235013
57	1	0	4.128785	-1.433940	-0.806950
58	1	0	3.920002	0.155667	-1.607323
59	1	0	-0.869684	-4.251207	2.577473
60	1	0	0.783290	-3.664033	2.909028
61	1	0	-0.415056	-1.762571	-2.116674
62	1	0	-0.595587	-2.822478	3.626398
63	1	0	3.191220	0.860602	3.041021
64	1	0	-8.478063	-1.264618	-0.220777
65	1	0	-7.667681	-1.991051	-1.616421
66	1	0	-7.534057	-2.740628	-0.018254