Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Data

Regioselective Baeyer-Villiger Oxidation of Lignin Model Compounds with Tin Beta Zeolite Catalyst and Hydrogen Peroxide

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Synthesis of 2-(4-methoxyphenoxy)-1-(4-methoxyphenyl)-ethanone (**6**)

A suspension of 4-methoxyphenol (16 g, 129 mmol), potassium carbonate (20 g, 144 mmol) and acetone (100 mL) was cooled to 0 °C and 2-bromo-4'-methoxyacetophenone (25 g, 110 mmol) was added slowly. After the addition, the reaction mixture was heated to reflux and held overnight. The reaction mixture was then allowed to cool, and was filtered through a pad of Celite® and was then concentrated *in vacuo*. The resulting solid was dissolved in chloroform (100 mL), washed with 1 M sodium hydroxide (50 mL x 3) followed by brine (100 mL x 2), and was dried over sodium sulfate. After filtration, the product was concentrated *in vacuo*, resulting in a red-brown solid. The solid was purified by recrystallization in water and acetone, resulting in a white solid (29.7 g, 94% yield). GCMS: *m/z* 272.1 (24%), 135.1 (100%), 77.1 (15%) and ^{1}H-NMR (400 MHz, $CDCl_3$) δ: 8.02-7.96 (m, 2H), 6.98-6.82 (m, 6H), 5.28 (s, 2H), 3.88 (s, 3H), 3.87 (s, 3H). The ^{1}H-NMR spectrum is consistent with the spectrum previously reported by Lee *et al.*[26]

Synthesis of 2-(2-methoxyphenoxy)-1-(4-methoxyphenyl)-ethanone (**7**)

A suspension of guaiacol (16.56 g, 138 mmol), potassium carbonate (21.1 g, 153 mmol) and acetone (140 mL) was cooled to 0 °C and 2-bromo-4'-methoxyacetophenone (24.3 g, 106 mmol) was added slowly. After the addition, the reaction was heated to reflux and held overnight. The mixture was then allowed to cool, and was filtered through a pad of Celite® and was then concentrated *in vacuo*. The resulting solid was dissolved in ethyl acetate (200 mL), washed with 1 M sodium hydroxide (75 mL x 3) followed by brine (100 mL x 2), and was dried over anhydrous sodium sulfate. After filtration, the product was concentrated *in vacuo*. The resulting solid was recrystallized from acetone, resulting in a white solid (20.3 g, 71% yield). GCMS: *m/z* 272.1 (20%), 135.1 (100%), 121.1 (7%) and ^{1}H-NMR (400 MHz, $CDCl_3$) δ: 8.04-7.98 (m, 2H), 6.98-6.94 (m, 2H), 6.92-6.78 (m, 4H),

5.15 (s, 2H), 3.36 (s, 3H), 3.17 (s, 3H). The ^{1}H-NMR spectrum is consistent with spectra previously reported by Dawange *et al.*[27]

Models **6a**[1] and **8a**[2] have been previously reported but were not completely characterized. NMR spectra provided below contain minor impurities corresponding to unreacted starting material. Spectra of contaminants have previously been reported.[3-5] Resonances resulting from unreacted starting material are indicated with an asterisk.

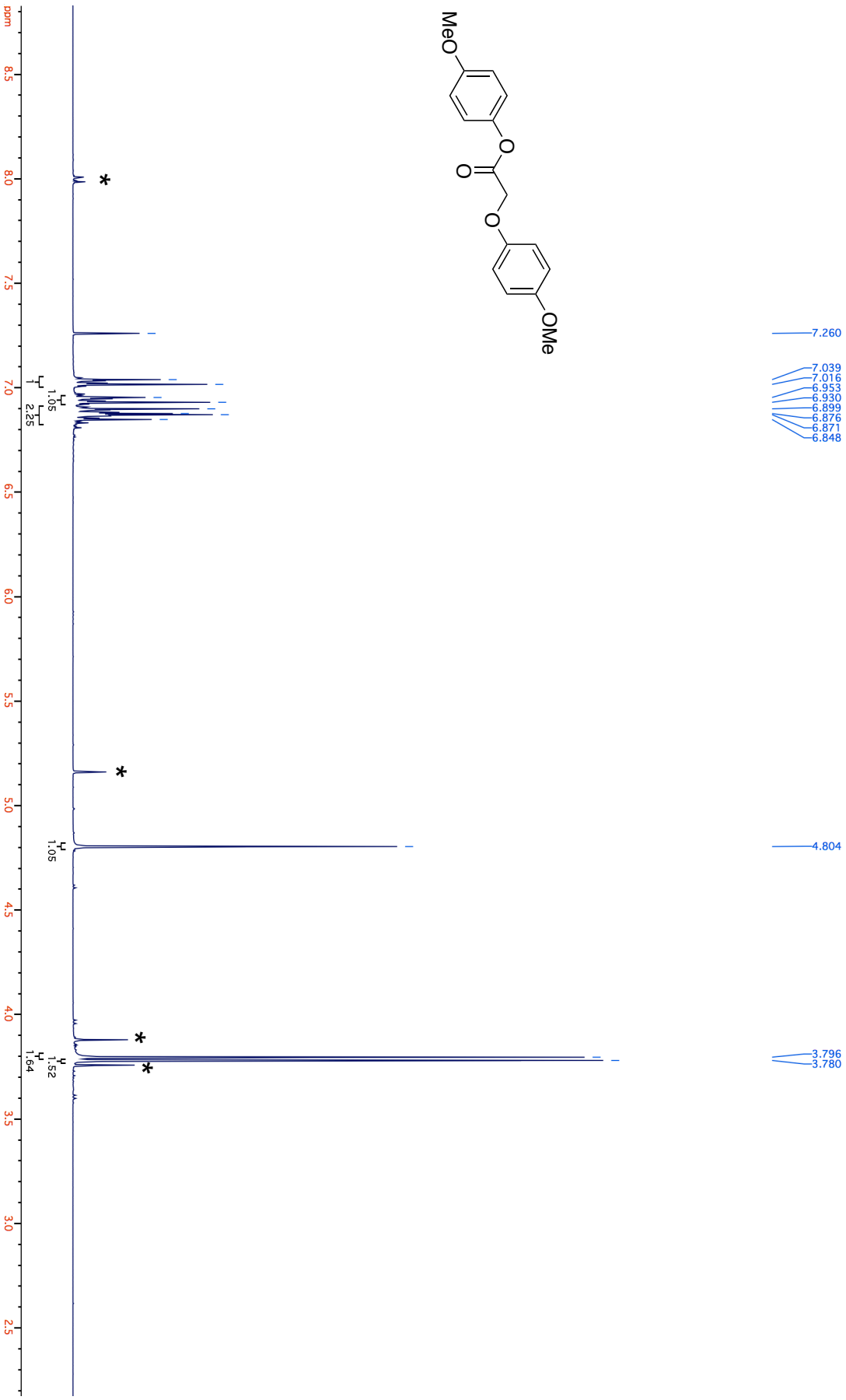

Figure S1. ^{1}H-NMR spectrum of compound **6a** in $CDCl_3$.

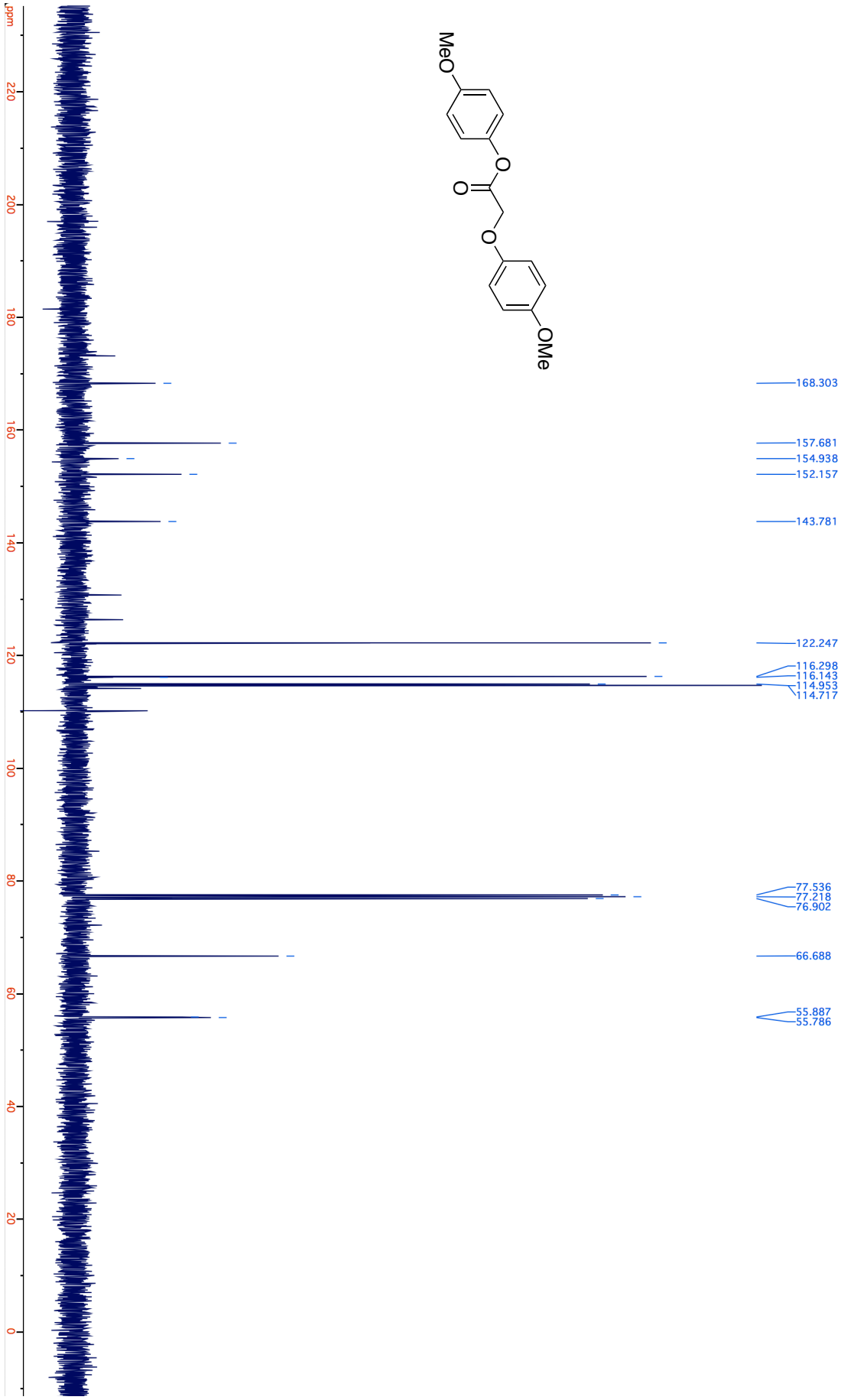

Figure S2. ^{13}C-NMR spectrum of compound **6a** in $CDCl_3$.

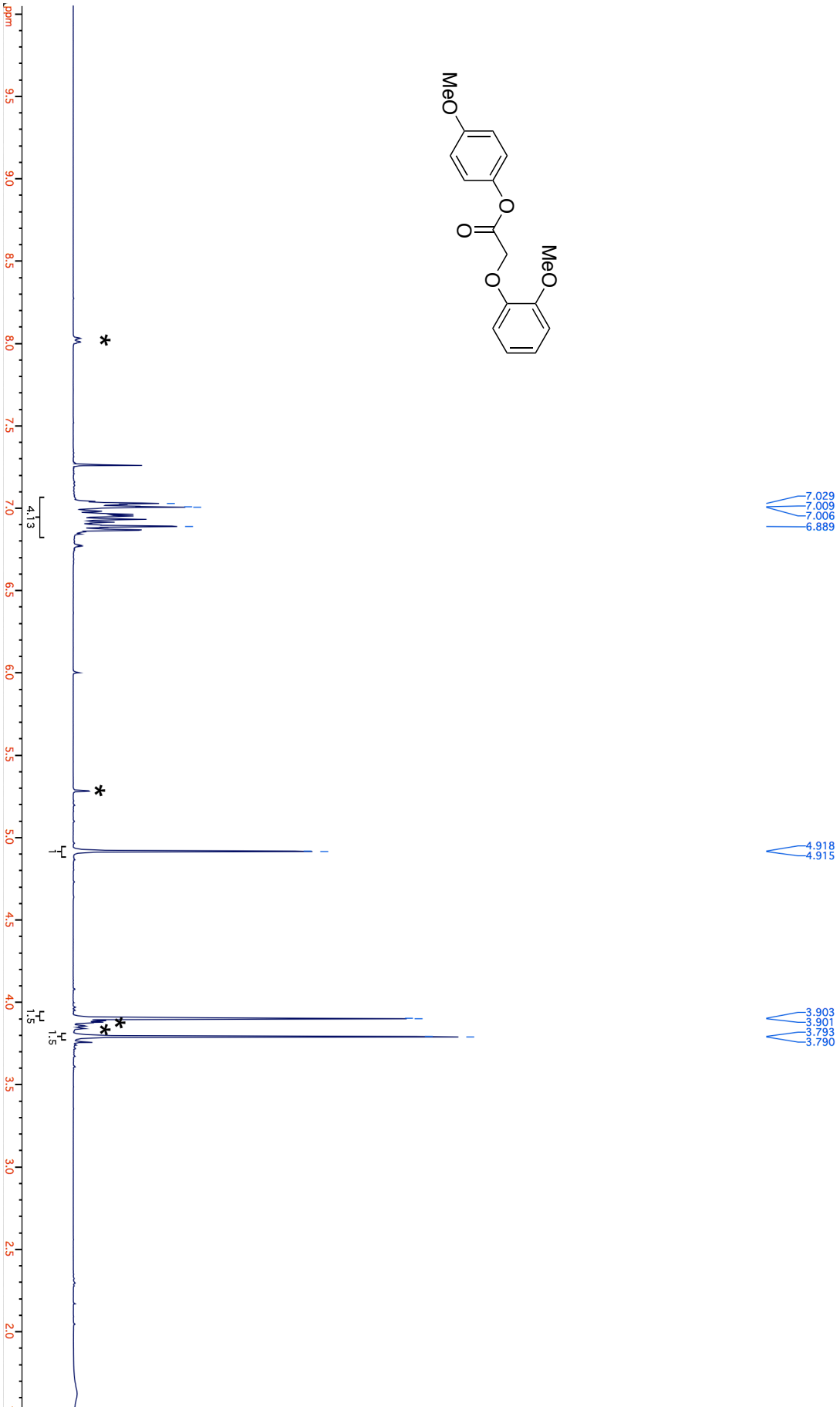

Figure S3. ^{1}H-NMR spectrum of compound **7a** in $CDCl_3$.

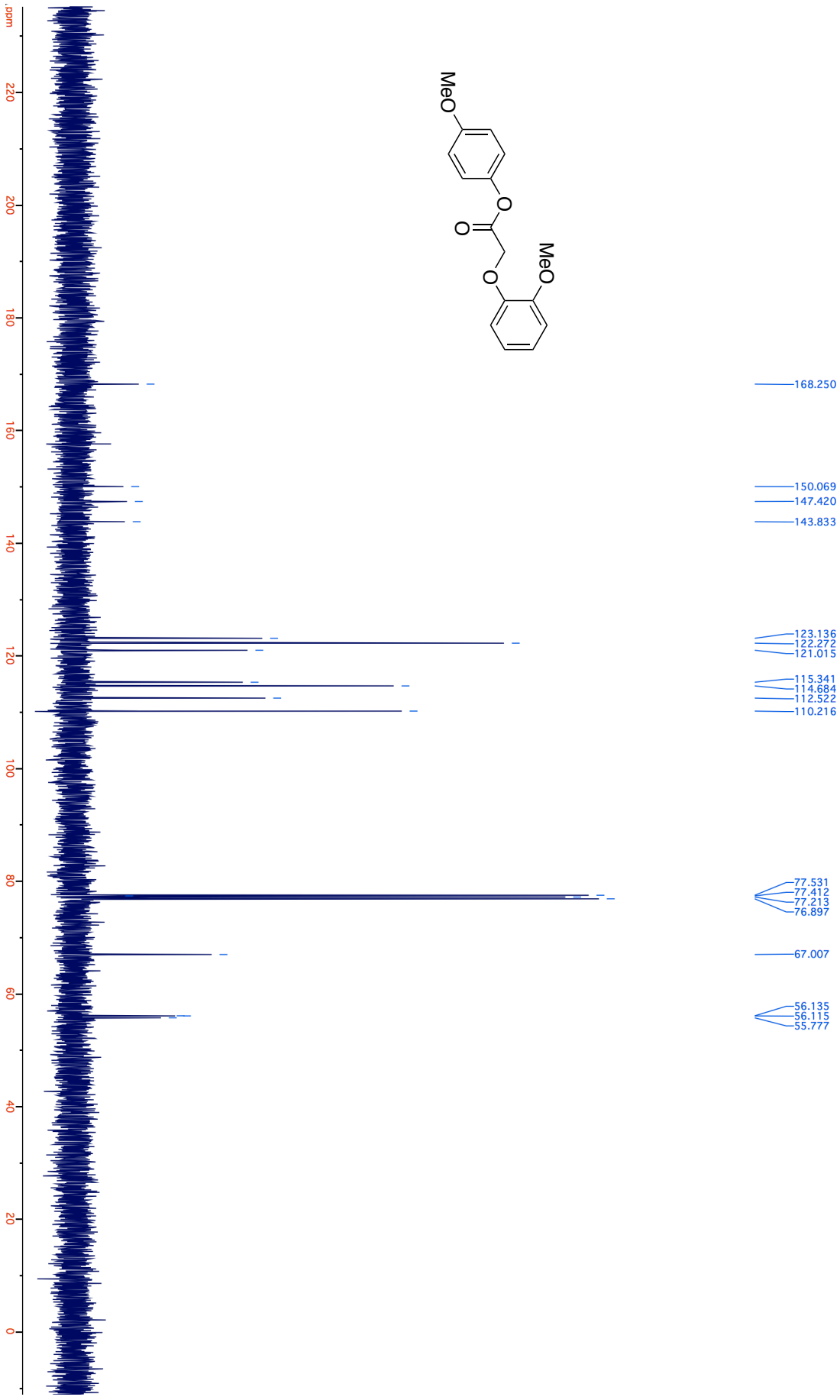

Figure S4. ^{13}C-NMR spectrum of compound **7a** in $CDCl_3$.

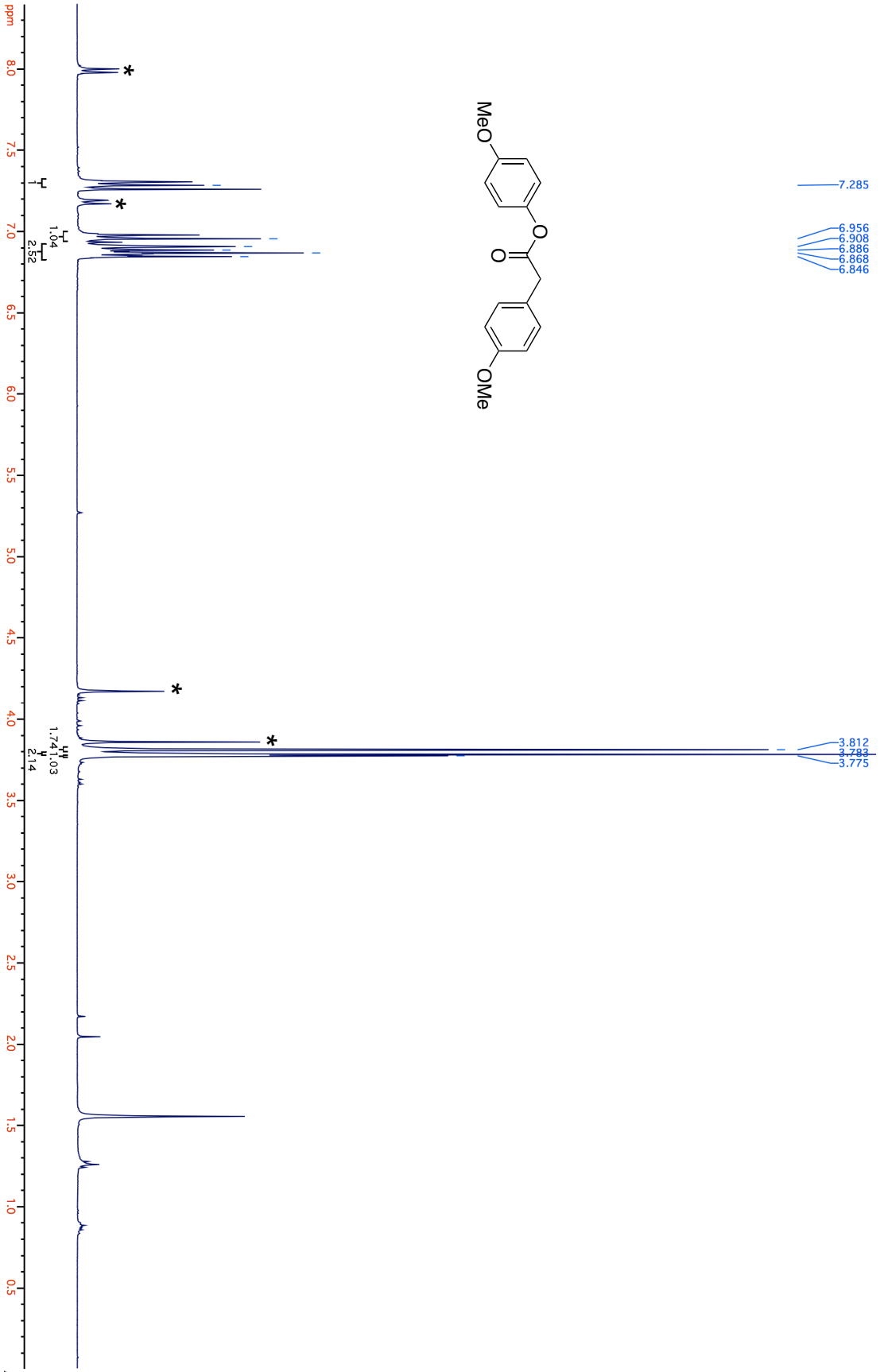

Figure S5. ^{1}H-NMR spectrum of compound **8a** in $CDCl_3$.

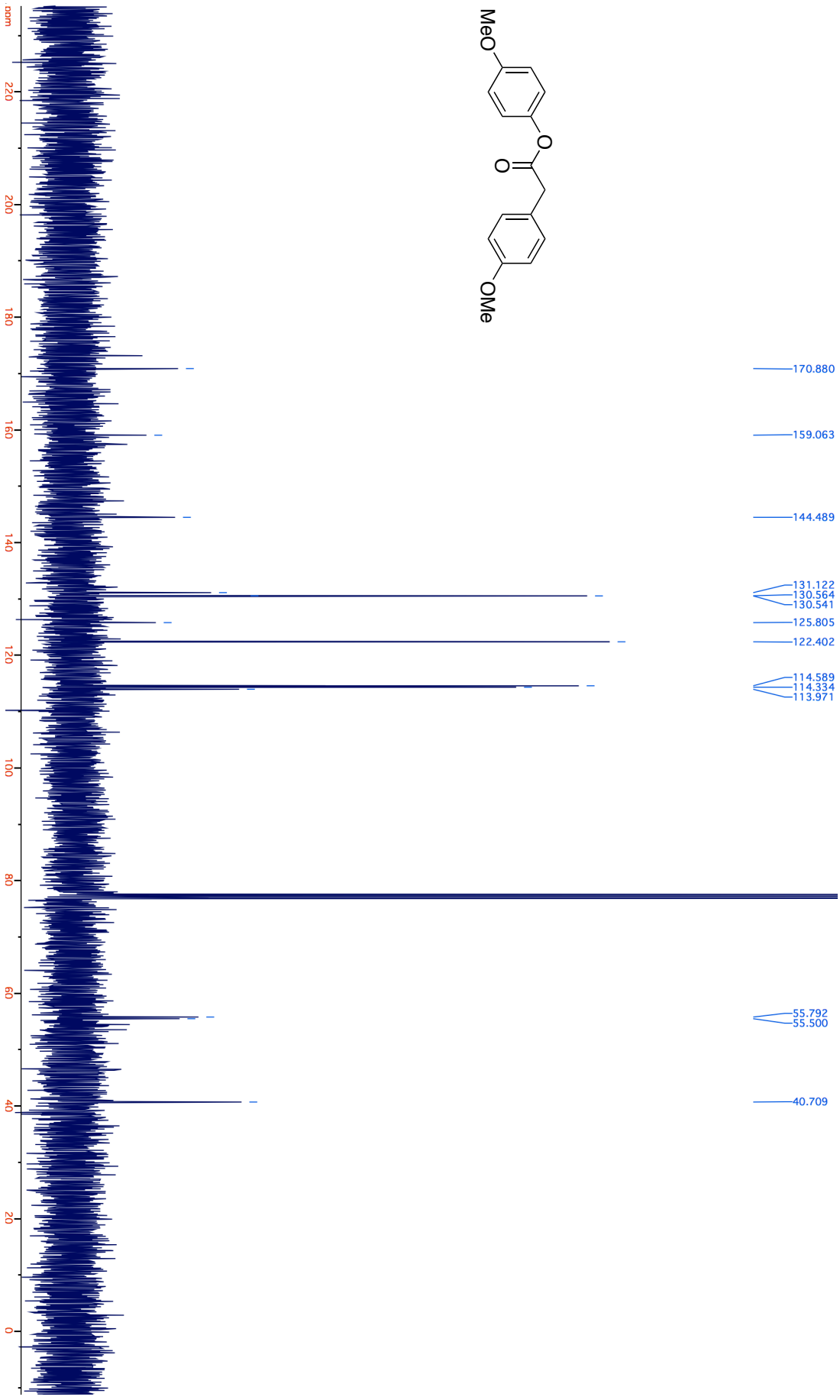

Figure S6. ^{13}C-NMR spectrum of compound **8a** in $CDCl_3$.

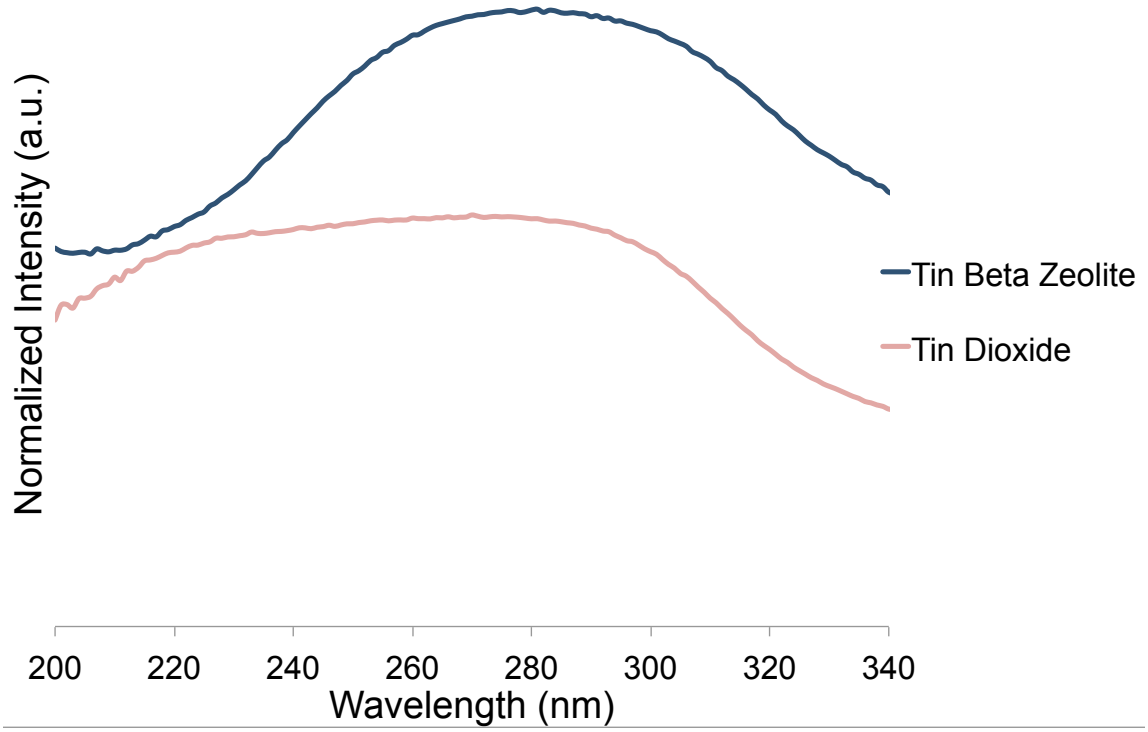

Figure S7. Diffuse Reflectance UV-vis spectra of tin beta zeolite and tin dioxide. Spectra were normalized and the zeolite background was subtracted.

Table 1 Crystal data and structure refinement for molecule **6a**.

Table 2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for molecule **6a**.

Table 3 Bond lengths [A] and angles [deg] for molecule **6a**.

Table 4 Anisotropic displacement parameters (A^2 x 10^3) for molecule **6a**.

Table 5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for molecule **6a**.

Table 6 Torsion angles [deg] for molecule **6a**.

Table 7 Crystal data and structure refinement for molecule **7a**.

Table 8 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for molecule **7a**.

Table 9 Bond lengths [A] and angles [deg] for molecule **7a**.

Table 7 Anisotropic displacement parameters (A^2 x 10^3) for molecule **7a**.

Table 8 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for molecule **7a**.

Table 9 Torsion angles [deg] for molecule **7a**.

Table 1. Crystal data and structure refinement for molecule 6a.

Identification code	**molecule 6a**
Empirical formula	C16 H16 O5
Formula weight	288.29
Temperature	90.0(2) K
Wavelength	1.54178 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 9.2686(2) A alpha = 90 deg. b = 17.7615(3) A beta = 96.374(1) deg. c = 8.3998(1) A gamma = 90 deg.
Volume	1374.26(4) A^3
Z, Calculated density	4, 1.393 Mg/m^3
Absorption coefficient	0.864 mm^-1
F(000)	608
Crystal size	0.340 x 0.250 x 0.170 mm
Theta range for data collection	4.801 to 68.365 deg.
Limiting indices	-7<=h<=11, -21<=k<=21, -10<=l<=8
Reflections collected / unique	18486 / 2504 [R(int) = 0.0423]
Completeness to theta = 67.679	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.929 and 0.762
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2504 / 0 / 192
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0962
R indices (all data)	R1 = 0.0385, wR2 = 0.0984
Extinction coefficient	n/a
Largest diff. peak and hole	0.211 and -0.226 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for molecule 6a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
O(1)	1310(1)	2724(1)	2964(1)	18(1)
O(2)	6083(1)	4408(1)	5334(1)	21(1)
O(3)	7566(1)	3417(1)	5974(1)	23(1)
O(4)	9705(1)	4370(1)	7139(1)	21(1)
O(5)	13923(1)	6104(1)	10565(1)	21(1)
C(1)	4902(1)	3943(1)	4781(2)	17(1)
C(2)	4714(1)	3733(1)	3192(2)	19(1)
C(3)	3496(1)	3325(1)	2620(1)	18(1)
C(4)	2467(1)	3132(1)	3646(1)	15(1)
C(5)	2657(1)	3361(1)	5241(1)	18(1)
C(6)	3890(1)	3768(1)	5804(2)	19(1)
C(7)	231(1)	2496(1)	3966(2)	20(1)
C(8)	7345(1)	4079(1)	5907(1)	16(1)
C(9)	8403(1)	4698(1)	6434(2)	18(1)
C(10)	10693(1)	4852(1)	7950(1)	17(1)
C(11)	11867(1)	4510(1)	8852(2)	18(1)
C(12)	12918(1)	4944(1)	9704(1)	18(1)
C(13)	12815(1)	5729(1)	9681(1)	17(1)
C(14)	11654(1)	6070(1)	8781(2)	18(1)
C(15)	10593(1)	5630(1)	7913(2)	19(1)
C(16)	13867(1)	6909(1)	10543(2)	23(1)

Table 3. Bond lengths [A] and angles [deg] for molecule 6a.

O(1)-C(4)	1.3668(14)
O(1)-C(7)	1.4347(14)
O(2)-C(8)	1.3488(15)
O(2)-C(1)	1.4084(14)
O(3)-C(8)	1.1926(15)
O(4)-C(10)	1.3776(14)
O(4)-C(9)	1.4105(14)
O(5)-C(13)	1.3721(15)
O(5)-C(16)	1.4295(15)
C(1)-C(6)	1.3763(18)
C(1)-C(2)	1.3788(18)
C(2)-C(3)	1.3815(18)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.3963(17)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.3925(17)
C(5)-C(6)	1.3904(17)
C(5)-H(5A)	0.9500
C(6)-H(6a)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(9)	1.5077(16)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.3846(18)
C(10)-C(11)	1.3948(17)
C(11)-C(12)	1.3777(17)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.3978(18)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.3838(17)
C(14)-C(15)	1.3960(17)
C(14)-H(14A)	0.9500
C(15)-H(15A)	0.9500
C(16)-H(16a)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(4)-O(1)-C(7)	118.05(9)
C(8)-O(2)-C(1)	118.31(9)
C(10)-O(4)-C(9)	116.15(9)
C(13)-O(5)-C(16)	117.06(9)
C(6)-C(1)-C(2)	121.46(11)
C(6)-C(1)-O(2)	119.04(11)
C(2)-C(1)-O(2)	119.22(11)
C(1)-C(2)-C(3)	119.29(11)
C(1)-C(2)-H(2A)	120.4
C(3)-C(2)-H(2A)	120.4
C(2)-C(3)-C(4)	120.10(11)
C(2)-C(3)-H(3A)	119.9
C(4)-C(3)-H(3A)	119.9
O(1)-C(4)-C(5)	124.53(10)
O(1)-C(4)-C(3)	115.46(10)
C(5)-C(4)-C(3)	120.02(11)
C(6)-C(5)-C(4)	119.37(11)
C(6)-C(5)-H(5A)	120.3

C(4)-C(5)-H(5A)	120.3
C(1)-C(6)-C(5)	119.74(11)
C(1)-C(6)-H(6a)	120.1
C(5)-C(6)-H(6a)	120.1
O(1)-C(7)-H(7A)	109.5
O(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
O(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
O(3)-C(8)-O(2)	125.59(11)
O(3)-C(8)-C(9)	127.07(11)
O(2)-C(8)-C(9)	107.33(10)
O(4)-C(9)-C(8)	108.63(10)
O(4)-C(9)-H(9A)	110.0
C(8)-C(9)-H(9A)	110.0
O(4)-C(9)-H(9B)	110.0
C(8)-C(9)-H(9B)	110.0
H(9A)-C(9)-H(9B)	108.3
O(4)-C(10)-C(15)	124.78(11)
O(4)-C(10)-C(11)	115.68(11)
C(15)-C(10)-C(11)	119.54(11)
C(12)-C(11)-C(10)	120.19(11)
C(12)-C(11)-H(11A)	119.9
C(10)-C(11)-H(11A)	119.9
C(11)-C(12)-C(13)	120.45(11)
C(11)-C(12)-H(12A)	119.8
C(13)-C(12)-H(12A)	119.8
O(5)-C(13)-C(14)	124.96(11)
O(5)-C(13)-C(12)	115.56(11)
C(14)-C(13)-C(12)	119.48(11)
C(13)-C(14)-C(15)	120.03(11)
C(13)-C(14)-H(14A)	120.0
C(15)-C(14)-H(14A)	120.0
C(10)-C(15)-C(14)	120.31(11)
C(10)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
O(5)-C(16)-H(16a)	109.5
O(5)-C(16)-H(16B)	109.5
H(16a)-C(16)-H(16B)	109.5
O(5)-C(16)-H(16C)	109.5
H(16a)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for molecule 6a. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

U11	U22	U33	U23	U13	U12	
O(1)	14(1)	24(1)	17(1)	-2(1)	2(1)	-4(1)
O(2)	14(1)	16(1)	31(1)	0(1)	-3(1)	-1(1)
O(3)	19(1)	18(1)	33(1)	-2(1)	-1(1)	1(1)
O(4)	15(1)	18(1)	30(1)	-3(1)	-4(1)	1(1)
O(5)	18(1)	18(1)	26(1)	-2(1)	-4(1)	0(1)
C(1)	14(1)	13(1)	25(1)	2(1)	-2(1)	0(1)
C(2)	15(1)	18(1)	24(1)	3(1)	5(1)	1(1)
C(3)	18(1)	20(1)	16(1)	1(1)	3(1)	1(1)
C(4)	13(1)	14(1)	19(1)	2(1)	0(1)	1(1)
C(5)	18(1)	20(1)	17(1)	2(1)	4(1)	0(1)
C(6)	21(1)	20(1)	16(1)	0(1)	0(1)	0(1)
C(7)	15(1)	24(1)	22(1)	0(1)	4(1)	-5(1)
C(8)	14(1)	20(1)	16(1)	0(1)	3(1)	1(1)
C(9)	14(1)	18(1)	21(1)	0(1)	0(1)	0(1)
C(10)	14(1)	19(1)	18(1)	-2(1)	2(1)	-1(1)
C(11)	17(1)	15(1)	22(1)	1(1)	4(1)	1(1)
C(12)	15(1)	20(1)	19(1)	3(1)	1(1)	2(1)
C(13)	14(1)	20(1)	16(1)	-1(1)	3(1)	0(1)
C(14)	17(1)	16(1)	22(1)	0(1)	3(1)	1(1)
C(15)	16(1)	19(1)	22(1)	2(1)	-1(1)	3(1)
C(16)	20(1)	18(1)	30(1)	-4(1)	0(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for molecule 6a.

x	y	z	U(eq)	
H(2A)	5414	3866	2497	23
H(3A)	3358	3176	1528	21
H(5A)	1951	3239	5937	22
H(6a)	4033	3925	6892	23
H(7A)	-505	2188	3342	30
H(7B)	-230	2943	4370	30
H(7C)	691	2201	4870	30
H(9A)	8595	5008	5501	21
H(9B)	7990	5029	7219	21
H(11A)	11943	3977	8880	22
H(12A)	13719	4707	10311	21
H(14A)	11579	6603	8753	22
H(15A)	9799	5866	7294	23
H(16a)	14735	7111	11169	34
H(16B)	13000	7079	11009	34
H(16C)	13827	7087	9435	34

Table 6. Torsion angles [deg] for molecule 6a.

C(8)-O(2)-C(1)-C(6)	95.46(13)
C(8)-O(2)-C(1)-C(2)	-90.58(13)
C(6)-C(1)-C(2)-C(3)	-1.21(18)
O(2)-C(1)-C(2)-C(3)	-175.02(10)
C(1)-C(2)-C(3)-C(4)	0.22(18)
C(7)-O(1)-C(4)-C(5)	-1.77(17)
C(7)-O(1)-C(4)-C(3)	178.76(10)
C(2)-C(3)-C(4)-O(1)	-179.5(1)
C(2)-C(3)-C(4)-C(5)	1.00(18)
O(1)-C(4)-C(5)-C(6)	179.31(11)
C(3)-C(4)-C(5)-C(6)	-1.24(18)
C(2)-C(1)-C(6)-C(5)	0.97(18)
O(2)-C(1)-C(6)-C(5)	174.79(10)
C(4)-C(5)-C(6)-C(1)	0.27(18)
C(1)-O(2)-C(8)-O(3)	0.99(17)
C(1)-O(2)-C(8)-C(9)	-179.09(10)
C(10)-O(4)-C(9)-C(8)	-168.50(9)
O(3)-C(8)-C(9)-O(4)	-3.94(17)
O(2)-C(8)-C(9)-O(4)	176.13(9)
C(9)-O(4)-C(10)-C(15)	-10.15(16)
C(9)-O(4)-C(10)-C(11)	170.22(10)
O(4)-C(10)-C(11)-C(12)	179.81(10)
C(15)-C(10)-C(11)-C(12)	0.17(17)
C(10)-C(11)-C(12)-C(13)	0.40(17)
C(16)-O(5)-C(13)-C(14)	-0.17(16)
C(16)-O(5)-C(13)-C(12)	178.8(1)
C(11)-C(12)-C(13)-O(5)	-179.72(10)
C(11)-C(12)-C(13)-C(14)	-0.68(17)
O(5)-C(13)-C(14)-C(15)	179.34(11)
C(12)-C(13)-C(14)-C(15)	0.40(17)
O(4)-C(10)-C(15)-C(14)	179.94(11)
C(11)-C(10)-C(15)-C(14)	-0.45(18)
C(13)-C(14)-C(15)-C(10)	0.16(18)

Symmetry transformations used to generate equivalent atoms:

Table 7. Crystal data and structure refinement for molecule 7a.

Identification code	molecule **7a**	
Empirical formula	C16 H16 O5	
Formula weight	288.29	
Temperature	90.0(2) K	
Wavelength	1.54178 A	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 5.8859(5) A	alpha = 87.423(4) deg.
	b = 12.7775(10) A	beta = 89.813(5) deg.
	c = 19.1219(14) A	gamma = 77.523(5) deg.
Volume	1402.69(19) A^3	
Z, Calculated density	4, 1.365 Mg/m^3	
Absorption coefficient	0.847 mm^-1	
F(000)	608	
Crystal size	0.200 x 0.140 x 0.120 mm	
Theta range for data collection	2.313 to 68.429 deg.	
Limiting indices	-7<=h<=7, -15<=k<=15, -21<=l<=23	
Reflections collected / unique	24835 / 24835 [R(int) = ?]	
Completeness to theta = 67.679	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.893 and 0.610	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	24835 / 0 / 385	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.2084	
R indices (all data)	R1 = 0.0835, wR2 = 0.2283	
Extinction coefficient	0.0022(7)	
Largest diff. peak and hole	0.389 and -0.347 e.A^-3	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for molecule 7a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
O(1A)	2150(5)	7404(2)	6646(1)	34(1)
O(2A)	5866(5)	6609(2)	5972(1)	33(1)
O(3A)	8031(5)	8072(2)	5414(1)	37(1)
O(4A)	10074(5)	6864(2)	4690(1)	34(1)
O(5A)	14437(5)	9738(2)	3266(1)	36(1)
C(1A)	2642(7)	6317(3)	6617(2)	28(1)
C(2A)	1354(7)	5634(3)	6926(2)	33(1)
C(3A)	2010(8)	4540(4)	6852(2)	37(1)
C(4A)	3939(7)	4109(3)	6471(2)	36(1)
C(5A)	5273(7)	4788(3)	6160(2)	33(1)
C(6A)	4641(7)	5876(3)	6236(2)	30(1)
C(7A)	54(7)	7876(3)	7004(2)	39(1)
C(8A)	7595(7)	6234(3)	5468(2)	32(1)
C(9A)	8535(7)	7184(3)	5211(2)	31(1)
C(10A)	11132(7)	7663(3)	4361(2)	31(1)
C(11A)	12588(7)	8144(3)	4726(2)	34(1)
C(12A)	13713(7)	8858(3)	4376(2)	33(1)
C(13A)	13366(7)	9069(3)	3661(2)	31(1)
C(14A)	11854(7)	8580(3)	3303(2)	35(1)
C(15A)	10734(7)	7873(3)	3655(2)	35(1)
C(16A)	15964(7)	10274(3)	3623(2)	38(1)
O(1B)	-3053(5)	7696(2)	-1489(1)	34(1)
O(2B)	783(5)	6767(2)	-879(1)	33(1)
O(3B)	2859(5)	8147(2)	-286(1)	35(1)
O(4B)	5010(5)	6830(2)	418(1)	34(1)
O(5B)	9295(5)	9583(2)	1810(1)	34(1)
C(1B)	-2510(7)	6606(3)	-1512(2)	29(1)
C(2B)	-3825(7)	6000(3)	-1850(2)	33(1)
C(3B)	-3109(7)	4891(3)	-1838(2)	35(1)
C(4B)	-1093(7)	4377(3)	-1488(2)	34(1)
C(5B)	253(7)	4990(3)	-1157(2)	32(1)
C(6B)	-439(7)	6083(3)	-1168(2)	28(1)
C(7B)	-5114(7)	8242(3)	-1857(2)	39(1)
C(8B)	2545(7)	6307(3)	-386(2)	31(1)
C(9B)	3436(7)	7225(3)	-100(2)	30(1)
C(10B)	6056(7)	7580(3)	747(2)	32(1)
C(11B)	7480(7)	8120(3)	372(2)	34(1)
C(12B)	8583(7)	8809(3)	712(2)	33(1)
C(13B)	8250(7)	8935(3)	1426(2)	30(1)
C(14B)	6796(7)	8387(3)	1792(2)	34(1)
C(15B)	5680(7)	7710(3)	1453(2)	33(1)
C(16B)	10812(7)	10162(3)	1447(2)	38(1)

Table 9. Bond lengths [A] and angles [deg] for molecule 7a.

O(1A)-C(1A)	1.360(4)
O(1A)-C(7A)	1.436(4)
O(2A)-C(6A)	1.378(4)
O(2A)-C(8A)	1.421(4)
O(3A)-C(9A)	1.191(5)
O(4A)-C(9A)	1.360(4)
O(4A)-C(10A)	1.428(4)
O(5A)-C(13A)	1.368(4)
O(5A)-C(16A)	1.433(4)
C(1A)-C(2A)	1.386(5)
C(1A)-C(6A)	1.406(5)
C(2A)-C(3A)	1.382(5)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.372(6)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.403(5)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.373(5)
C(5A)-H(5A)	0.9500
C(7A)-H(7A1)	0.9800
C(7A)-H(7A2)	0.9800
C(7A)-H(7A3)	0.9800
C(8A)-C(9A)	1.502(5)
C(8A)-H(8A1)	0.9900
C(8A)-H(8A2)	0.9900
C(10A)-C(11A)	1.367(5)
C(10A)-C(15A)	1.376(5)
C(11A)-C(12A)	1.385(5)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.390(5)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.389(5)
C(14A)-C(15A)	1.380(5)
C(14A)-H(14A)	0.9500
C(15A)-H(15A)	0.9500
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
O(1B)-C(1B)	1.363(4)
O(1B)-C(7B)	1.432(4)
O(2B)-C(6B)	1.381(4)
O(2B)-C(8B)	1.415(4)
O(3B)-C(9B)	1.191(5)
O(4B)-C(9B)	1.361(5)
O(4B)-C(10B)	1.416(4)
O(5B)-C(13B)	1.370(4)
O(5B)-C(16B)	1.436(4)
C(1B)-C(2B)	1.387(5)
C(1B)-C(6B)	1.407(5)
C(2B)-C(3B)	1.387(5)
C(2B)-H(2B)	0.9500
C(3B)-C(4B)	1.384(6)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.400(5)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.367(5)

C(5B)-H(5B)	0.9500
C(7B)-H(7B1)	0.9800
C(7B)-H(7B2)	0.9800
C(7B)-H(7B3)	0.9800
C(8B)-C(9B)	1.509(5)
C(8B)-H(8B1)	0.9900
C(8B)-H(8B2)	0.9900
C(10B)-C(11B)	1.376(5)
C(10B)-C(15B)	1.379(5)
C(11B)-C(12B)	1.386(5)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.391(5)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.386(5)
C(14B)-C(15B)	1.379(5)
C(14B)-H(14B)	0.9500
C(15B)-H(15B)	0.9500
C(16B)-H(16D)	0.9800
C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(1A)-O(1A)-C(7A)	116.4(3)
C(6A)-O(2A)-C(8A)	116.4(3)
C(9A)-O(4A)-C(10A)	117.0(3)
C(13A)-O(5A)-C(16A)	117.2(3)
O(1A)-C(1A)-C(2A)	125.7(3)
O(1A)-C(1A)-C(6A)	115.5(3)
C(2A)-C(1A)-C(6A)	118.9(4)
C(3A)-C(2A)-C(1A)	120.4(4)
C(3A)-C(2A)-H(2A)	119.8
C(1A)-C(2A)-H(2A)	119.8
C(4A)-C(3A)-C(2A)	120.8(4)
C(4A)-C(3A)-H(3A)	119.6
C(2A)-C(3A)-H(3A)	119.6
C(3A)-C(4A)-C(5A)	119.5(4)
C(3A)-C(4A)-H(4A)	120.2
C(5A)-C(4A)-H(4A)	120.2
C(6A)-C(5A)-C(4A)	120.0(4)
C(6A)-C(5A)-H(5A)	120.0
C(4A)-C(5A)-H(5A)	120.0
C(5A)-C(6A)-O(2A)	124.6(3)
C(5A)-C(6A)-C(1A)	120.4(3)
O(2A)-C(6A)-C(1A)	115.0(4)
O(1A)-C(7A)-H(7A1)	109.5
O(1A)-C(7A)-H(7A2)	109.5
H(7A1)-C(7A)-H(7A2)	109.5
O(1A)-C(7A)-H(7A3)	109.5
H(7A1)-C(7A)-H(7A3)	109.5
H(7A2)-C(7A)-H(7A3)	109.5
O(2A)-C(8A)-C(9A)	106.9(3)
O(2A)-C(8A)-H(8A1)	110.4
C(9A)-C(8A)-H(8A1)	110.4
O(2A)-C(8A)-H(8A2)	110.4
C(9A)-C(8A)-H(8A2)	110.4
H(8A1)-C(8A)-H(8A2)	108.6
O(3A)-C(9A)-O(4A)	124.9(4)
O(3A)-C(9A)-C(8A)	127.0(4)
O(4A)-C(9A)-C(8A)	108.1(3)
C(11A)-C(10A)-C(15A)	121.8(3)

C(11A)-C(10A)-O(4A)	121.1(3)
C(15A)-C(10A)-O(4A)	116.9(3)
C(10A)-C(11A)-C(12A)	119.4(3)
C(10A)-C(11A)-H(11A)	120.3
C(12A)-C(11A)-H(11A)	120.3
C(11A)-C(12A)-C(13A)	119.7(4)
C(11A)-C(12A)-H(12A)	120.1
C(13A)-C(12A)-H(12A)	120.1
O(5A)-C(13A)-C(14A)	115.9(3)
O(5A)-C(13A)-C(12A)	124.2(3)
C(14A)-C(13A)-C(12A)	119.8(3)
C(15A)-C(14A)-C(13A)	120.1(3)
C(15A)-C(14A)-H(14A)	120.0
C(13A)-C(14A)-H(14A)	120.0
C(10A)-C(15A)-C(14A)	119.1(4)
C(10A)-C(15A)-H(15A)	120.4
C(14A)-C(15A)-H(15A)	120.4
O(5A)-C(16A)-H(16A)	109.5
O(5A)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
O(5A)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
C(1B)-O(1B)-C(7B)	116.5(3)
C(6B)-O(2B)-C(8B)	116.9(3)
C(9B)-O(4B)-C(10B)	116.7(3)
C(13B)-O(5B)-C(16B)	117.5(3)
O(1B)-C(1B)-C(2B)	124.9(4)
O(1B)-C(1B)-C(6B)	116.0(3)
C(2B)-C(1B)-C(6B)	119.1(4)
C(3B)-C(2B)-C(1B)	120.0(4)
C(3B)-C(2B)-H(2B)	120.0
C(1B)-C(2B)-H(2B)	120.0
C(4B)-C(3B)-C(2B)	120.7(4)
C(4B)-C(3B)-H(3B)	119.7
C(2B)-C(3B)-H(3B)	119.7
C(3B)-C(4B)-C(5B)	119.3(4)
C(3B)-C(4B)-H(4B)	120.4
C(5B)-C(4B)-H(4B)	120.4
C(6B)-C(5B)-C(4B)	120.3(4)
C(6B)-C(5B)-H(5B)	119.8
C(4B)-C(5B)-H(5B)	119.8
C(5B)-C(6B)-O(2B)	125.2(3)
C(5B)-C(6B)-C(1B)	120.5(4)
O(2B)-C(6B)-C(1B)	114.2(3)
O(1B)-C(7B)-H(7B1)	109.5
O(1B)-C(7B)-H(7B2)	109.5
H(7B1)-C(7B)-H(7B2)	109.5
O(1B)-C(7B)-H(7B3)	109.5
H(7B1)-C(7B)-H(7B3)	109.5
H(7B2)-C(7B)-H(7B3)	109.5
O(2B)-C(8B)-C(9B)	106.4(3)
O(2B)-C(8B)-H(8B1)	110.4
C(9B)-C(8B)-H(8B1)	110.4
O(2B)-C(8B)-H(8B2)	110.4
C(9B)-C(8B)-H(8B2)	110.4
H(8B1)-C(8B)-H(8B2)	108.6
O(3B)-C(9B)-O(4B)	125.0(4)

O(3B)-C(9B)-C(8B)	126.4(4)
O(4B)-C(9B)-C(8B)	108.6(3)
C(11B)-C(10B)-C(15B)	121.8(3)
C(11B)-C(10B)-O(4B)	120.2(3)
C(15B)-C(10B)-O(4B)	117.9(3)
C(10B)-C(11B)-C(12B)	119.3(3)
C(10B)-C(11B)-H(11B)	120.4
C(12B)-C(11B)-H(11B)	120.4
C(11B)-C(12B)-C(13B)	119.6(3)
C(11B)-C(12B)-H(12B)	120.2
C(13B)-C(12B)-H(12B)	120.2
O(5B)-C(13B)-C(14B)	116.2(3)
O(5B)-C(13B)-C(12B)	123.8(3)
C(14B)-C(13B)-C(12B)	120.1(3)
C(15B)-C(14B)-C(13B)	120.5(3)
C(15B)-C(14B)-H(14B)	119.8
C(13B)-C(14B)-H(14B)	119.8
C(14B)-C(15B)-C(10B)	118.8(3)
C(14B)-C(15B)-H(15B)	120.6
C(10B)-C(15B)-H(15B)	120.6
O(5B)-C(16B)-H(16D)	109.5
O(5B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
O(5B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for molecule 7a. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

U11	U22	U33	U23	U13	U12	
O(1A)	31(2)	33(2)	40(2)	-5(1)	9(1)	-8(1)
O(2A)	31(2)	35(2)	34(1)	-3(1)	10(1)	-11(1)
O(3A)	34(2)	36(2)	42(2)	-6(1)	9(1)	-9(1)
O(4A)	37(2)	32(2)	35(2)	-3(1)	11(1)	-11(1)
O(5A)	44(2)	36(2)	32(1)	-1(1)	6(1)	-16(1)
C(1A)	27(2)	31(2)	28(2)	-2(2)	1(2)	-9(2)
C(2A)	31(2)	41(3)	29(2)	-5(2)	3(2)	-13(2)
C(3A)	38(2)	40(3)	37(2)	-5(2)	5(2)	-17(2)
C(4A)	38(2)	34(2)	35(2)	-4(2)	5(2)	-10(2)
C(5A)	30(2)	37(3)	33(2)	-4(2)	4(2)	-8(2)
C(6A)	27(2)	37(2)	27(2)	0(2)	1(2)	-11(2)
C(7A)	32(2)	38(3)	46(2)	-10(2)	12(2)	-5(2)
C(8A)	30(2)	36(2)	29(2)	-3(2)	7(2)	-9(2)
C(9A)	27(2)	37(2)	29(2)	-3(2)	2(2)	-6(2)
C(10A)	32(2)	31(2)	33(2)	2(2)	6(2)	-11(2)
C(11A)	38(2)	37(2)	28(2)	-1(2)	4(2)	-9(2)
C(12A)	36(2)	31(2)	33(2)	-2(2)	3(2)	-10(2)
C(13A)	33(2)	27(2)	32(2)	-1(2)	8(2)	-6(2)
C(14A)	39(2)	38(2)	28(2)	1(2)	1(2)	-9(2)
C(15A)	35(2)	38(2)	33(2)	-2(2)	0(2)	-11(2)
C(16A)	37(2)	37(3)	41(2)	1(2)	5(2)	-14(2)
O(1B)	27(2)	34(2)	38(2)	0(1)	-5(1)	-4(1)
O(2B)	28(1)	34(2)	37(1)	-1(1)	-6(1)	-9(1)
O(3B)	32(2)	33(2)	41(2)	3(1)	-4(1)	-9(1)
O(4B)	36(2)	33(2)	34(1)	-2(1)	-8(1)	-10(1)
O(5B)	38(2)	33(2)	34(1)	-3(1)	-4(1)	-12(1)
C(1B)	27(2)	32(2)	27(2)	-2(2)	4(2)	-8(2)
C(2B)	27(2)	44(3)	30(2)	-2(2)	0(2)	-12(2)
C(3B)	35(2)	40(3)	35(2)	-2(2)	1(2)	-18(2)
C(4B)	39(2)	34(2)	32(2)	-1(2)	2(2)	-14(2)
C(5B)	28(2)	36(2)	33(2)	-3(2)	2(2)	-7(2)
C(6B)	25(2)	35(2)	27(2)	-4(2)	2(2)	-10(2)
C(7B)	30(2)	42(3)	43(2)	4(2)	-4(2)	-4(2)
C(8B)	29(2)	35(2)	30(2)	-1(2)	-5(2)	-7(2)
C(9B)	25(2)	36(2)	29(2)	-3(2)	2(2)	-7(2)
C(10B)	29(2)	32(2)	35(2)	-5(2)	-4(2)	-9(2)
C(11B)	33(2)	41(3)	29(2)	-2(2)	0(2)	-9(2)
C(12B)	30(2)	36(2)	35(2)	-3(2)	2(2)	-11(2)
C(13B)	30(2)	29(2)	32(2)	-3(2)	-5(2)	-5(2)
C(14B)	36(2)	38(2)	27(2)	-2(2)	-1(2)	-7(2)
C(15B)	33(2)	32(2)	34(2)	1(2)	-1(2)	-8(2)
C(16B)	35(2)	37(3)	44(2)	-2(2)	-3(2)	-12(2)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for molecule 7a.

x	y	z	U(eq)	
H(2A)	10	5921	7189	39
H(3A)	1115	4080	7067	44
H(4A)	4368	3356	6418	43
H(5A)	6614	4495	5897	39
H(7A1)	-1268	7644	6798	58
H(7A2)	-199	8660	6957	58
H(7A3)	201	7646	7500	58
H(8A1)	6908	5927	5074	38
H(8A2)	8855	5672	5683	38
H(11A)	12827	7991	5214	41
H(12A)	14718	9202	4625	39
H(14A)	11591	8734	2816	42
H(15A)	9701	7536	3413	42
H(16A)	15062	10772	3948	57
H(16B)	16730	10674	3280	57
H(16C)	17142	9742	3884	57
H(2B)	-5215	6344	-2090	39
H(3B)	-4012	4480	-2073	42
H(4B)	-629	3617	-1472	41
H(5B)	1654	4645	-923	39
H(7B1)	-4995	8057	-2350	58
H(7B2)	-5287	9018	-1826	58
H(7B3)	-6472	8023	-1648	58
H(8B1)	3818	5804	-615	38
H(8B2)	1905	5909	-5	38
H(11B)	7705	8021	-115	41
H(12B)	9559	9192	460	40
H(14B)	6567	8480	2279	40
H(15B)	4671	7339	1701	40
H(16D)	12063	9655	1224	57
H(16E)	11483	10573	1780	57
H(16F)	9923	10654	1088	57

Table 12. Torsion angles [deg] for molecule 7a.

C(7A)-O(1A)-C(1A)-C(2A)	-2.8(5)
C(7A)-O(1A)-C(1A)-C(6A)	177.1(3)
O(1A)-C(1A)-C(2A)-C(3A)	179.1(3)
C(6A)-C(1A)-C(2A)-C(3A)	-0.8(6)
C(1A)-C(2A)-C(3A)-C(4A)	-0.2(6)
C(2A)-C(3A)-C(4A)-C(5A)	0.8(6)
C(3A)-C(4A)-C(5A)-C(6A)	-0.2(6)
C(4A)-C(5A)-C(6A)-O(2A)	177.9(3)
C(4A)-C(5A)-C(6A)-C(1A)	-0.8(6)
C(8A)-O(2A)-C(6A)-C(5A)	13.9(5)
C(8A)-O(2A)-C(6A)-C(1A)	-167.3(3)
O(1A)-C(1A)-C(6A)-C(5A)	-178.6(3)
C(2A)-C(1A)-C(6A)-C(5A)	1.3(6)
O(1A)-C(1A)-C(6A)-O(2A)	2.6(5)
C(2A)-C(1A)-C(6A)-O(2A)	-177.5(3)
C(6A)-O(2A)-C(8A)-C(9A)	175.0(3)
C(10A)-O(4A)-C(9A)-O(3A)	-0.7(6)
C(10A)-O(4A)-C(9A)-C(8A)	178.6(3)
O(2A)-C(8A)-C(9A)-O(3A)	3.6(5)
O(2A)-C(8A)-C(9A)-O(4A)	-175.6(3)
C(9A)-O(4A)-C(10A)-C(11A)	64.9(5)
C(9A)-O(4A)-C(10A)-C(15A)	-119.0(4)
C(15A)-C(10A)-C(11A)-C(12A)	-0.5(6)
O(4A)-C(10A)-C(11A)-C(12A)	175.4(3)
C(10A)-C(11A)-C(12A)-C(13A)	-0.6(6)
C(16A)-O(5A)-C(13A)-C(14A)	178.5(4)
C(16A)-O(5A)-C(13A)-C(12A)	-1.7(6)
C(11A)-C(12A)-C(13A)-O(5A)	-178.3(4)
C(11A)-C(12A)-C(13A)-C(14A)	1.4(6)
O(5A)-C(13A)-C(14A)-C(15A)	178.6(4)
C(12A)-C(13A)-C(14A)-C(15A)	-1.2(6)
C(11A)-C(10A)-C(15A)-C(14A)	0.7(6)
O(4A)-C(10A)-C(15A)-C(14A)	-175.3(4)
C(13A)-C(14A)-C(15A)-C(10A)	0.1(6)
C(7B)-O(1B)-C(1B)-C(2B)	-1.4(5)
C(7B)-O(1B)-C(1B)-C(6B)	177.9(3)
O(1B)-C(1B)-C(2B)-C(3B)	-179.8(3)
C(6B)-C(1B)-C(2B)-C(3B)	0.9(5)
C(1B)-C(2B)-C(3B)-C(4B)	0.3(5)
C(2B)-C(3B)-C(4B)-C(5B)	-1.4(6)
C(3B)-C(4B)-C(5B)-C(6B)	1.2(5)
C(4B)-C(5B)-C(6B)-O(2B)	-177.9(3)
C(4B)-C(5B)-C(6B)-C(1B)	0.0(5)
C(8B)-O(2B)-C(6B)-C(5B)	-17.0(5)
C(8B)-O(2B)-C(6B)-C(1B)	165.0(3)
O(1B)-C(1B)-C(6B)-C(5B)	179.6(3)
C(2B)-C(1B)-C(6B)-C(5B)	-1.1(5)
O(1B)-C(1B)-C(6B)-O(2B)	-2.3(4)
C(2B)-C(1B)-C(6B)-O(2B)	177.1(3)
C(6B)-O(2B)-C(8B)-C(9B)	-174.5(3)
C(10B)-O(4B)-C(9B)-O(3B)	-1.2(5)
C(10B)-O(4B)-C(9B)-C(8B)	179.4(3)
O(2B)-C(8B)-C(9B)-O(3B)	-4.1(5)
O(2B)-C(8B)-C(9B)-O(4B)	175.2(3)
C(9B)-O(4B)-C(10B)-C(11B)	-65.0(5)
C(9B)-O(4B)-C(10B)-C(15B)	117.8(4)

C(15B)-C(10B)-C(11B)-C(12B)	0.4(6)
O(4B)-C(10B)-C(11B)-C(12B)	-176.7(4)
C(10B)-C(11B)-C(12B)-C(13B)	0.6(6)
C(16B)-O(5B)-C(13B)-C(14B)	-179.9(4)
C(16B)-O(5B)-C(13B)-C(12B)	0.2(6)
C(11B)-C(12B)-C(13B)-O(5B)	178.9(4)
C(11B)-C(12B)-C(13B)-C(14B)	-1.0(6)
O(5B)-C(13B)-C(14B)-C(15B)	-179.5(4)
C(12B)-C(13B)-C(14B)-C(15B)	0.4(6)
C(13B)-C(14B)-C(15B)-C(10B)	0.6(6)
C(11B)-C(10B)-C(15B)-C(14B)	-1.0(6)
O(4B)-C(10B)-C(15B)-C(14B)	176.1(4)

Symmetry transformations used to generate equivalent atoms:

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