

Appendix 2

X-Ray Crystallography Reports Relevant to Chapter 2

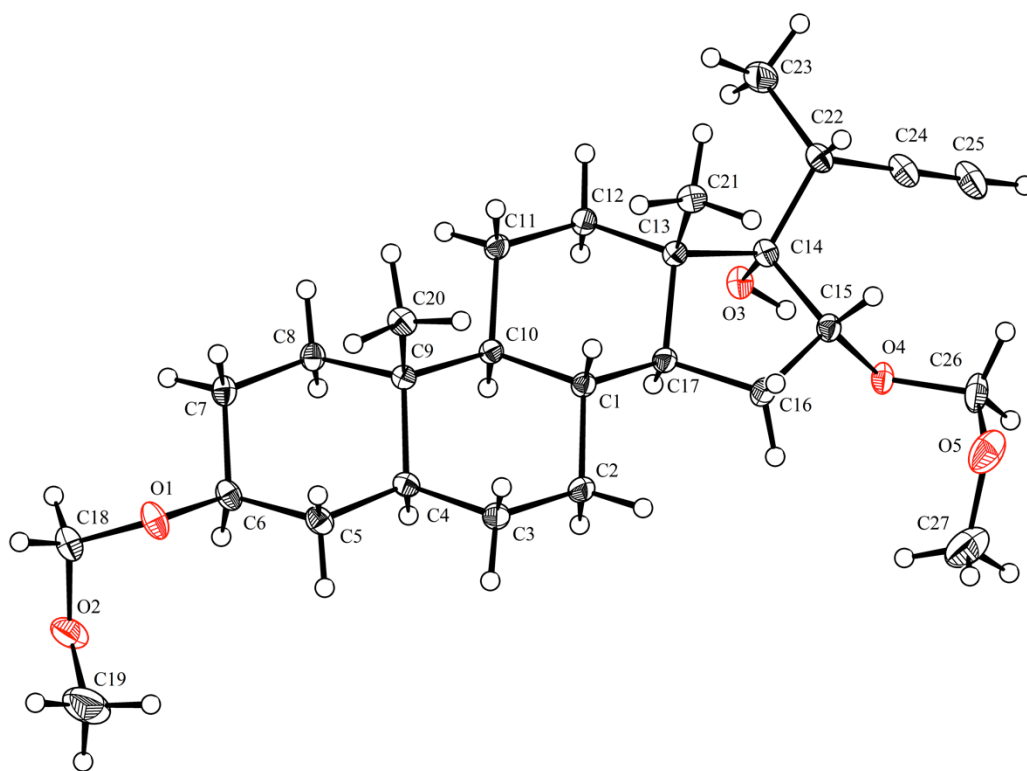
Figure 4. X-ray structure of alcohol **87**.

Table 1. Crystal data and structure refinement for a14213.

Identification code	a14213	
Empirical formula	$C_{27}H_{44}O_5$	
Formula weight	448.62	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P 41 21 2	
Unit cell dimensions	$a = 12.1458(4)$ Å	$a = 90^\circ$
	$b = 12.1458(4)$ Å	$b = 90^\circ$
	$c = 34.4196(16)$ Å	$g = 90^\circ$
Volume	$5077.6(4)$ Å ³	
Z	8	
Density (calculated)	1.174 Mg/m ³	
Absorption coefficient	0.079 mm ⁻¹	

F(000)	1968
Crystal size	0.53 x 0.40 x 0.19 mm ³
Theta range for data collection	1.778 to 37.056°.
Index ranges	-20<=h<=20, -20<=k<=19, -58<=l<=57
Reflections collected	233885
Independent reflections	12739 [R(int) = 0.0650]
Completeness to theta = 25.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.9201
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12739 / 0 / 409
Goodness-of-fit on F ²	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.1003
R indices (all data)	R1 = 0.0461, wR2 = 0.1047
Absolute structure parameter	-0.12(14)
Extinction coefficient	n/a
Largest diff. peak and hole	0.375 and -0.224 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁵) and equivalent isotropic displacement parameters (Å²x 10⁴) for a14213. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	129946(8)	149003(7)	56096(2)	195(2)
O(2)	135140(9)	157278(8)	50225(3)	265(2)
O(3)	90398(7)	75451(7)	53158(2)	162(1)
O(4)	68988(6)	79928(7)	53810(2)	163(1)
O(5)	51853(8)	86741(11)	55854(3)	329(2)
C(1)	95261(8)	107761(8)	57862(3)	131(2)
C(2)	89567(9)	117708(9)	56012(3)	173(2)
C(3)	95505(9)	128430(8)	56965(3)	169(2)
C(4)	107604(9)	127728(8)	55763(3)	138(2)
C(5)	113396(9)	138808(8)	56244(3)	164(2)
C(6)	125280(9)	138611(8)	54868(3)	156(2)
C(7)	131681(9)	128993(9)	56614(3)	159(2)

C(8)	125595(8)	117994(8)	56125(3)	143(2)
C(9)	113794(8)	118157(8)	57802(3)	121(1)
C(10)	107635(8)	107272(8)	56784(3)	122(1)
C(11)	113061(8)	96825(8)	58470(3)	143(2)
C(12)	106897(8)	86081(8)	57478(3)	142(2)
C(13)	94677(8)	86716(8)	58659(3)	125(1)
C(14)	86905(8)	77591(8)	57015(3)	134(2)
C(15)	75328(8)	83374(9)	57110(3)	145(2)
C(16)	77380(8)	95900(9)	57160(3)	168(2)
C(17)	89837(8)	96998(8)	56619(3)	134(2)
C(18)	138626(10)	152948(10)	53821(3)	197(2)
C(19)	127984(18)	166497(16)	50724(7)	479(5)
C(20)	114429(9)	119834(9)	62240(3)	158(2)
C(21)	93401(9)	87327(9)	63099(3)	161(2)
C(22)	86402(9)	66577(9)	59331(3)	166(2)
C(23)	97569(11)	60829(10)	59779(4)	242(2)
C(24)	78585(11)	59023(9)	57405(3)	206(2)
C(25)	72478(12)	52766(11)	55777(4)	257(2)
C(26)	57925(10)	77554(12)	54678(3)	239(2)
C(27)	49571(14)	94156(19)	52751(6)	400(4)