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Supplementary Information

Structural Analysis and Antitumor Activity of Androstane D-Seco-mesyloxy Derivatives

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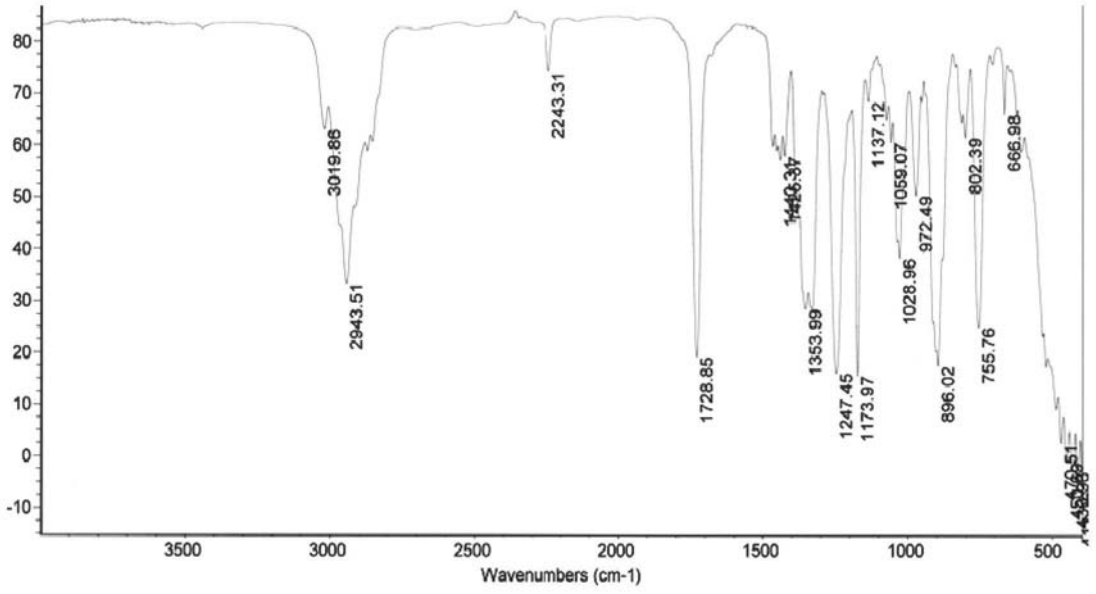

Figure S1. IR spectrum of 3β-acetoxy-(*17S*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**5**).

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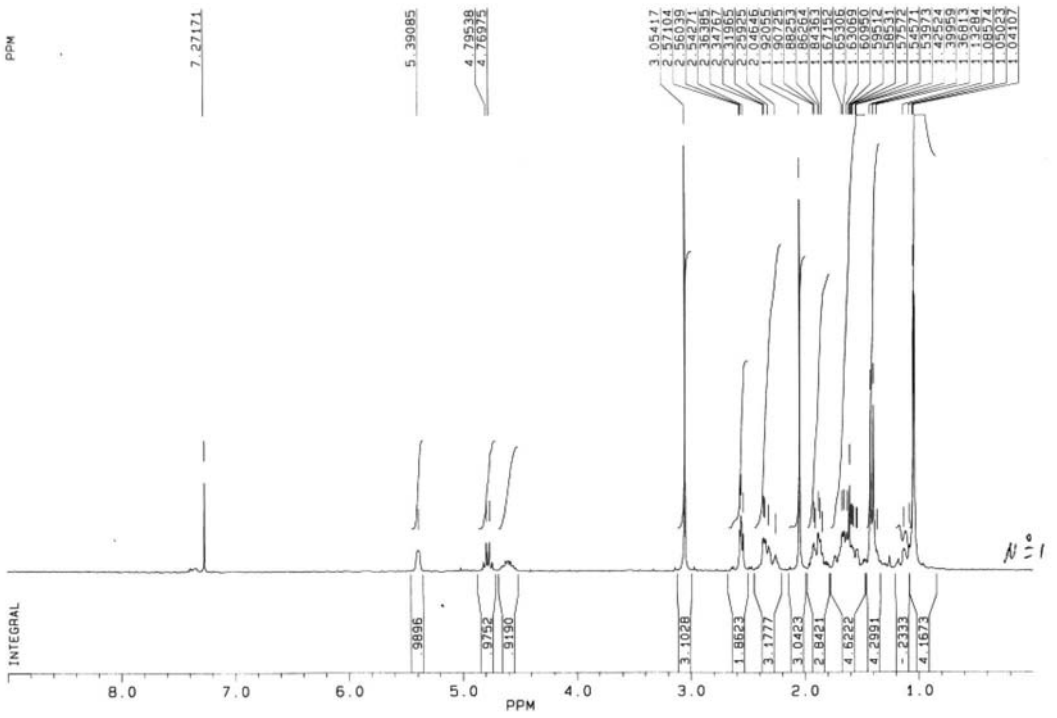


Figure S2. ^{1}H NMR spectrum (250 MHz, $CDCl_3$) of 3β-acetoxy-(*17S*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**5**).

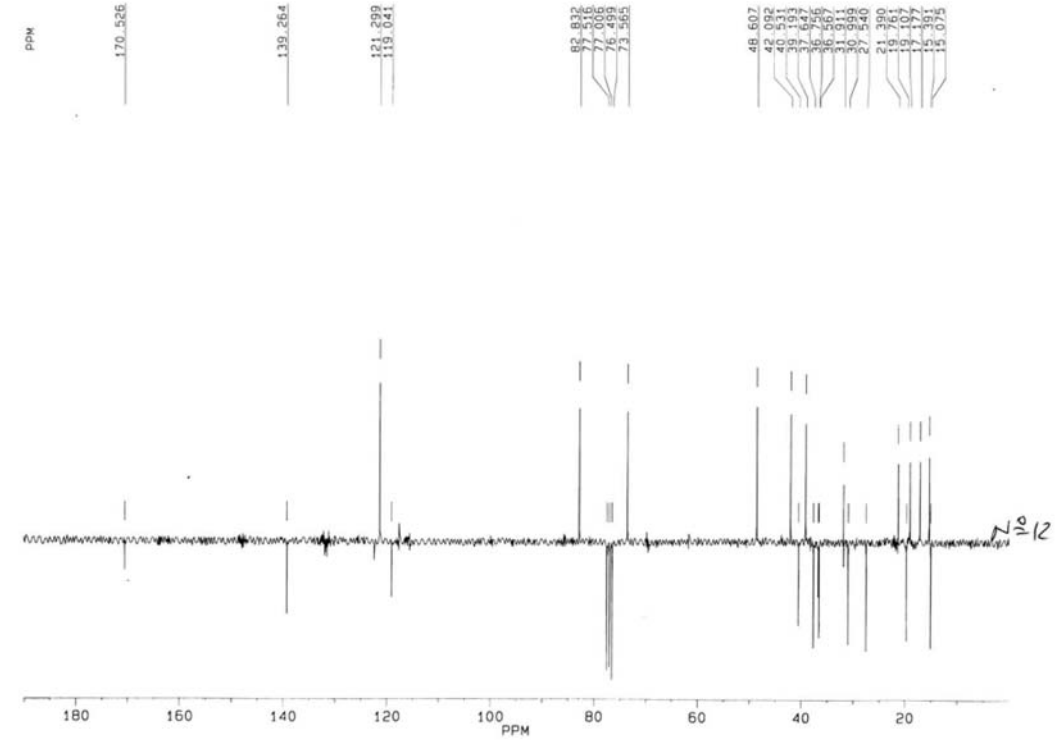


Figure S3. ^{13}C NMR spectrum (62.5 MHz, $CDCl_3$) of 3β-acetoxy-(*17S*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**5**).

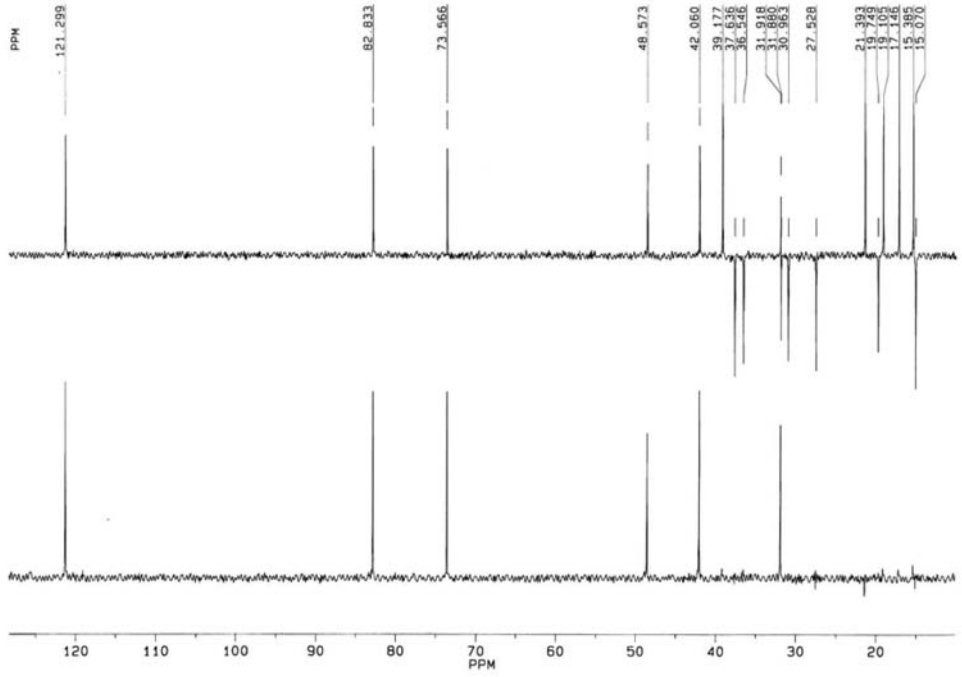
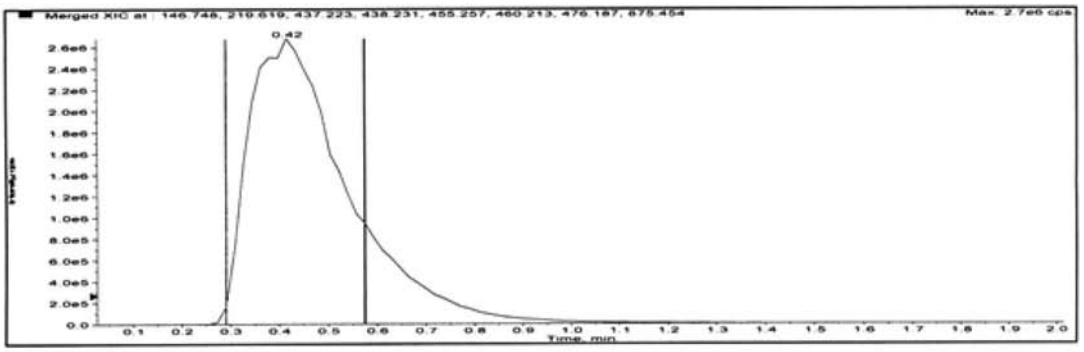
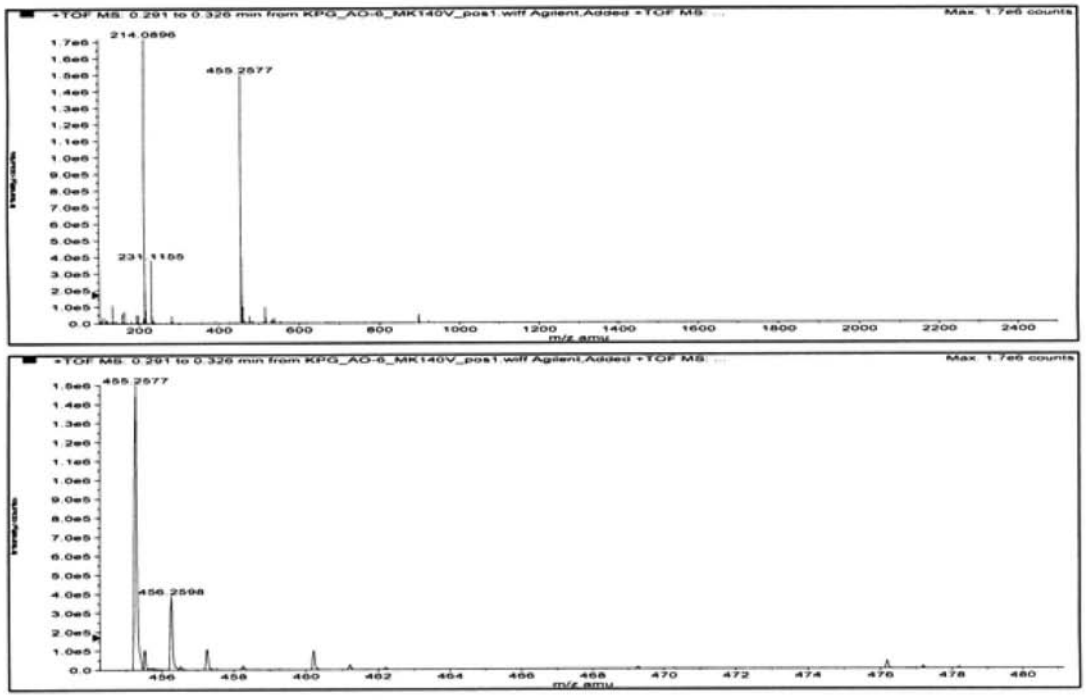


Figure S4. DEPT 135 and DEPT 90 spectrum (62.5 MHz, $CDCl_3$) of 3β-acetoxy-(*17S*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**5**).



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H35NO5S	--	437.22359	0.42	3.75659 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+NH4]+	1506511.36	455.25742	455.25771	0.28895	0.63	--
[M+Na]+	101743.68	460.21282	460.21217	-0.64697	-1.41	--
[M+K]+	41807.72	476.18675	476.18622	-0.52749	-1.11	--

Figure S5. HRMS (ESI$^+$/TOF) spectrum of 3β-acetoxy-(*17S*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**5**).

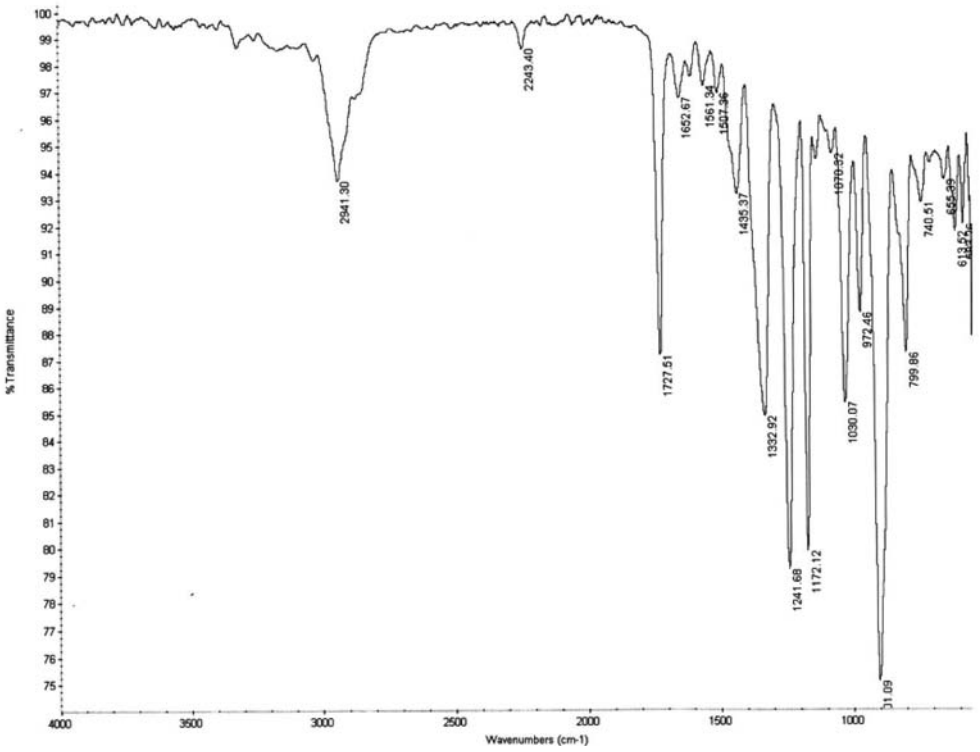


Figure S6. IR spectrum of 3β-acetoxy-(17*R*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**6**).

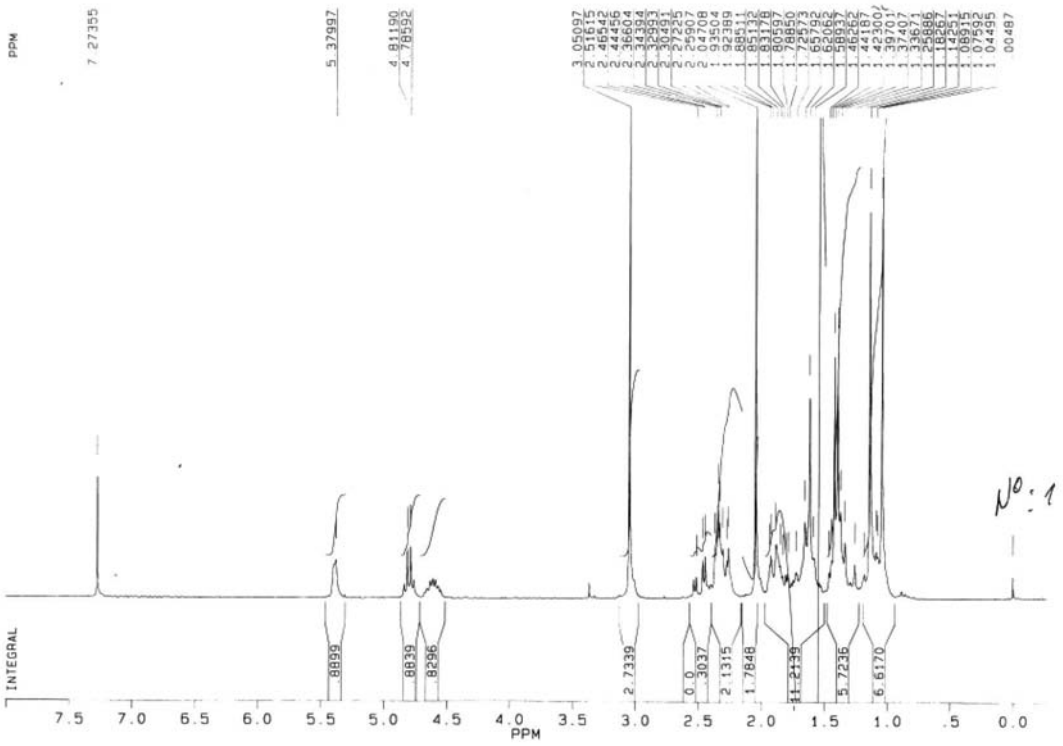


Figure S7. ^{1}H NMR spectrum (250 MHz, $CDCl_3$) of 3β-acetoxy-(17*R*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**6**).

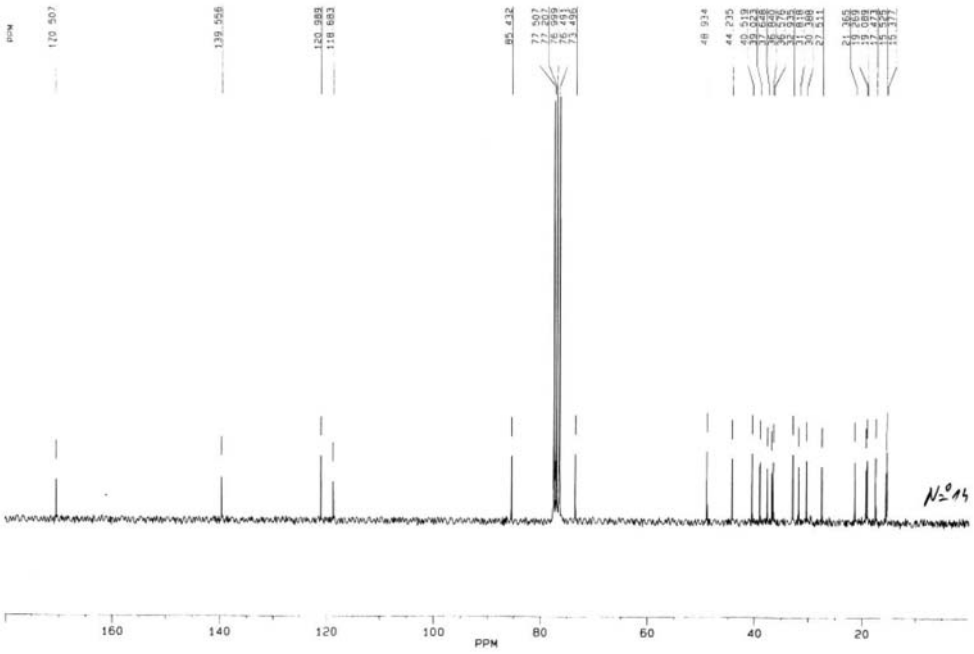


Figure S8. ^{13}C NMR spectrum (62.5 MHz, $CDCl_3$) of 3β-acetoxy-(17*R*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**6**).

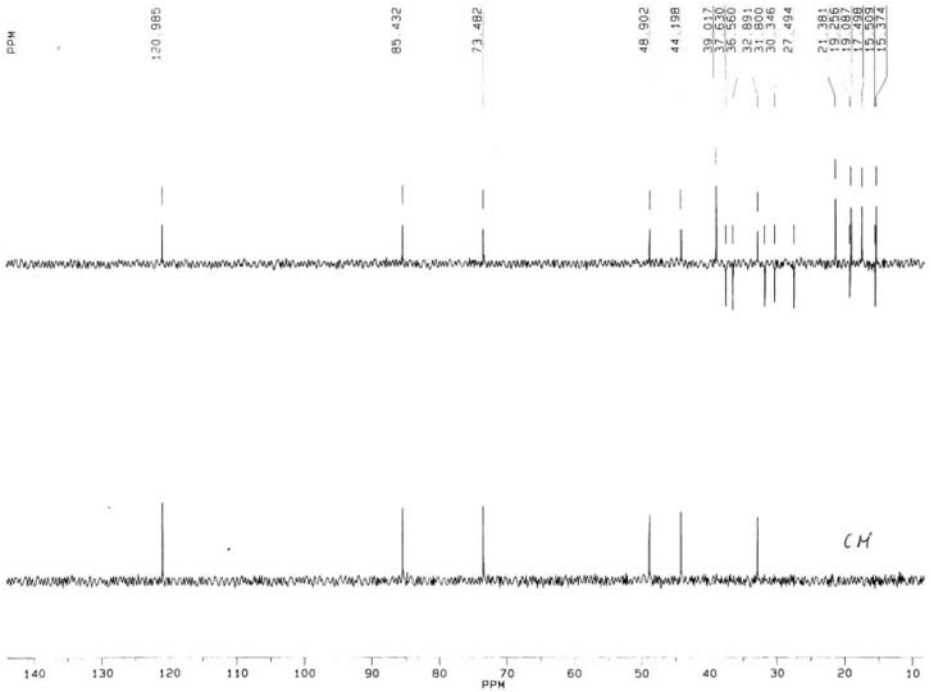
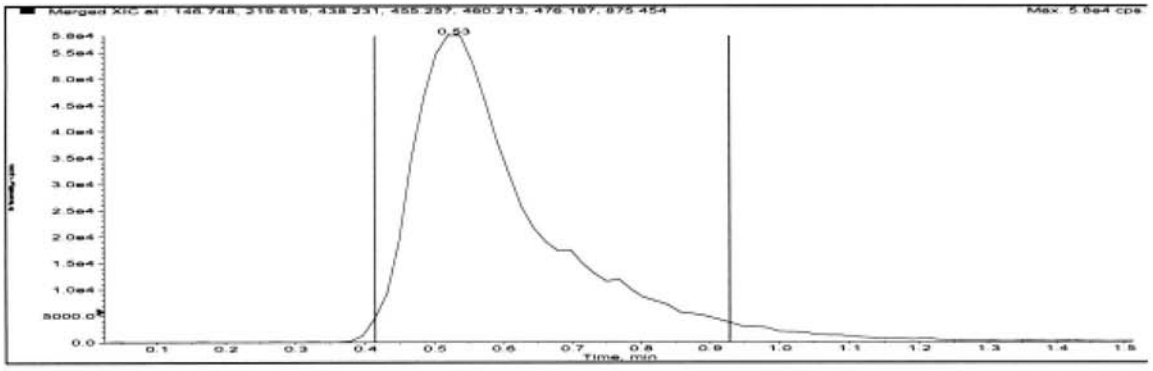
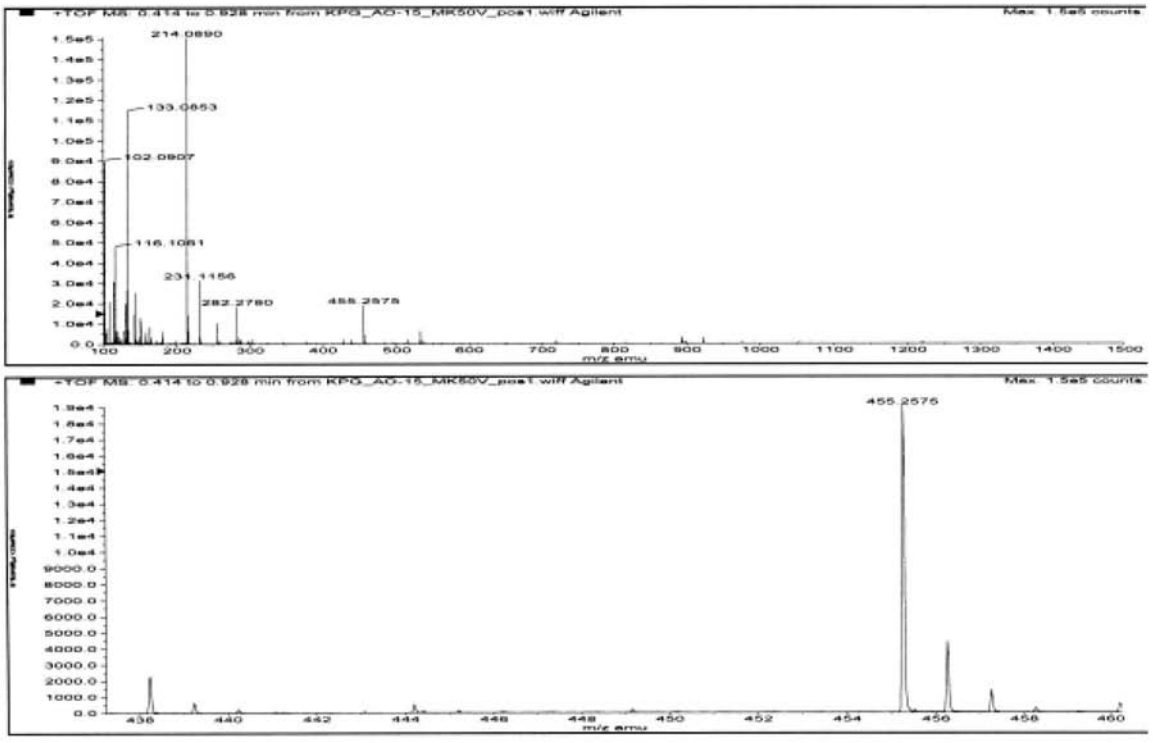


Figure S9. DEPT 135 and DEPT 90 spectrum (62.5 MHz, $CDCl_3$) of 3β-acetoxy-(17*R*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**6**).



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H35NO5S	--	437.22359	0.53	7.22937 E5	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H]+	2416.57	438.23087	438.23088	0.01272	0.03	--
[M+NH4]+	19680.11	455.25742	455.25753	0.10898	0.24	--

Figure S10. HRMS (ESI$^+$/TOF) spectrum of 3β-acetoxy-(17*R*)-mesyloxy-17-methyl-16,17-secoandrost-5-ene-16-nitrile (**6**).

Table S1. Crystal data and structure refinement for compound **5**

Identification code	Compound **5**	
Empirical formula	$C_{23}H_{35}NO_5S$	
Formula weight	437.58	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.539(5) Å	α = 90°
	b = 9.190(5) Å	β = 90°
	c = 30.024(5) Å	γ = 90°
Volume	2356.1(19) Å^3	
Z	4	
Density (calculated)	1.234 mg m^{-3}	
Absorption coefficient	0.170 mm^{-1}	
F(000)	944	
Crystal size	0.569 × 0.328 × 0.082 mm^3	
Theta range for data collection	3.14 to 25.00°	
Index ranges	$-10 \leq h \leq 7$, $-9 \leq k \leq 10$, $-31 \leq l \leq 35$	
Reflections collected	6767	
Independent reflections	3816 [R(int) = 0.0261]	
Completeness to theta = 25.00°	99.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.91093	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	3816 / 0 / 279	
Goodness-of-fit on F^2	1.122	
Final R indices [I > 2sigma(I)]	R1 = 0.0581, wR2 = 0.1217	
R indices (all data)	R1 = 0.0680, wR2 = 0.1267	
Absolute structure parameter	–0.05(12)	
Largest diff. peak and hole	0.198 and –0.238 e Å^{-3}	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
S(1)	–3506(1)	8472(1)	7900(1)	51(1)
O(1)	237(3)	2182(2)	10881(1)	48(1)
O(3)	–2358(3)	8724(3)	8297(1)	47(1)
C(10)	731(4)	5245(3)	9791(1)	32(1)
C(13)	210(4)	8079(3)	8582(1)	33(1)
O(2)	–1903(4)	2824(4)	11263(1)	75(1)
O(5)	–2624(4)	8233(4)	7505(1)	83(1)
O(4)	–4565(4)	7386(3)	8035(1)	92(1)
N(1)	–1793(5)	3929(4)	7773(1)	63(1)
C(14)	–285(4)	6451(3)	8558(1)	32(1)
C(6)	–121(5)	3121(3)	9335(1)	42(1)
C(11)	571(4)	7760(3)	9417(1)	37(1)
C(9)	29(4)	6171(3)	9408(1)	30(1)
C(8)	337(4)	5511(3)	8945(1)	30(1)
C(5)	384(4)	3633(3)	9720(1)	32(1)
C(4)	666(5)	2647(3)	10113(1)	41(1)
C(1)	–67(5)	5699(3)	10232(1)	46(1)
C(15)	199(5)	5769(3)	8103(1)	42(1)
C(17)	–672(5)	8979(3)	8230(1)	39(1)
C(12)	–184(5)	8641(3)	9048(1)	40(1)
C(16)	–936(5)	4725(4)	7922(1)	44(1)
C(22)	–747(5)	2095(4)	11228(1)	49(1)
C(7)	–386(5)	3986(3)	8923(1)	45(1)
C(2)	287(5)	4721(3)	10631(1)	46(1)
C(3)	–189(4)	3175(3)	10522(1)	42(1)
C(18)	1965(4)	8257(4)	8485(1)	50(1)
C(21)	–4537(6)	10104(4)	7860(2)	71(1)
C(19)	2504(4)	5465(4)	9831(1)	50(1)
C(23)	–215(6)	981(5)	11556(1)	73(1)
C(20)	–394(6)	10611(4)	8242(1)	69(1)

Table S3. Bond lengths (Å) and angles (degree) for compound **5**

S(1)-O(4)	1.406(3)	C(18)-H(18C)	0.9600	C(7)-C(8)-C(9)	109.3(2)
S(1)-O(5)	1.422(3)	C(21)-H(21A)	0.9600	C(7)-C(8)-C(14)	110.0(3)
S(1)-O(3)	1.561(3)	C(21)-H(21B)	0.9600	C(9)-C(8)-C(14)	113.5(2)
S(1)-C(21)	1.743(4)	C(21)-H(21C)	0.9600	C(7)-C(8)-H(8)	108.0
O(1)-C(22)	1.342(4)	C(19)-H(19A)	0.9600	C(9)-C(8)-H(8)	108.0
O(1)-C(3)	1.457(4)	C(19)-H(19B)	0.9600	C(14)-C(8)-H(8)	108.0
O(3)-C(17)	1.473(4)	C(19)-H(19C)	0.9600	C(6)-C(5)-C(4)	121.5(3)
C(10)-C(5)	1.525(4)	C(23)-H(23A)	0.9600	C(6)-C(5)-C(10)	122.1(3)
C(10)-C(19)	1.533(5)	C(23)-H(23B)	0.9600	C(4)-C(5)-C(10)	116.3(3)
C(10)-C(1)	1.546(4)	C(23)-H(23C)	0.9600	C(5)-C(4)-C(3)	111.5(3)
C(10)-C(9)	1.552(4)	C(20)-H(20A)	0.9600	C(5)-C(4)-H(4A)	109.3
C(13)-C(12)	1.530(4)	C(20)-H(20B)	0.9600	C(3)-C(4)-H(4A)	109.3
C(13)-C(18)	1.535(5)	C(20)-H(20C)	0.9600	C(5)-C(4)-H(4B)	109.3
C(13)-C(17)	1.538(5)	O(4)-S(1)-O(5)	118.1(2)	C(3)-C(4)-H(4B)	109.3
C(13)-C(14)	1.556(4)	O(4)-S(1)-O(3)	106.82(19)	H(4A)-C(4)-H(4B)	108.0
O(2)-C(22)	1.197(5)	O(5)-S(1)-O(3)	109.09(16)	C(2)-C(1)-C(10)	115.2(3)
N(1)-C(16)	1.127(4)	O(4)-S(1)-C(21)	107.8(2)	C(2)-C(1)-H(1A)	108.5
C(14)-C(8)	1.541(4)	O(5)-S(1)-C(21)	110.1(2)	C(10)-C(1)-H(1A)	108.5
C(14)-C(15)	1.560(4)	O(3)-S(1)-C(21)	103.96(19)	C(2)-C(1)-H(1B)	108.5
C(14)-H(14)	0.9800	C(22)-O(1)-C(3)	117.1(3)	C(10)-C(1)-H(1B)	108.5
C(6)-C(5)	1.320(4)	C(17)-O(3)-S(1)	122.3(2)	H(1A)-C(1)-H(1B)	107.5
C(6)-C(7)	1.488(4)	C(5)-C(10)-C(19)	109.3(3)	C(16)-C(15)-C(14)	114.4(3)
C(6)-H(6)	0.96(3)	C(5)-C(10)-C(1)	107.2(3)	C(16)-C(15)-H(15A)	108.7
C(11)-C(12)	1.515(4)	C(19)-C(10)-C(1)	109.4(3)	C(14)-C(15)-H(15A)	108.7
C(11)-C(9)	1.532(4)	C(5)-C(10)-C(9)	110.8(2)	C(16)-C(15)-H(15B)	108.7
C(11)-H(11A)	0.9700	C(19)-C(10)-C(9)	111.5(3)	C(14)-C(15)-H(15B)	108.7
C(11)-H(11B)	0.9700	C(1)-C(10)-C(9)	108.5(2)	H(15A)-C(15)-H(15B)	107.6
C(9)-C(8)	1.540(4)	C(12)-C(13)-C(18)	110.6(3)	O(3)-C(17)-C(20)	107.9(3)
C(9)-H(9)	0.9800	C(12)-C(13)-C(17)	109.8(3)	O(3)-C(17)-C(13)	107.4(3)
C(8)-C(7)	1.533(4)	C(18)-C(13)-C(17)	106.9(3)	C(20)-C(17)-C(13)	116.1(3)
C(8)-H(8)	0.9800	C(12)-C(13)-C(14)	107.8(2)	O(3)-C(17)-H(17)	106.0(19)
C(5)-C(4)	1.507(4)	C(18)-C(13)-C(14)	111.0(3)	C(20)-C(17)-H(17)	109.2(17)
C(4)-C(3)	1.509(5)	C(17)-C(13)-C(14)	110.7(3)	C(13)-C(17)-H(17)	109.7(17)
C(4)-H(4A)	0.9700	C(8)-C(14)-C(13)	114.3(2)	C(11)-C(12)-C(13)	113.3(3)
C(4)-H(4B)	0.9700	C(8)-C(14)-C(15)	110.0(3)	C(11)-C(12)-H(12A)	108.9
C(1)-C(2)	1.529(4)	C(13)-C(14)-C(15)	110.7(2)	C(13)-C(12)-H(12A)	108.9
C(1)-H(1A)	0.9700	C(8)-C(14)-H(14)	107.1	C(11)-C(12)-H(12B)	108.9
C(1)-H(1B)	0.9700	C(13)-C(14)-H(14)	107.1	C(13)-C(12)-H(12B)	108.9
C(15) -C(16)	1.468(5)	C(15)-C(14)-H(14)	107.1	H(12A)-C(12)-H(12B)	107.7
C(15)-H(15A)	0.9700	C(5)-C(6)-C(7)	126.0(3)	N(1)-C(16)-C(15)	178.3(4)
C(15)-H(15B)	0.9700	C(5)-C(6)-H(6)	117.3(17)	O(2)-C(22)-O(1)	123.5(3)
C(17)-C(20)	1.519(5)	C(7)-C(6)-H(6)	116.7(18)	O(2)-C(22)-C(23)	125.2(4)
C(17)-H(17)	0.94(3)	C(12)-C(11)-C(9)	111.6(3)	O(1)-C(22)-C(23)	111.3(4)
C(12)-H(12A)	0.9700	C(12)-C(11)-H(11A)	109.3	C(6)-C(7)-C(8)	113.0(3)
C(12)-H(12B)	0.9700	C(9)-C(11)-H(11A)	109.3	C(6)-C(7)-H(7A)	109.0
C(22)-C(23)	1.493(5)	C(12)-C(11)-H(11B)	109.3	C(8)-C(7)-H(7A)	109.0
C(7)-H(7A)	0.9700	C(9)-C(11)-H(11B)	109.3	C(6)-C(7)-H(7B)	109.0
C(7)-H(7B)	0.9700	H(11A)-C(11)-H(11B)	108.0	C(8)-C(7)-H(7B)	109.0
C(2)-C(3)	1.513(5)	C(11)-C(9)-C(8)	109.9(2)	H(7A)-C(7)-H(7B)	107.8
C(2)-H(2A)	0.9700	C(11)-C(9)-C(10)	113.2(2)	C(3)-C(2)-C(1)	109.2(3)
C(2)-H(2B)	0.9700	C(8)-C(9)-C(10)	112.8(2)	C(3)-C(2)-H(2A)	109.8
C(3)-H(3)	0.9800	C(11)-C(9)-H(9)	106.9	C(1)-C(2)-H(2A)	109.8
C(18)-H(18A)	0.9600	C(8)-C(9)-H(9)	106.9	C(3)-C(2)-H(2B)	109.8
C(18)-H(18B)	0.9600	C(10)-C(9)-H(9)	106.9	C(1)-C(2)-H(2B)	109.8

Table S3. continuation

H(2A)-C(2)-H(2B)	108.3	S(1)-C(21)-H(21A)	109.5	C(22)-C(23)-H(23B)	109.5
O(1)-C(3)-C(4)	106.2(3)	S(1)-C(21)-H(21B)	109.5	H(23A)-C(23)-H(23B)	109.5
O(1)-C(3)-C(2)	111.2(3)	H(21A)-C(21)-H(21B)	109.5	C(22)-C(23)-H(23C)	109.5
C(4)-C(3)-C(2)	110.4(3)	S(1)-C(21)-H(21C)	109.5	H(23A)-C(23)-H(23C)	109.5
O(1)-C(3)-H(3)	109.7	H(21A)-C(21)-H(21C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(4)-C(3)-H(3)	109.7	H(21B)-C(21)-H(21C)	109.5	C(17)-C(20)-H(20A)	109.5
C(2)-C(3)-H(3)	109.7	C(10)-C(19)-H(19A)	109.5	C(17)-C(20)-H(20B)	109.5
C(13)-C(18)-H(18A)	109.5	C(10)-C(19)-H(19B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(13)-C(18)-H(18B)	109.5	H(19A)-C(19)-H(19B)	109.5	C(17)-C(20)-H(20C)	109.5
H(18A)-C(18)-H(18B)	109.5	C(10)-C(19)-H(19C)	109.5	H(20A)-C(20)-H(20C)	109.5
C(13)-C(18)-H(18C)	109.5	H(19A)-C(19)-H(19C)	109.5	H(20B)-C(20)-H(20C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(19B)-C(19)-H(19C)	109.5		
H(18B)-C(18)-H(18C)	109.5	C(22)-C(23)-H(23A)	109.5		

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **5**. The anisotropic displacement factor exponent takes the form: $2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	47(1)	51(1)	54(1)	0(1)	−12(1)	7(1)
O(1)	47(2)	58(1)	40(1)	13(1)	4(1)	4(1)
O(3)	42(2)	63(2)	34(1)	5(1)	1(1)	9(1)
C(10)	30(2)	32(2)	35(2)	–5(1)	–2(2)	3(1)
C(13)	35(2)	32(2)	31(2)	−1(1)	2(2)	−2(2)
O(2)	58(2)	112(2)	55(2)	15(2)	19(2)	19(2)
O(5)	68(2)	134(3)	47(2)	−32(2)	−13(2)	24(2)
O(4)	66(2)	68(2)	144(3)	11(2)	−17(2)	−14(2)
N(1)	76(3)	67(2)	46(2)	−18(2)	–7(2)	−10(2)
C(14)	31(2)	35(2)	31(2)	–9(1)	3(2)	0(2)
C(6)	56(2)	24(2)	45(2)	–2(1)	1(2)	−1(2)
C(11)	44(2)	34(2)	32(2)	–6(1)	–6(2)	2(2)
C(9)	31(2)	28(1)	32(2)	–5(1)	−1(2)	3(1)
C(8)	32(2)	27(1)	32(2)	–5(1)	2(2)	1(2)
C(5)	30(2)	31(2)	35(2)	0(1)	5(2)	2(2)
C(4)	40(2)	36(2)	46(2)	5(1)	5(2)	−3(2)
C(1)	66(3)	40(2)	31(2)	–3(1)	−3(2)	6(2)
C(15)	51(2)	44(2)	30(2)	–6(1)	4(2)	−2(2)
C(17)	49(2)	38(2)	30(2)	–3(1)	3(2)	−3(2)
C(12)	54(2)	31(2)	34(2)	–8(1)	–6(2)	5(2)
C(16)	62(3)	41(2)	29(2)	−10(2)	−3(2)	4(2)
C(22)	48(2)	67(2)	32(2)	0(2)	−2(2)	−11(2)
C(7)	64(3)	33(2)	37(2)	−10(1)	–4(2)	–4(2)
C(2)	55(3)	55(2)	28(2)	–4(1)	0(2)	1(2)
C(3)	39(2)	49(2)	37(2)	9(2)	2(2)	4(2)
C(18)	43(2)	52(2)	55(2)	2(2)	−3(2)	−16(2)
C(21)	65(3)	72(3)	77(3)	13(2)	−12(3)	26(2)
C(19)	46(3)	46(2)	58(2)	12(2)	−15(2)	–4(2)
C(23)	83(4)	86(3)	49(2)	23(2)	11(3)	1(3)
C(20)	98(4)	40(2)	70(3)	14(2)	−24(3)	–8(2)

Table S5. Torsion angles (degree) for compound **5**

O(4)-S(1)-O(3)-C(17)	140.7(3)	C(15)-C(14)-C(8)-C(7)	–61.9(4)	C(14)-C(13)-C(17)-O(3)	54.5(3)
O(5)-S(1)-O(3)-C(17)	12.0(3)	C(13)-C(14)-C(8)-C(9)	49.9(4)	C(12)-C(13)-C(17)-C(20)	56.4(4)
C(21)-S(1)-O(3)-C(17)	−105.4(3)	C(15)-C(14)-C(8)-C(9)	175.3(3)	C(18)-C(13)-C(17)-C(20)	–63.7(4)
C(12)-C(13)-C(14)-C(8)	–50.7(4)	C(7)-C(6)-C(5)-C(4)	−177.8(3)	C(14)-C(13)-C(17)-C(20)	175.3(3)
C(18)-C(13)-C(14)-C(8)	70.6(3)	C(7)-C(6)-C(5)-C(10)	1.5(6)	C(9)-C(11)-C(12)-C(13)	–60.8(4)
C(17)-C(13)-C(14)-C(8)	−170.8(3)	C(19)-C(10)-C(5)-C(6)	−109.2(4)	C(18)-C(13)-C(12)-C(11)	–65.3(4)
C(12)-C(13)-C(14)-C(15)	−175.7(3)	C(1)-C(10)-C(5)-C(6)	132.3(3)	C(17)-C(13)-C(12)-C(11)	176.9(3)
C(18)-C(13)-C(14)-C(15)	–54.4(4)	C(9)-C(10)-C(5)-C(6)	14.1(5)	C(14)-C(13)-C(12)-C(11)	56.3(4)
C(17)-C(13)-C(14)-C(15)	64.2(4)	C(19)-C(10)-C(5)-C(4)	70.2(4)	C(14)-C(15)-C(16)-N(1)	158(14)
C(12)-C(11)-C(9)-C(8)	55.0(4)	C(1)-C(10)-C(5)-C(4)	–48.3(4)	C(3)-O(1)-C(22)-O(2)	–3.0(5)
C(12)-C(11)-C(9)-C(10)	−177.9(3)	C(9)-C(10)-C(5)-C(4)	−166.5(3)	C(3)-O(1)-C(22)-C(23)	176.8(3)
C(5)-C(10)-C(9)-C(11)	−170.2(3)	C(6)-C(5)-C(4)-C(3)	−127.0(4)	C(5)-C(6)-C(7)-C(8)	13.3(6)
C(19)-C(10)-C(9)-C(11)	–48.2(4)	C(10)-C(5)-C(4)-C(3)	53.6(4)	C(9)-C(8)-C(7)-C(6)	–42.2(4)
C(1)-C(10)-C(9)-C(11)	72.4(3)	C(5)-C(10)-C(1)-C(2)	50.5(4)	C(14)-C(8)-C(7)-C(6)	−167.5(3)
C(5)-C(10)-C(9)-C(8)	–44.7(4)	C(19)-C(10)-C(1)-C(2)	–67.9(4)	C(10)-C(1)-C(2)-C(3)	–57.4(5)
C(19)-C(10)-C(9)-C(8)	77.3(3)	C(9)-C(10)-C(1)-C(2)	170.2(3)	C(22)-O(1)-C(3)-C(4)	−157.4(3)
C(1)-C(10)-C(9)-C(8)	−162.1(3)	C(8)-C(14)-C(15)-C(16)	89.9(4)	C(22)-O(1)-C(3)-C(2)	82.5(4)
C(11)-C(9)-C(8)-C(7)	−173.3(3)	C(13)-C(14)-C(15)-C(16)	−142.7(3)	C(5)-C(4)-C(3)-O(1)	−177.3(3)
C(10)-C(9)-C(8)-C(7)	59.5(4)	S(1)-O(3)-C(17)-C(20)	97.0(3)	C(5)-C(4)-C(3)-C(2)	–56.7(4)
C(11)-C(9)-C(8)-C(14)	–50.1(4)	S(1)-O(3)-C(17)-C(13)	−137.2(2)	C(1)-C(2)-C(3)-O(1)	175.6(3)
C(10)-C(9)-C(8)-C(14)	−177.3(3)	C(12)-C(13)-C(17)-O(3)	–64.4(3)	C(1)-C(2)-C(3)-C(4)	58.1(4)
C(13)-C(14)-C(8)-C(7)	172.7(3)	C(18)-C(13)-C(17)-O(3)	175.6(3)		

Table S6. Crystal data and structure refinement for compound **6**

Identification code	Compound **6**	
Empirical formula	$C_{23}H_{35}NO_5S$	
Formula weight	437.58	
Temperature	293(2) K	
Wavelength	0.71069 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 10.644(5) Å	α = 90°
	b = 9.823(5) Å	β = 94.995(5)°
	c = 11.068(5) Å	γ = 90°
Volume	1152.8(10) Å^3	
Z	2	
Density (calculated)	1.261 mg m^{-3}	
Absorption coefficient	0.174 mm^{1}	
F(000)	472	
Crystal size	0.532 × 0.178 × 0.079 mm^3	
Theta range for data collection	3.28 to 25.00°	
Index ranges	8 ≤ h ≤ 12, 11 ≤ k ≤ 11, 13 ≤ l ≤ 12	
Reflections collected	4336	
Independent reflections	3448 [R(int) = 0.0249]	
Completeness to theta = 25.00°	99.7%	
Absorption correction	semiempirical from equivalents	
Max. and min. transmission	1.00000 and 0.74065	
Refinement method	full matrix least squares on F^2	
Data / restraints / parameters	3448 / 1 / 275	
Goodnessoffit on *F2*	1.058	
Final R indices [I > 2sigma(I)]	R1 = 0.0535, wR2 = 0.1017	
R indices (all data)	R1 = 0.0678, wR2 = 0.1108	
Absolute structure parameter	0.01(10)	
Largest diff. peak and hole	0.169 and 0.200 e Å^3	

Table S7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
S(1)	10266(1)	7848(1)	5579(1)	52(1)
O(3)	9606(2)	8391(2)	6687(2)	47(1)
O(1)	849(3)	8888(3)	11208(2)	55(1)
O(5)	10936(3)	6673(3)	6002(3)	77(1)
C(9)	5251(3)	9044(3)	8542(3)	35(1)
C(8)	5071(3)	9556(3)	7227(3)	34(1)
O(4)	9383(3)	7722(3)	4561(3)	72(1)
C(13)	7373(3)	8856(3)	6900(3)	37(1)
C(11)	6300(3)	7986(4)	8712(4)	46(1)
C(14)	6322(3)	9957(3)	6723(3)	34(1)
C(10)	3991(3)	8562(3)	9016(3)	37(1)
C(5)	2955(3)	9594(3)	8692(3)	38(1)
C(20)	9115(3)	10708(3)	7172(3)	47(1)
C(3)	1986(4)	9309(4)	10662(3)	49(1)
O(2)	-72(3)	10907(3)	10828(3)	88(1)
C(7)	4168(3)	10776(3)	7159(3)	41(1)
C(12)	7520(4)	8504(4)	8252(3)	46(1)
C(6)	3074(4)	10579(4)	7900(3)	42(1)
C(16)	5236(4)	9660(4)	4607(4)	51(1)
C(17)	8612(3)	9450(3)	6500(3)	41(1)
C(4)	1753(4)	9426(4)	9309(3)	50(1)
C(18)	7026(4)	7583(3)	6134(4)	53(1)
C(15)	6083(4)	10494(4)	5402(3)	45(1)
C(1)	4171(4)	8469(4)	10412(3)	51(1)
C(2)	2955(4)	8212(4)	11009(4)	56(1)
C(21)	11347(4)	9112(5)	5278(4)	72(1)
C(22)	−110(4)	9763(4)	11217(4)	60(1)
C(23)	−1217(4)	9131(5)	11716(4)	73(1)
C(19)	3580(4)	7164(3)	8483(4)	57(1)
N(1)	4557(4)	9017(4)	4005(3)	85(1)

Table S8. Bond lengths (Å) and angles (degree) for compound **6**

S(1)-O(4)	1.409(3)	C(1)-H(1B)	0.9700	C(5)-C(10)-C(9)	110.3(3)
S(1)-O(5)	1.415(3)	C(2)-H(2A)	0.9700	C(19)-C(10)-C(9)	111.4(3)
S(1)-O(3)	1.559(3)	C(2)-H(2B)	0.9700	C(1)-C(10)-C(9)	108.7(3)
S(1)-C(21)	1.744(4)	C(21)-H(21A)	0.9600	C(6)-C(5)-C(4)	121.0(3)
O(3)-C(17)	1.486(4)	C(21)-H(21B)	0.9600	C(6)-C(5)-C(10)	122.5(3)
O(1)-C(22)	1.336(5)	C(21)-H(21C)	0.9600	C(4)-C(5)-C(10)	116.5(3)
O(1)-C(3)	1.459(4)	C(22)-C(23)	1.481(6)	C(17)-C(20)-H(20A)	109.5
C(9)-C(11)	1.526(5)	C(23)-H(23A)	0.9600	C(17)-C(20)-H(20B)	109.5
C(9)-C(8)	1.535(4)	C(23)-H(23B)	0.9600	H(20A)-C(20)-H(20B)	109.5
C(9)-C(10)	1.556(5)	C(23)-H(23C)	0.9600	C(17)-C(20)-H(20C)	109.5
C(9)-H(9)	0.9800	C(19)-H(19A)	0.9600	H(20A)-C(20)-H(20C)	109.5
C(8)-C(7)	1.534(5)	C(19)-H(19B)	0.9600	H(20B)-C(20)-H(20C)	109.5
C(8)-C(14)	1.538(5)	C(19)-H(19C)	0.9600	O(1)-C(3)-C(4)	111.3(3)
C(8)-H(8)	0.9800	O(4)-S(1)-O(5)	118.3(2)	O(1)-C(3)-C(2)	105.3(3)
C(13)-C(12)	1.530(5)	O(4)-S(1)-O(3)	110.11(16)	C(4)-C(3)-C(2)	110.9(3)
C(13)-C(18)	1.538(5)	O(5)-S(1)-O(3)	105.52(17)	O(1)-C(3)-H(3)	109.8
C(13)-C(17)	1.542(5)	O(4)-S(1)-C(21)	108.4(2)	C(4)-C(3)-H(3)	109.8
C(13)-C(14)	1.556(5)	O(5)-S(1)-C(21)	108.8(2)	C(2)-C(3)-H(3)	109.8
C(11)-C(12)	1.523(5)	O(3)-S(1)-C(21)	104.88(18)	C(6)-C(7)-C(8)	112.8(3)
C(11)-H(11A)	0.9700	C(17)-O(3)-S(1)	119.6(2)	C(6)-C(7)-H(7A)	109.0
C(11)-H(11B)	0.9700	C(22)-O(1)-C(3)	118.9(3)	C(8)-C(7)-H(7A)	109.0
C(14)-C(15)	1.555(4)	C(11)-C(9)-C(8)	111.7(3)	C(6)-C(7)-H(7B)	109.0
C(14)-H(14)	0.9800	C(11)-C(9)-C(10)	113.2(3)	C(8)-C(7)-H(7B)	109.0
C(10)-C(5)	1.518(5)	C(8)-C(9)-C(10)	112.3(3)	H(7A)-C(7)-H(7B)	107.8
C(10)-C(19)	1.542(5)	C(11)-C(9)-H(9)	106.3	C(11)-C(12)-C(13)	112.6(3)
C(10)-C(1)	1.542(5)	C(8)-C(9)-H(9)	106.3	C(11)-C(12)-H(12A)	109.1
C(5)-C(6)	1.320(5)	C(10)-C(9)-H(9)	106.3	C(13)-C(12)-H(12A)	109.1
C(5)-C(4)	1.511(5)	C(7)-C(8)-C(9)	109.1(3)	C(11)-C(12)-H(12B)	109.1
C(20)-C(17)	1.516(5)	C(7)-C(8)-C(14)	109.9(3)	C(13)-C(12)-H(12B)	109.1
C(20)-H(20A)	0.9600	C(9)-C(8)-C(14)	112.8(3)	H(12A)-C(12)-H(12B)	107.8
C(20)-H(20B)	0.9600	C(7)-C(8)-H(8)	108.3	C(5)-C(6)-C(7)	125.7(3)
C(20)-H(20C)	0.9600	C(9)-C(8)-H(8)	108.3	C(5)-C(6)-H(6)	118(2)
C(3)-C(4)	1.501(5)	C(14)-C(8)-H(8)	108.3	C(7)-C(6)-H(6)	116(2)
C(3)-C(2)	1.517(5)	C(12)-C(13)-C(18)	110.8(3)	N(1)-C(16)-C(15)	178.4(5)
C(3)-H(3)	0.9800	C(12)-C(13)-C(17)	110.5(3)	O(3)-C(17)-C(20)	106.6(3)
O(2)-C(22)	1.205(5)	C(18)-C(13)-C(17)	108.6(3)	O(3)-C(17)-C(13)	108.2(3)
C(7)-C(6)	1.493(5)	C(12)-C(13)-C(14)	107.0(3)	C(20)-C(17)-C(13)	116.2(3)
C(7)-H(7A)	0.9700	C(18)-C(13)-C(14)	111.1(3)	O(3)-C(17)-H(17)	108.6
C(7)-H(7B)	0.9700	C(17)-C(13)-C(14)	108.9(3)	C(20)-C(17)-H(17)	108.6
C(12)-H(12A)	0.9700	C(12)-C(11)-C(9)	111.6(3)	C(13)-C(17)-H(17)	108.6
C(12)-H(12B)	0.9700	C(12)-C(11)-H(11A)	109.3	C(3)-C(4)-C(5)	112.7(3)
C(6)-H(6)	0.89(3)	C(9)-C(11)-H(11A)	109.3	C(3)-C(4)-H(4A)	109.0
C(16)-N(1)	1.132(5)	C(12)-C(11)-H(11B)	109.3	C(5)-C(4)-H(4A)	109.0
C(16)-C(15)	1.456(6)	C(9)-C(11)-H(11B)	109.3	C(3)-C(4)-H(4B)	109.0
C(17)-H(17)	0.9800	H(11A)-C(11)-H(11B)	108.0	C(5)-C(4)-H(4B)	109.0
C(4)-H(4A)	0.9700	C(8)-C(14)-C(15)	110.6(3)	H(4A)-C(4)-H(4B)	107.8
C(4)-H(4B)	0.9700	C(8)-C(14)-C(13)	114.3(2)	C(13)-C(18)-H(18A)	109.5
C(18)-H(18A)	0.9600	C(15)-C(14)-C(13)	114.3(3)	C(13)-C(18)-H(18B)	109.5
C(18)-H(18B)	0.9600	C(8)-C(14)-H(14)	105.6	H(18A)-C(18)-H(18B)	109.5
C(18)-H(18C)	0.9600	C(15)-C(14)-H(14)	105.6	C(13)-C(18)-H(18C)	109.5
C(15)-H(15A)	0.9700	C(13)-C(14)-H(14)	105.6	H(18A)-C(18)-H(18C)	109.5
C(15)-H(15B)	0.9700	C(5)-C(10)-C(19)	109.2(3)	H(18B)-C(18)-H(18C)	109.5
C(1)-C(2)	1.525(5)	C(5)-C(10)-C(1)	107.5(3)	C(16)-C(15)-C(14)	114.8(3)
C(1)-H(1A)	0.9700	C(19)-C(10)-C(1)	109.7(3)	C(16)-C(15)-H(15A)	108.6

Table S8. continuation

C(14)-C(15)-H(15A)	108.6	C(3)-C(2)-H(2B)	109.5	C(22)-C(23)-H(23B)	109.5
C(16)-C(15)-H(15B)	108.6	C(1)-C(2)-H(2B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(14)-C(15)-H(15B)	108.6	H(2A)-C(2)-H(2B)	108.1	C(22)-C(23)-H(23C)	109.5
H(15A)-C(15)-H(15B)	107.5	S(1)-C(21)-H(21A)	109.5	H(23A)-C(23)-H(23C)	109.5
C(2)-C(1)-C(10)	114.0(3)	S(1)-C(21)-H(21B)	109.5	H(23B)-C(23)-H(23C)	109.5
C(2)-C(1)-H(1A)	108.7	H(21A)-C(21)-H(21B)	109.5	C(10)-C(19)-H(19A)	109.5
C(10)-C(1)-H(1A)	108.7	S(1)-C(21)-H(21C)	109.5	C(10)-C(19)-H(19B)	109.5
C(2)-C(1)-H(1B)	108.7	H(21A)-C(21)-H(21C)	109.5	H(19A)-C(19)-H(19B)	109.5
C(10)-C(1)-H(1B)	108.7	H(21B)-C(21)-H(21C)	109.5	C(10)-C(19)-H(19C)	109.5
H(1A)-C(1)-H(1B)	107.6	O(2)-C(22)-O(1)	123.2(4)	H(19A)-C(19)-H(19C)	109.5
C(3)-C(2)-C(1)	110.9(3)	O(2)-C(22)-C(23)	125.3(4)	H(19B)-C(19)-H(19C)	109.5
C(3)-C(2)-H(2A)	109.5	O(1)-C(22)-C(23)	111.5(3)		
C(1)-C(2)-H(2A)	109.5	C(22)-C(23)-H(23A)	109.5		

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **6**. The anisotropic displacement factor exponent takes the form: $2\pi\ 2[h^2\ a^{*2}\ U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	53(1)	50(1)	54(1)	–8(1)	11(1)	9(1)
O(3)	48(2)	48(1)	45(2)	–1(1)	5(1)	9(1)
O(1)	52(2)	53(2)	61(2)	11(1)	16(2)	–4(1)
O(5)	91(3)	54(2)	88(2)	7(2)	16(2)	30(2)
C(9)	35(2)	27(2)	41(2)	4(2)	–6(2)	–2(2)
C(8)	36(2)	27(2)	39(2)	–1(2)	–3(2)	–5(2)
O(4)	68(2)	97(2)	52(2)	–19(2)	5(2)	8(2)
C(13)	36(2)	34(2)	41(2)	1(2)	0(2)	1(2)
C(11)	40(2)	44(2)	54(2)	19(2)	3(2)	5(2)
C(14)	42(2)	27(2)	32(2)	1(2)	–3(2)	–3(2)
C(10)	36(2)	33(2)	43(2)	11(2)	2(2)	–4(2)
C(5)	34(2)	42(2)	38(2)	4(2)	1(2)	2(2)
C(20)	44(2)	43(2)	54(2)	–5(2)	11(2)	–4(2)
C(3)	49(2)	47(2)	51(2)	5(2)	12(2)	–9(2)
O(2)	97(3)	56(2)	118(3)	23(2)	50(2)	19(2)
C(7)	49(2)	37(2)	36(2)	6(2)	1(2)	6(2)
C(12)	37(2)	48(2)	51(2)	14(2)	–1(2)	7(2)
C(6)	42(2)	39(2)	44(2)	7(2)	0(2)	15(2)
C(16)	60(3)	60(3)	31(2)	–6(2)	–6(2)	10(2)
C(17)	41(2)	36(2)	44(2)	2(2)	0(2)	6(2)
C(4)	45(2)	55(2)	50(2)	6(2)	5(2)	–1(2)
C(18)	48(2)	37(2)	73(3)	–9(2)	1(2)	3(2)
C(15)	47(2)	44(2)	43(2)	6(2)	5(2)	7(2)
C(1)	42(2)	62(3)	48(2)	20(2)	–1(2)	3(2)
C(2)	51(3)	73(3)	45(2)	17(2)	7(2)	–2(2)
C(21)	72(3)	72(3)	75(3)	–7(3)	31(3)	–3(3)
C(22)	72(3)	52(3)	58(3)	5(2)	17(2)	4(2)
C(23)	56(3)	82(3)	83(3)	27(3)	21(2)	7(3)
C(19)	57(3)	38(2)	77(3)	2(2)	9(2)	–5(2)
N(1)	109(4)	78(3)	61(3)	–13(2)	–26(2)	19(3)

Table S10. Torsion angles (degree) for compound **6**

O(4)-S(1)-O(3)-C(17)	−38.6(3)	C(8)-C(9)-C(10)-C(19)	75.3(3)	C(12)-C(13)-C(17)-O(3)	62.3(4)
O(5)-S(1)-O(3)-C(17)	−167.4(3)	C(11)-C(9)-C(10)-C(1)	68.7(4)	C(18)-C(13)-C(17)-O(3)	–59.4(4)
C(21)-S(1)-O(3)-C(17)	77.8(3)	C(8)-C(9)-C(10)-C(1)	−163.6(3)	C(14)-C(13)-C(17)-O(3)	179.4(3)
C(11)-C(9)-C(8)-C(7)	−170.7(3)	C(19)-C(10)-C(5)-C(6)	−109.2(4)	C(12)-C(13)-C(17)-C(20)	–57.5(4)
C(10)-C(9)-C(8)-C(7)	60.9(3)	C(1)-C(10)-C(5)-C(6)	131.8(4)	C(18)-C(13)-C(17)-C(20)	−179.2(3)
C(11)-C(9)-C(8)-C(14)	–48.2(4)	C(9)-C(10)-C(5)-C(6)	13.5(5)	C(14)-C(13)-C(17)-C(20)	59.7(4)
C(10)-C(9)-C(8)-C(14)	−176.6(3)	C(19)-C(10)-C(5)-C(4)	69.7(4)	O(1)-C(3)-C(4)-C(5)	−169.0(3)
C(8)-C(9)-C(11)-C(12)	52.8(4)	C(1)-C(10)-C(5)-C(4)	–49.3(4)	C(2)-C(3)-C(4)-C(5)	–52.1(4)
C(10)-C(9)-C(11)-C(12)	−179.2(3)	C(9)-C(10)-C(5)-C(4)	−167.6(3)	C(6)-C(5)-C(4)-C(3)	−129.5(4)
C(7)-C(8)-C(14)-C(15)	–56.8(4)	C(22)-O(1)-C(3)-C(4)	–70.1(5)	C(10)-C(5)-C(4)-C(3)	51.6(4)
C(9)-C(8)-C(14)-C(15)	−178.8(3)	C(22)-O(1)-C(3)-C(2)	169.7(3)	N(1)-C(16)-C(15)-C(14)	63(16)
C(7)-C(8)-C(14)-C(13)	172.5(3)	C(9)-C(8)-C(7)-C(6)	–41.6(4)	C(8)-C(14)-C(15)-C(16)	–46.8(4)
C(9)-C(8)-C(14)-C(13)	50.4(4)	C(14)-C(8)-C(7)-C(6)	−165.8(3)	C(13)-C(14)-C(15)-C(16)	83.9(4)
C(12)-C(13)-C(14)-C(8)	–53.8(4)	C(9)-C(11)-C(12)-C(13)	–60.2(4)	C(5)-C(10)-C(1)-C(2)	52.0(4)
C(18)-C(13)-C(14)-C(8)	67.2(4)	C(18)-C(13)-C(12)-C(11)	–62.8(4)	C(19)-C(10)-C(1)-C(2)	–66.6(4)
C(17)-C(13)-C(14)-C(8)	−173.2(3)	C(17)-C(13)-C(12)-C(11)	176.8(3)	C(9)-C(10)-C(1)-C(2)	171.4(3)
C(12)-C(13)-C(14)-C(15)	177.2(3)	C(14)-C(13)-C(12)-C(11)	58.4(4)	O(1)-C(3)-C(2)-C(1)	175.6(3)
C(18)-C(13)-C(14)-C(15)	–61.7(4)	C(4)-C(5)-C(6)-C(7)	−174.5(4)	C(4)-C(3)-C(2)-C(1)	55.1(4)
C(17)-C(13)-C(14)-C(15)	57.9(4)	C(10)-C(5)-C(6)-C(7)	4.3(6)	C(10)-C(1)-C(2)-C(3)	–57.2(4)
C(11)-C(9)-C(10)-C(5)	−173.7(3)	C(8)-C(7)-C(6)-C(5)	10.5(5)	C(3)-O(1)-C(22)-O(2)	–2.3(6)
C(8)-C(9)-C(10)-C(5)	–46.1(4)	S(1)-O(3)-C(17)-C(20)	−115.6(3)	C(3)-O(1)-C(22)-C(23)	175.6(3)
C(11)-C(9)-C(10)-C(19)	–52.3(4)	S(1)-O(3)-C(17)-C(13)	118.8(3)		

Table S11. Selected bond lengths and bond angles for compounds **5** and **6**

Bond	Compound **5**	Compound **6**	Angle / degree	Compound **5**	Compound **6**
	Bond length / Å			Bond angle / degree	
S1-O4	1.406 (3)	1.409 (3)	O4-S1-O5	118.1 (2)	118.3 (2)
S1-O5	1.422 (3)	1.415 (3)	O4-S1-O3	106.82 (19)	110.11 (16)
S1-O3	1.561 (3)	1.559 (3)	O5-S1-O3	109.09 (16)	105.52 (17)
S1-C21	1.743 (4)	1.744 (4)	O4-S1-C21	107.8 (2)	108.4 (2)
O3-C17	1.473 (4)	1.486 (4)	O5-S1-C21	110.1 (2)	108.8 (2)
C13-C18	1.535 (5)	1.538 (5)	O3-S1-C21	103.96 (19)	104.88 (18)
C13-C17	1.538 (5)	1.542 (5)	C17-O3-S1	122.3 (2)	119.6 (2)
C17-C20	1.519 (5)	1.516 (5)	O3-C17-C20	107.9 (3)	106.6 (3)
C13-C12	1.530 (4)	1.530 (5)	C12-C13-C17	109.8 (3)	110.5 (3)
C13-C18	1.535 (5)	1.538 (5)	C18-C13-C17	106.9 (3)	108.6 (3)
C13-C14	1.556 (4)	1.556 (5)	C17-C13-C14	110.7 (3)	108.9 (3)

Table S12. Selected torsion angles for compounds **5** and **6**

	Compound **5**	Compound **6**
	Torsion angle / degree	
O4-S1-O3-C17	140.7 (3)	38.6 (3)
O5-S1-O3-C17	12.0 (3)	167.4 (3)
C21-S1-O3-C17	105.4 (3)	77.8 (3)
S1-O3-C17-C13	137.2 (2)	118.8 (3)
S1-O3-C17-C20	97.0 (3)	115.6 (3)
C12-C13-C17-C20	56.4 (4)	57.5 (4)
C18-C13-C17-C20	63.7 (4)	179.2 (3)
C14-C13-C17-C20	175.3 (3)	59.7 (4)
C12-C13-C17-O3	64.4 (3)	62.3 (4)
C18-C13-C17-O3	175.6 (3)	59.4 (4)
C14-C13-C17-O3	54.5 (3)	179.4 (3)
C8-C14-C15-C16	89.9 (4)	46.8 (4)
C13-C14-C15-C16	142.7 (3)	83.9 (4)
C14-C15-C16-N1	158 (14)	63 (16)