Table. Crystal data and structure refinement for Mosher ester **10**.

Identification code	nik13t	
Empirical formula	C28 H30 F3 N O7	
Formula weight	549.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.6205(4) Å	α= 90°.
	b = 13.0233(6) Å	β= 90°.
	c = 21.4135(10) Å	γ= 90°.
Volume	2682.9(2) $Å^3$	
Z	4	
Density (calculated)	1.360 Mg/m^3	
Absorption coefficient	0.111 mm^{-1}	
F(000)	1152	
Crystal size	0.25 x 0.20 x 0.15 mm^3	
Theta range for data collection	1.83 to 27.90°.	
Index ranges	-12<=h<=4, -16<=k<=16, -27<=l<=27	
Reflections collected	17124	
Independent reflections	5764 [R(int) = 0.0540]	
Completeness to theta = 27.90°	92.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5764 / 0 / 352	
Goodness-of-fit on F2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0946	
R indices (all data)	R1 = 0.0627, wR2 = 0.1042	
Absolute structure parameter	-0.2(7)	
Largest diff. peak and hole	0.179 and -0.210 e. $Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	9563(1)	931(1)	9003(1)	37(1)
O(7)	5635(2)	982(1)	10151(1)	43(1)

F(1)	2825(1)	-240(1)	9347(1)	60(1)
O(5)	6820(1)	1088(1)	9029(1)	36(1)
C(28)	5495(2)	819(2)	9013(1)	36(1)
O(2)	8480(2)	-306(1)	8430(1)	38(1)
C(7)	8845(2)	752(2)	8436(1)	30(1)
O(4)	7622(2)	100(1)	6867(1)	42(1)
F(3)	3068(2)	229(1)	10298(1)	69(1)
C(5)	11242(2)	747(2)	7981(1)	37(1)
N(1)	8048(2)	1678(1)	7180(1)	37(1)
O(3)	5858(2)	1262(2)	6885(1)	60(1)
C(20)	5546(2)	-692(2)	9721(1)	34(1)
O(6)	4760(2)	839(2)	8569(1)	67(1)
C(8)	7483(2)	1367(2)	8438(1)	35(1)
C(19)	5053(2)	414(2)	9661(1)	34(1)
C(12)	7055(2)	1019(2)	6963(1)	42(1)
C(4)	12211(2)	874(2)	7513(1)	46(1)
F(2)	2921(2)	1354(1)	9571(1)	83(1)
C(25)	5328(2)	-1388(2)	9241(1)	46(1)
C(6)	9845(2)	986(2)	7895(1)	31(1)
C(18)	9151(2)	-797(2)	8944(1)	47(1)
C(3)	11801(3)	1245(2)	6941(1)	51(1)
C(2)	10432(2)	1490(2)	6844(1)	45(1)
C(9)	7686(2)	2503(2)	8438(1)	41(1)
C(21)	6228(2)	-1017(2)	10257(1)	46(1)
C(17)	9372(2)	62(2)	9401(1)	43(1)
C(11)	7722(3)	2767(2)	7275(1)	50(1)
C(1)	9451(2)	1364(2)	7311(1)	34(1)
C(26)	5444(3)	2075(2)	10142(1)	60(1)
C(13)	6765(3)	-826(2)	6773(1)	50(1)
C(27)	3458(2)	442(2)	9717(1)	49(1)
C(24)	5774(3)	-2388(2)	9295(2)	61(1)
C(10)	7792(2)	3095(2)	7940(1)	48(1)
C(22)	6696(3)	-2018(2)	10298(1)	64(1)
C(15)	5858(3)	-1001(2)	7339(1)	63(1)
C(16)	7867(4)	-1654(2)	6729(2)	74(1)
C(23)	6467(3)	-2700(2)	9821(2)	70(1)
C(14)	5946(4)	-745(3)	6176(1)	85(1)

Table 3. Bond lengths [Å] and angles [°] for Mosher ester 10.

O(1)-C(7)	1.415(2)
O(1)-C(17)	1.428(3)
O(7)-C(19)	1.400(3)
O(7)-C(26)	1.436(3)
F(1)-C(27)	1.337(3)

O(5)-C(28)	1.322(2)
O(5)-C(8)	1.463(2)
C(28)-O(6)	1.186(3)
C(28)-C(19)	1.544(3)
O(2)-C(7)	1.422(3)
O(2)-C(18)	1.426(3)
C(7)-C(6)	1.536(3)
C(7)-C(8)	1.537(3)
O(4)-C(12)	1.331(3)
O(4)-C(13)	1.474(3)
F(3)-C(27)	1.328(3)
C(5)-C(4)	1.379(3)
C(5)-C(6)	1.392(3)
N(1)-C(12)	1.365(3)
N(1)-C(1)	1.438(3)
N(1)-C(11)	1.467(3)
O(3)-C(12)	1.206(3)
C(20)-C(25)	1.388(3)
C(20)-C(21)	1.388(3)
C(20)-C(19)	1.522(3)
C(8)-C(9)	1.491(3)
C(19)-C(27)	1.540(3)
C(4)-C(3)	1.374(4)
F(2)-C(27)	1.332(3)
C(25)-C(24)	1.376(4)
C(6)-C(1)	1.397(3)
C(18)-C(17)	1.502(4)
C(3)-C(2)	1.372(4)
C(2)-C(1)	1.385(3)
C(9)-C(10)	1.320(3)
C(21)-C(22)	1.383(4)
C(11)-C(10)	1.490(4)
C(13)-C(14)	1.505(4)
C(13)-C(15)	1.512(3)
C(13)-C(16)	1.516(4)
C(24)-C(23)	1.370(4)
C(22)-C(23)	1.370(4)

C(7)-O(1)-C(17)	108.61(16)
C(19)-O(7)-C(26)	117.50(19)
C(28)-O(5)-C(8)	117.60(16)
O(6)-C(28)-O(5)	126.2(2)
O(6)-C(28)-C(19)	124.28(19)
O(5)-C(28)-C(19)	109.44(17)
C(7)-O(2)-C(18)	108.39(17)
O(1)-C(7)-O(2)	106.71(16)

O(1)-C(7)-C(6)	107.98(16)
O(2)-C(7)-C(6)	109.89(16)
O(1)-C(7)-C(8)	109.14(16)
O(2)-C(7)-C(8)	107.13(16)
C(6)-C(7)-C(8)	115.64(17)
C(12)-O(4)-C(13)	121.85(18)
C(4)-C(5)-C(6)	122.0(2)
C(12)-N(1)-C(1)	123.00(19)
C(12)-N(1)-C(11)	120.36(19)
C(1)-N(1)-C(11)	116.63(19)
C(25)-C(20)-C(21)	119.0(2)
C(25)-C(20)-C(19)	120.5(2)
C(21)-C(20)-C(19)	120.4(2)
O(5)-C(8)-C(9)	107.64(18)
O(5)-C(8)-C(7)	104.14(16)
C(9)-C(8)-C(7)	113.92(17)
O(7)-C(19)-C(20)	108.10(17)
O(7)-C(19)-C(27)	109.12(18)
C(20)-C(19)-C(27)	109.02(19)
O(7)-C(19)-C(28)	112.54(18)
C(20)-C(19)-C(28)	108.28(17)
C(27)-C(19)-C(28)	109.70(18)
O(3)-C(12)-O(4)	127.2(2)
O(3)-C(12)-N(1)	123.4(2)
O(4)-C(12)-N(1)	109.36(18)
C(3)-C(4)-C(5)	119.7(2)
C(24)-C(25)-C(20)	120.5(2)
C(5)-C(6)-C(1)	117.31(19)
C(5)-C(6)-C(7)	117.43(18)
C(1)-C(6)-C(7)	125.15(18)
O(2)-C(18)-C(17)	103.46(18)
C(2)-C(3)-C(4)	119.6(2)
C(3)-C(2)-C(1)	121.1(2)
C(10)-C(9)-C(8)	126.1(2)
C(22)-C(21)-C(20)	119.6(2)
O(1)-C(17)-C(18)	102.64(17)
N(1)-C(11)-C(10)	113.58(19)
C(2)-C(1)-C(6)	120.3(2)
C(2)-C(1)-N(1)	117.71(19)
C(6)-C(1)-N(1)	121.94(18)
O(4)-C(13)-C(14)	110.6(2)
O(4)-C(13)-C(15)	109.7(2)
C(14)-C(13)-C(15)	113.0(2)
O(4)-C(13)-C(16)	101.5(2)
C(14)-C(13)-C(16)	111.3(3)
C(15)-C(13)-C(16)	110.2(2)

F(3)-C(27)-F(2)	107.2(2)
F(3)-C(27)-F(1)	106.7(2)
F(2)-C(27)-F(1)	106.1(2)
F(3)-C(27)-C(19)	110.5(2)
F(2)-C(27)-C(19)	112.9(2)
F(1)-C(27)-C(19)	113.1(2)
C(23)-C(24)-C(25)	120.2(3)
C(9)-C(10)-C(11)	127.0(2)
C(23)-C(22)-C(21)	120.8(3)
C(24)-C(23)-C(22)	119.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Mosher ester 10. The anisotropic displacement factor exponent takes the form: $-2\ p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	35(1)	46(1)	31(1)	-3(1)	-4(1)	-2(1)
O(7)	56(1)	38(1)	36(1)	-5(1)	2(1)	-5(1)
F(1)	30(1)	79(1)	70(1)	6(1)	-4(1)	-10(1)
O(5)	27(1)	53(1)	30(1)	1(1)	2(1)	-1(1)
C(28)	26(1)	43(1)	39(1)	4(1)	-1(1)	3(1)
O(2)	48(1)	30(1)	37(1)	3(1)	1(1)	-7(1)
C(7)	31(1)	31(1)	30(1)	-2(1)	-1(1)	-5(1)
O(4)	37(1)	46(1)	44(1)	-4(1)	-1(1)	-3(1)
F(3)	50(1)	92(1)	64(1)	-2(1)	28(1)	-6(1)
C(5)	34(1)	40(1)	39(1)	-1(1)	0(1)	-1(1)
N(1)	39(1)	37(1)	34(1)	6(1)	-1(1)	4(1)
O(3)	41(1)	74(1)	64(1)	6(1)	-15(1)	8(1)
C(20)	30(1)	37(1)	36(1)	0(1)	6(1)	-2(1)
O(6)	36(1)	121(2)	45(1)	26(1)	-10(1)	-15(1)
C(8)	31(1)	44(1)	29(1)	2(1)	3(1)	-2(1)
C(19)	32(1)	38(1)	34(1)	-2(1)	2(1)	-1(1)
C(12)	36(1)	57(2)	32(1)	9(1)	-4(1)	1(1)
C(4)	32(1)	54(2)	52(1)	-7(1)	5(1)	0(1)
F(2)	45(1)	69(1)	133(2)	19(1)	15(1)	21(1)
C(25)	40(1)	49(2)	47(1)	-8(1)	1(1)	-1(1)
C(6)	31(1)	29(1)	34(1)	-3(1)	1(1)	-4(1)
C(18)	43(1)	46(2)	52(1)	14(1)	7(1)	7(1)
C(3)	46(1)	61(2)	46(1)	-1(1)	15(1)	-9(1)
C(2)	48(1)	51(2)	34(1)	5(1)	7(1)	-6(1)
C(9)	41(1)	38(1)	44(1)	-4(1)	2(1)	5(1)
C(21)	48(1)	50(2)	39(1)	6(1)	2(1)	3(1)
C(17)	34(1)	61(2)	34(1)	12(1)	3(1)	4(1)

C(11)	57(2)	41(1)	52(1)	15(1)	4(1)	10(1)
C(1)	34(1)	36(1)	33(1)	2(1)	1(1)	-3(1)
C(26)	82(2)	38(1)	59(2)	-8(1)	14(2)	-7(1)
C(13)	52(1)	57(2)	42(1)	-2(1)	-2(1)	-20(1)
C(27)	35(1)	53(2)	58(2)	7(1)	11(1)	6(1)
C(24)	61(2)	46(2)	75(2)	-17(1)	20(2)	-4(1)
C(10)	51(1)	31(1)	61(2)	-2(1)	0(1)	4(1)
C(22)	73(2)	58(2)	61(2)	23(2)	7(2)	17(2)
C(15)	56(2)	79(2)	53(2)	1(2)	8(1)	-23(2)
C(16)	85(2)	56(2)	80(2)	-13(2)	19(2)	-8(2)
C(23)	81(2)	42(2)	87(2)	11(2)	28(2)	14(2)
C(14)	103(3)	102(3)	49(2)	-3(2)	-22(2)	-39(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Mosher ester 10.

	x	y	z	U(eq)
H(5A)	11530	494	8366	45
H(8A)	6895	1161	8085	42
H(4A)	13138	709	7584	55
H(25A)	4877	-1177	8878	55
H(18A)	10029	-1098	8817	56
H(18B)	8567	-1330	9121	56
H(3A)	12448	1329	6623	61
H(2A)	10157	1746	6457	53
H(9A)	7743	2823	8825	49
H(21A)	6369	-564	10587	55
H(17A)	8569	151	9670	51
H(17B)	10188	-59	9657	51
H(11A)	6795	2902	7117	60
H(11B)	8369	3179	7033	60
H(26A)	5881	2373	10502	90
H(26B)	4468	2230	10148	90
H(26C)	5854	2354	9770	90
H(24A)	5605	-2853	8975	73
H(10A)	7924	3792	8013	57
H(22A)	7172	-2232	10653	77
H(15A)	5158	-476	7360	94
H(15B)	6419	-976	7710	94
H(15C)	5420	-1661	7309	94
H(16A)	8366	-1692	7116	110
H(16B)	8501	-1492	6397	110
H(16C)	7432	-2303	6645	110

H(23A)	6782	-3373	9854	84
H(14A)	5251	-220	6218	127
H(14B)	5504	-1390	6090	127
H(14C)	6560	-572	5838	127

Table 6. Torsion angles [°] for Mosher ester 10.

C(8)-O(5)-C(28)-O(6)	-4.8(4)
C(8)-O(5)-C(28)-C(19)	172.29(17)
C(17)-O(1)-C(7)-O(2)	-12.7(2)
C(17)-O(1)-C(7)-C(6)	-130.80(18)
C(17)-O(1)-C(7)-C(8)	102.74(18)
C(18)-O(2)-C(7)-O(1)	-8.6(2)
C(18)-O(2)-C(7)-C(6)	108.25(18)
C(18)-O(2)-C(7)-C(8)	-125.38(17)
C(28)-O(5)-C(8)-C(9)	107.1(2)
C(28)-O(5)-C(8)-C(7)	-131.62(19)
O(1)-C(7)-C(8)-O(5)	-51.6(2)
O(2)-C(7)-C(8)-O(5)	63.56(19)
C(6)-C(7)-C(8)-O(5)	-173.57(16)
O(1)-C(7)-C(8)-C(9)	65.3(2)
O(2)-C(7)-C(8)-C(9)	-179.47(17)
C(6)-C(7)-C(8)-C(9)	-56.6(2)
C(26)-O(7)-C(19)-C(20)	172.60(19)
C(26)-O(7)-C(19)-C(27)	-69.0(3)
C(26)-O(7)-C(19)-C(28)	53.1(2)
C(25)-C(20)-C(19)-O(7)	-168.84(18)
C(21)-C(20)-C(19)-O(7)	10.7(3)
C(25)-C(20)-C(19)-C(27)	72.7(3)
C(21)-C(20)-C(19)-C(27)	-107.8(2)
C(25)-C(20)-C(19)-C(28)	-46.7(2)
C(21)-C(20)-C(19)-C(28)	132.9(2)
O(6)-C(28)-C(19)-O(7)	-143.4(2)
O(5)-C(28)-C(19)-O(7)	39.5(2)
O(6)-C(28)-C(19)-C(20)	97.2(3)
O(5)-C(28)-C(19)-C(20)	-80.0(2)
O(6)-C(28)-C(19)-C(27)	-21.7(3)
O(5)-C(28)-C(19)-C(27)	161.2(2)
C(13)-O(4)-C(12)-O(3)	-13.3(4)
C(13)-O(4)-C(12)-N(1)	165.67(17)
C(1)-N(1)-C(12)-O(3)	175.7(2)
C(11)-N(1)-C(12)-O(3)	-6.0(3)
C(1)-N(1)-C(12)-O(4)	-3.3(3)
C(11)-N(1)-C(12)-O(4)	174.95(18)
C(6)-C(5)-C(4)-C(3)	-0.1(4)

C(21)-C(20)-C(25)-C(24)	0.4(3)
C(19)-C(20)-C(25)-C(24)	180.0(2)
C(4)-C(5)-C(6)-C(1)	-0.1(3)
C(4)-C(5)-C(6)-C(7)	176.4(2)
O(1)-C(7)-C(6)-C(5)	35.2(2)
O(2)-C(7)-C(6)-C(5)	-80.8(2)
C(8)-C(7)-C(6)-C(5)	157.77(19)
O(1)-C(7)-C(6)-C(1)	-148.7(2)
O(2)-C(7)-C(6)-C(1)	95.3(2)
C(8)-C(7)-C(6)-C(1)	-26.1(3)
C(7)-O(2)-C(18)-C(17)	25.1(2)
C(5)-C(4)-C(3)-C(2)	0.3(4)
C(4)-C(3)-C(2)-C(1)	-0.4(4)
O(5)-C(8)-C(9)-C(10)	-155.2(2)
C(7)-C(8)-C(9)-C(10)	89.8(3)
C(25)-C(20)-C(21)-C(22)	1.1(3)
C(19)-C(20)-C(21)-C(22)	-178.5(2)
C(7)-O(1)-C(17)-C(18)	27.5(2)
O(2)-C(18)-C(17)-O(1)	-31.6(2)
C(12)-N(1)-C(11)-C(10)	115.1(2)
C(1)-N(1)-C(11)-C(10)	-66.5(3)
C(3)-C(2)-C(1)-C(6)	0.3(4)
C(3)-C(2)-C(1)-N(1)	177.5(2)
C(5)-C(6)-C(1)-C(2)	0.0(3)
C(7)-C(6)-C(1)-C(2)	-176.2(2)
C(5)-C(6)-C(1)-N(1)	-177.2(2)
C(7)-C(6)-C(1)-N(1)	6.7(3)
C(12)-N(1)-C(1)-C(2)	94.0(3)
C(11)-N(1)-C(1)-C(2)	-84.4(3)
C(12)-N(1)-C(1)-C(6)	-88.8(3)
C(11)-N(1)-C(1)-C(6)	92.9(2)
C(12)-O(4)-C(13)-C(14)	65.3(3)
C(12)-O(4)-C(13)-C(15)	-59.9(3)
C(12)-O(4)-C(13)-C(16)	-176.5(2)
O(7)-C(19)-C(27)-F(3)	-47.9(3)
C(20)-C(19)-C(27)-F(3)	70.0(3)
C(28)-C(19)-C(27)-F(3)	-171.60(19)
O(7)-C(19)-C(27)-F(2)	72.2(3)
C(20)-C(19)-C(27)-F(2)	-170.0(2)
C(28)-C(19)-C(27)-F(2)	-51.6(3)
O(7)-C(19)-C(27)-F(1)	-167.38(18)
C(20)-C(19)-C(27)-F(1)	-49.5(3)
C(28)-C(19)-C(27)-F(1)	68.9(3)
C(20)-C(25)-C(24)-C(23)	-1.5(4)
C(8)-C(9)-C(10)-C(11)	0.5(4)
N(1)-C(11)-C(10)-C(9)	-22.2(4)

C(20)-C(21)-C(22)-C(23)	-1.5(4)
C(25)-C(24)-C(23)-C(22)	1.1(4)
C(21)-C(22)-C(23)-C(24)	0.4(4)

Symmetry transformations used to generate equivalent atoms: