Structural characterization of LASSBio-1289: A novel vasoactive *N*-methyl-*N*-acylhydrazone derivative

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Supporting Information

Table S1 - Final coordinates and equivalent isotropic displacement parameters ($U_{iso} = B_{iso}/8\pi^2$) for all atoms in the LASSBio-1289 crystal structure.

Atom	*x*	*y*	*z*	U_{iso} (Å^2)
S(26)	0.1496(4)	0.0015(4)	0.1368(6)	0.0488
O(6)	0.4843(7)	0.5557(7)	0.2247(13)	0.0488
O(23)	0.0768(10)	0.5662(9)	0.1626(11)	0.0488
O(28)	0.0925(10)	0.7188(8)	-0.0200(12)	0.0488
N(1)	0.4142(10)	0.3906(13)	0.2439(18)	0.0488
N(3)	0.3405(9)	0.3285(11)	0.1848(15)	0.0488
C(2)	0.4135(12)	0.5026(18)	0.206(2)	0.0488
C(4)	0.4957(10)	0.3394(10)	0.3329(15)	0.0488
C(5)	0.3303(16)	0.5582(18)	0.130(3)	0.0488
C(7)	0.3405(13)	0.2234(14)	0.2119(17)	0.0488
C(11)	0.3390(11)	0.6523(18)	0.028(2)	0.0488
C(12)	0.2437(16)	0.5268(15)	0.1869(19)	0.0488
C(13)	0.2607(16)	0.1572(14)	0.161(2)	0.0488
C(15)	0.2617(17)	0.7114(12)	-0.0289(17)	0.0488
C(17)	0.1679(14)	0.586(2)	0.129(3)	0.0488
C(19)	0.1784(13)	0.1978(13)	0.076(2)	0.0488
C(20)	0.2507(10)	0.0493(14)	0.2083(15)	0.0488
C(21)	0.1768(15)	0.6730(19)	0.019(3)	0.0488
C(24)	0.1110(12)	0.1124(14)	0.0397(15)	0.0488
C(29)	0.0257(11)	0.6524(15)	0.0733(18)	0.0488
H(8)	0.4736(10)	0.3134(10)	0.4337(15)	0.0586
H(9)	0.5383(10)	0.3992(10)	0.3495(15)	0.0586
H(10)	0.5159(10)	0.2847(10)	0.2494(15)	0.0586
H(14)	0.3900(13)	0.1909(14)	0.2801(17)	0.0586

H(16)	0.3982(11)	0.6740(18)	-0.015(2)	0.0586
H(18)	0.2385(16)	0.4668(15)	0.2688(19)	0.0586
H(22)	0.2671(17)	0.7690(12)	-0.1153(17)	0.0586
H(25)	0.1712(13)	0.2725(13)	0.039(2)	0.0586
H(27)	0.2921(10)	0.0127(14)	0.2911(15)	0.0586
H(30)	0.0608(12)	0.1184(14)	-0.0438(15)	0.0586
H(31)	-0.0185(11)	0.6203(15)	-0.0067(18)	0.0586
H(32)	-0.0037(11)	0.6987(15)	0.1584(18)	0.0586

Table S2 - Some selected bond distances for LASSBio-1289.

Bonds	Lengths (Å)
S(26)-C(20)	1.658(16)
S(26)-C(24)	1.627(17)
O(6)-C(2)	1.22(2)
O(23)-C(17)	1.37(3)
O(23)-C(29)	1.44(2)
O(28)-C(21)	1.37(3)
O(28)-C(29)	1.45(2)
N(1)-N(3)	1.38(2)
N(1)-C(2)	1.39(3)
N(1)-C(4)	1.49(2)
N(3)-C(7)	1.29(2)
C(2)-C(5)	1.49(3)
C(5)-C(11)	1.39(3)
C(5)-C(12)	1.39(3)
C(7)-C(13)	1.46(3)
C(11)-C(15)	1.39(3)
C(12)-C(17)	1.38(3)
C(13)-C(19)	1.43(3)
C(13)-C(20)	1.37(2)
C(15)-C(21)	1.37(3)
C(17)-C(21)	1.35(3)
C(19)-C(24)	1.45(2)

Table S3 - Some selected bond angles for LASSBio-1289.

Bonds	Angles (°)
C(20)-S(26)-C(24)	98.7(9)
C(17)-O(23)-C(29)	106.0(14)
C(21)-O(28)-C(29)	105.8(13)
N(3)-N(1)-C(2)	117.8(14)
N(3)-N(1)-C(4)	121.7(13)
C(2)-N(1)-C(4)	120.4(13)
N(1)-N(3)-C(7)	119.5(14)
O(6)-C(2)-N(1)	119.4(16)
O(6)-C(2)-C(5)	118.7(19)
N(1)-C(2)-C(5)	121.7(17)
C(2)-C(5)-C(11)	120.4(19)
C(2)-C(5)-C(12)	119.2(18)
C(11)-C(5)-C(12)	119.4(19)
N(3)-C(7)-C(13)	120.4(16)
C(5)-C(11)-C(15)	121.0(17)
C(5)-C(12)-C(17)	118.7(18)
C(7)-C(13)-C(19)	125.5(15)
C(7)-C(13)-C(20)	123.3(17)
C(19)-C(13)-C(20)	110.8(17)
C(11)-C(15)-C(21)	117.8(16)
O(23)-C(17)-C(12)	128(2)
O(23)-C(17)-C(21)	110.8(18)
C(12)-C(17)-C(21)	121(2)
C(13)-C(19)-C(24)	113.1(14)
S(26)-C(20)-C(13)	110.4(13)
O(28)-C(21)-C(15)	127.4(19)
O(28)-C(21)-C(17)	110.7(18)
C(15)-C(21)-C(17)	122(2)
S(26)-C(24)-C(19)	106.4(12)
O(23)-C(29)-O(28)	106.7(13)

Table S4 - Morphology predictions for LASSBio-1289 by means of GM calculations. Percentage of total facet area (TFA) is calculated as 100× (*hkl* facet area)/(total surface area).

hkl	Multiplicity	d_{hkl}	% Total facet area
(1 0 0)	2	14.5091	40.0
(1 1 0)	4	9.3095	31.9
(0 1 1)	4	6.4099	27.2
(1 1 -1)	4	5.8993	0.9

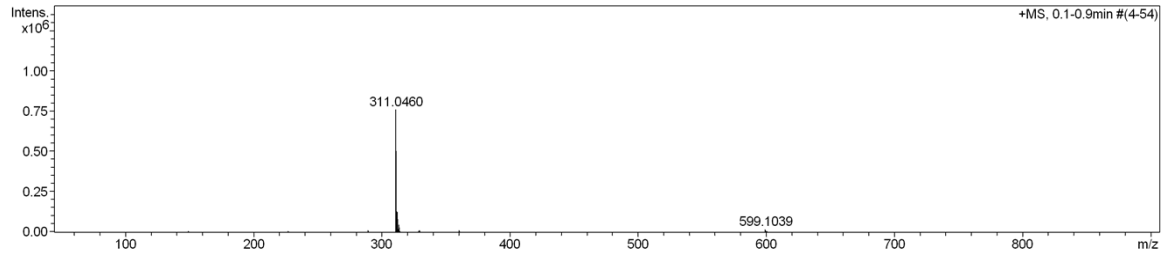
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Usuarios\Externas\MiguelDR_LasBio-Mansur_ESI_pos_LB-1289_08-07-14.d	Acquisition Date	7/8/2014 10:40:53 AM
Method	NaFormate_ESI_pos_100-900_Lab-Mass.m	Operator	LabMass-Central Analitica IPPN
Sample Name	MiguelDR_LasBio-Mansur_ESI_pos_LB-1289_08-07-14	Instrument / Ser#	micrOTOF 10368
Comment	Fluxo:180uL/h Faixa de varredura: 100-900 FM proposta:C14 H12 N2 O3 S MM:288.056863 M+H:289.064139 M+Na:311.046084 2M+H:577.121002 2M+Na:599.102947		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	900 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
289.0647	1	C 14 H 13 N 2 O 3 S	100.00	289.0641	-2.1	-2.9	5.0	9.5	even	ok
311.0460	1	C 14 H 12 N 2 Na O 3 S	100.00	311.0461	0.4	-0.4	1.9	9.5	even	ok
599.1039	1	C 28 H 24 N 4 Na O 6 S 2	100.00	599.1029	-1.7	-2.8	17.6	18.5	even	ok
	2	C 30 H 23 N 4 O 6 S 2	72.47	599.1054	2.4	1.2	20.8	21.5	even	ok
	3	C 12 H 31 N 4 O 19 S 2	8.56	599.1018	-3.5	-4.6	75.6	-0.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 7/10/2014 10:38:46 AM Page 1 of 1

Fig. S1 – Accurate mass spectrum of LASSBio-1289.