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Supporting information for

Mixed Carboxylic-Sulfonic Anhydride in Reactions with Imines: A Straightforward Route to Water-Soluble β-Lactams via a Staudinger-Type Reaction

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Crystallographic data for compound trans-20h

Suitable crystals of *trans*-20h were studied using SuperNova, Dual, Cu at zero, Atlas diffractometer (monochromated Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å). The structure has been solved with the ShelXT [1] structure solution program using Intrinsic Phasing and refined with the ShelXL [1] refinement package incorporated in the OLEX2 program package [2] using Least Squares minimization. Empirical absorption correction was applied in CrysAlisPro [3] program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. CCDC 1548177 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <u>http://www.ccdc.cam.ac.uk</u>.





Identification code	trans-20h
Empirical formula	C ₂₄ H ₃₃ N ₃ O ₆ S
Formula weight	491.59
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	19.0398(14)
b/Å	8.7917(5)
c/Å	15.4377(11)
α/°	90
β/°	103.834(7)
γ/°	90
Volume/Å ³	2509.2(3)
Z	4
$\rho_{calc}g/cm^3$	1.301
μ/mm^{-1}	1.513
F(000)	1048.0
Crystal size/mm ³	$0.12\times0.06\times0.04$
Radiation	$Cu K\alpha (\lambda = 1.5418)$
2Θ range for data collection/°	9.568 to 144.976
Index ranges	$-23 \le h \le 19, -10 \le k \le 9, -16 \le l \le 19$
Reflections collected	10954
Independent reflections	$4956 [R_{int} = 0.0418, R_{sigma} = 0.0494]$

Data/restraints/parameters	4956/3/315
Goodness-of-fit on F ²	1.020
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0557, wR_2 = 0.1369$
Final R indexes [all data]	$R_1 = 0.0673, wR_2 = 0.1480$
Largest diff. peak/hole / e•Å ⁻³	1.04/-0.98
CCDC	1548177

References

- 1. Sheldrick, G. M. Acta Crystallographica Section C 2015, 71, 3-8.
- 2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, J. Appl. Cryst., 2009, 42, 339–341.
- 3. CrysAlisPro, Agilent Technologies Ltd., Version 1.171.36.32 (release 02-08-2013 CrysAlis171.NET).

¹H and ¹³C NMR of compound **14**



¹H and ¹³C NMR of compound *trans/cis-20a*

¹H and ¹³C NMR of compound *trans*-20b

S7

¹H and ¹³C NMR of compound *trans/cis-20d*

¹H and ¹³C NMR of compound *cis***-20d**

¹H and ¹³C NMR of compound *trans/cis-20e* C 806 - 10.07 < 558 558 558 558 1 548 7 528 7 528 SO₃H * NEt₃ Q MeO MeÓ TET - 070 - 0.0 - 620 ¥ 650 - 45 1601 7447 1054 ۲ 2 5.5 3.0 5.0 f1 (MA) 11.0 10.5 10.0 9.5 9.0 7.5 7.0 6.5 4.0 3.5 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 8.5 8.0 13061 13061 13023 13023 12023 12023 <111.08 110.55 C 149.00
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¹H and ¹³C NMR of compound *trans/cis-20f* - 10.22 £ 4.85 113 SO₃H * NEt₃ 0 Ph OMe 1.07 4 74 00 T ¥-0172 70 1-950 10.954 8 T 68 0.12 -Ŧ 11.0 10.5 10.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 0.5 0.0 -0.5 -1.0 9.5 9.0 8.5 8.0 1.0 - 170.09 - 158.26 - 110.97 1 55.59 14006 - 8.50 SO₃H * NEt₃ 0 ∠Ph Ň. OMe 0 170 50 140 130 120 110 100 80 70 60 40 30 20 10 180 160 150 90

¹H and ¹³C NMR of compound *trans/cis-20g*

¹H and ¹³C NMR of compound *trans*-20h

¹H and ¹³C NMR of compound *trans/cis-20*h

¹H and ¹³C NMR of compound *trans*-20i

¹H and ¹³C NMR of compound *trans*-201

¹H and ¹³C NMR of compound *trans*-200

¹H and ¹³C NMR of compound *cis*-20p

¹H and ¹³C NMR of compound *trans/cis*-20q

¹H and ¹³C NMR of compound *trans/cis-20*r

¹H and ¹³C NMR of compound **24b**

¹H and ¹³C NMR of compound **24c**

