Crystal Data compound **3**

Single crystal of **3**were mounted under oil on a MiTeGen mount. X-ray diffraction data was collected at 150(1)K with Mo-Kα radiation (λ = 0.71073 Å) using Bruker Nonius X-8 diffractometer with ApexII detector and FR591 rotating anode generator. Data reduction was carried out by means of a standard procedure by using the Apex2 software package. Data sets were corrected for absorption using a multi-scan method, and structures were solved by direct methods using SHELXS-97,[1] and refined by full-matrix least-squares on F^2 using the SHELXL-97,[1] interfaced through the program X-Seed.[2] all non-hydrogen atoms were refined anisotropically and hydrogen atoms were included as invariants at geometrically estimated positions.

Compound reference	**xxxx**
Chemical formula	$C_{17}H_{23}NO_4S$
Formula Mass	337.42
Crystal system	Orthorhombic
a/Å	12.491(2)
b/Å	9.1019(17)
c/Å	30.464(6)
α/°	90.00
β/°	90.00
γ/°	90.00
Unit cell volume/Å^3	3463.5(11)
Temperature/K	150(2)
Space group	*Pbca*
No. of formula units per unit cell, *Z*	8
Radiation type	MoKα
Absorption coefficient, μ/mm^{-1}	0.206
No. of reflections measured	44819
No. of independent reflections	3438
R_{int}	0.0389
Final R_1 values ($I > 2\sigma(I)$)	0.0552
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1510
Final R_1 values (all data)	0.0618
Final $wR(F^2)$ values (all data)	0.1581
Goodness of fit on F^2	1.043
CCDC number	892870

In the crystal structure of compound **3**the methyl ether was disordered over two positions as was one cyclic -CH_2- group.

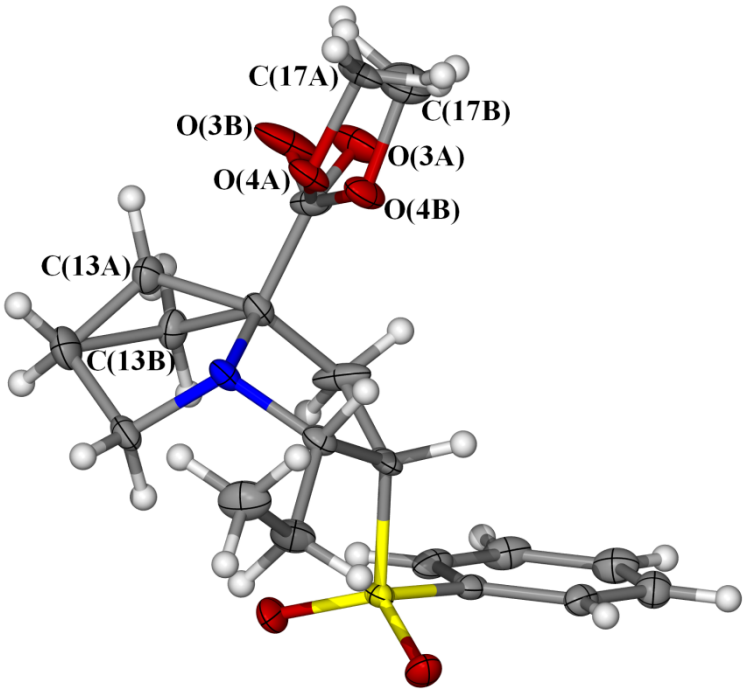

Figure S1. Ellipsoid plot of the asymmetric unit of compound **xxxx** showing disorder model for methyl ether and cyclic -CH_2- group. The disordered atoms have been labelled. Ellipsoids shown at 30% probability level. Carbon (grey), hydrogen (white), nitrogen (blue) sulphur (yellow) and oxygen (red).

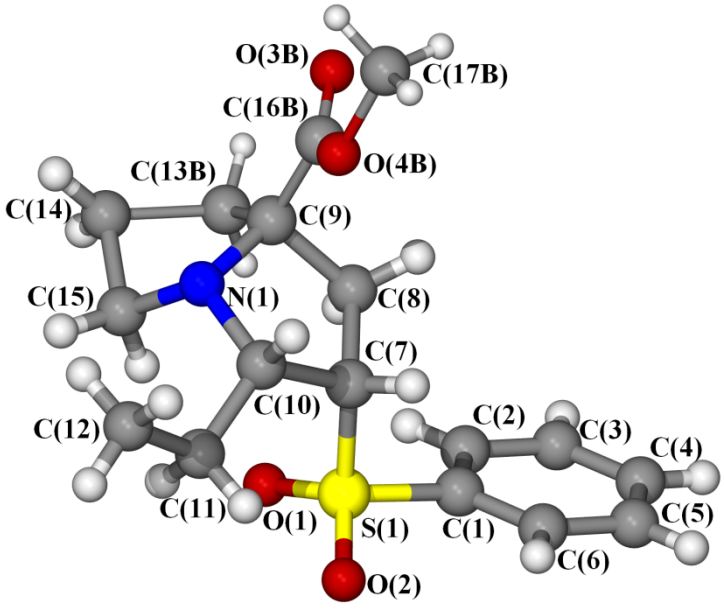

Figure S2. Fully labelled ball and stick model of compound **xxxx** showing part A only.

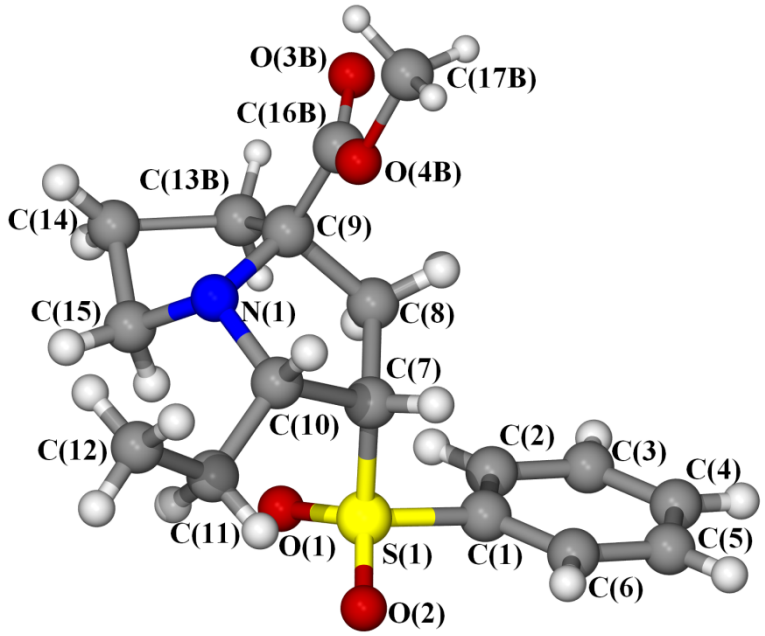

Figure S3. Fully labelled ball and stick model of compound **xxxx** showing part B only.

References

1 Sheldrick, G. M. SHELXS-97; *Acta Crystallogr*. 2008, **A64**, 112.

2 Barbour, L. J. J. *Supramol. Chem*. 2003, **1**, 189.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

```
Bond precision: C-C = 0.0039 A Wavelength=0.71073
Cell: a=12.491(2) b=9.1019(17) c=30.464(6)
alpha=90 beta=90 gamma=90
Temperature: 150 K
Calculated Reported
Volume 3463.5(11) 3463.5(11)
Space group P b c a Pbca
Hall group -P 2ac 2ab -P 2ac 2ab
Moiety formula C17 H23 N O4 S C17 H23 N O4 S
Sum formula C17 H23 N O4 S C17 H23 N O4 S
Mr 337.43 337.42
Dx,g cm-3 1.294 1.294
Z 8 8
Mu (mm-1) 0.206 0.206
F000 1440.0 1440.0
F000' 1441.65
h,k,lmax 15,11,37 15,11,37
Nref 3452 3438
Tmin,Tmax 0.968,0.978 0.958,0.978
Tmin' 0.958
Correction method= MULTI-SCAN
Data completeness= 0.996 Theta(max)= 26.130
```

R(reflections)= 0.0552(3028) wR2(reflections)= 0.1581(3438)
S = 1.043 Npar= 247
The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C8

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 6
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for C16B
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 22 Perc.
PLAT793_ALERT_4_G The Model has Chirality at C7 (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C10 (Verify) .... S
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 26
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.
1 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your

paper, to upload your CIF via our web site.

PLATON version of 04/07/2012; check.def file version of 28/06/2012

Datablock I - ellipsoid plot