Supporting Informations

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Contents:

1. Instrumentation and Chemicals
2. Crystallographic description.
3. Spectra of all compounds

Instrumentation and Chemicals
All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulfate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F\textsubscript{254} (0.25mm). Melting points were recorded on melting point apparatus and are uncorrected. IR spectra were recorded on IR spectrophotometer. NMR spectra were recorded in CDCl\textsubscript{3} with tetramethylsilane as the internal standard for \textsuperscript{1}H NMR (400 MHz) CDCl\textsubscript{3} solvent as the internal standard for \textsuperscript{13}C NMR (100 MHz.) MS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat. \textsuperscript{1}H and \textsuperscript{13}C NMR spectra were recorded on Varian 400 and Brucker 600 spectrometer by using TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm).
Elemental analyses were carried out using analyzer. Column chromatographic separations were performed using Merck silica gel (60-120 mesh).

**Crystallographic Description**

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions.

Table S1.Crystal data and structure refinement for 4a and 6d. For atomic coordinates and equivalent isotropic displacement parameters and bond angles, please check the CIF.

<table>
<thead>
<tr>
<th></th>
<th>Compound (CCDC)</th>
<th>Compound (CCDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identification code</td>
<td>SS-4a</td>
<td>SS-6d</td>
</tr>
<tr>
<td>Empirical formula</td>
<td>'C₁₉H₁₉N₅'</td>
<td>'C₂₀H₁₆ClN₅'</td>
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<td>Formula weight</td>
<td>318.1719</td>
<td>362.1172</td>
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<td>Temperature</td>
<td>298(2) K</td>
<td>296(2) K</td>
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<tr>
<td>Wavelength</td>
<td>0.71073Å</td>
<td>0.71073Å</td>
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<td>Crystal system</td>
<td>Triclinic</td>
<td>Monoclinic</td>
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<tr>
<td>Space group</td>
<td>P-1</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
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<td></td>
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<tr>
<td>------------------------------------------</td>
<td>----------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>a</td>
<td>8.5845(3) Å</td>
<td>12.968(2) Å</td>
</tr>
<tr>
<td>b</td>
<td>10.8223(3) Å</td>
<td>10.2902(18) Å</td>
</tr>
<tr>
<td>c</td>
<td>12.5073(4) Å</td>
<td>13.385(2) Å</td>
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<tr>
<td>α</td>
<td>84.207(2) °</td>
<td>90.00 °</td>
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<tr>
<td>β</td>
<td>72.287(2) °</td>
<td>98.889(12) °</td>
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<td>γ</td>
<td>75.180(2) °</td>
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<td>Volume</td>
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<td>1764.7(5) Å³</td>
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<tr>
<td>Z</td>
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<td>4</td>
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<td>Density (calculated)</td>
<td>1.228 g/cm³</td>
<td>1.362 g/cm³</td>
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<td>Absorption coefficient</td>
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<td>0.230 mm⁻¹</td>
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<td>F(000)</td>
<td>420.0</td>
<td>752</td>
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<tr>
<td>Theta range for data collection</td>
<td>1.71 to 28.42 °</td>
<td>2.04 to 24.99 °</td>
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<td>-11&lt;=h&lt;=11, -13&lt;=k&lt;=13, -16&lt;=l&lt;=14</td>
<td>-15&lt;=h&lt;=15, -11&lt;=k&lt;=12, -15&lt;=l&lt;=15</td>
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<td>Reflections collected</td>
<td>13065</td>
<td>12046</td>
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<td>Independent reflections</td>
<td>5294 R_{int} = 0.0606</td>
<td>2962 R_{int} = 0.1004</td>
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<td>Completeness to θ°</td>
<td>98.3 % (θ = 28.42°)</td>
<td>95.4 % (θ = 24.99°)</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F2</td>
<td>Full-matrix least-squares on F2</td>
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<td>Data / restraints / parameters</td>
<td>5294 / 0 / 268</td>
<td>2962 / 0 / 237</td>
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<tr>
<td>-------------------------------</td>
<td>----------------</td>
<td>----------------</td>
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<tr>
<td>Goodness-of-fit on F2</td>
<td>1.086</td>
<td>1.010</td>
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<tr>
<td>Final R indices [&gt;2sigma(I)]</td>
<td>R_{obs} = 0.0772, wR_{obs} = 0.2353</td>
<td>R_{obs} = 0.1537, wR_{obs} = 0.3668</td>
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<tr>
<td>R indices (all data)</td>
<td>R_{all} = 0.0952, wR_{all} = 0.2513</td>
<td>R_{all} = 0.1914, wR_{all} = 0.3821</td>
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<tr>
<td>Largest diff. peak and hole</td>
<td>1.109 and -1.204e.Å^{-3}</td>
<td>0.964 and -0.525e.Å^{-3}</td>
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</table>
$^1$H-NMR spectra of compound 4a
13C-NMR spectra of compound 4a
HRMS spectra of compound 4a
$^1$H-NMR spectra of compound 4b
13C-NMR spectra of compound 4b
HRMS spectra of compound 4b
$^1$H-NMR spectra of compound 4c
$^{13}$C-NMR spectra of compound 4c
HRMS-spectra of compound 4c
$^1$H-NMR spectra of compound 4d
$^{13}$C-NMR spectra of compound 4d
HRMS spectra of compound 4d

Chemical structure:

![Chemical structure of compound 4d]

- The molecular formula of compound 4d is C24H14ClN4.
- The molecular weight is 352.1336.
- Major peaks observed at m/z values of 130.1593 and 225.1949.

Graphical representation:

- ESI Scan (15.4 sec) Frag=175.0V SS-4Cl-CY.d
- Counts vs. Mass-to-Charge (m/z)
$^1$H-NMR spectra of compound 4e
$^{13}$C-NMR spectra of compound 4e
HRMS-spectra of compound 4e
$^1$H-NMR spectra of compound 4g
$^{13}$C-NMR spectra of compound 4g
HRMS spectra of compound 4g
$^1$H-NMR spectra of compound $4h$
$^{13}$C-NMR spectra of compound 4h

SS-3F-CY-13C

Current Data Parameters
NAME SS-3F-CY-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140502
Time 12.33
INSTRUM spect
PROBD 5 mm PABBO BB/
PULPROG zgq30
TD 32768
SOLVENT DMSO
NS 138
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.26
DW 13.867 usec
DE 6.50 usec
TE 300.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1
SFO1 150.9279571 MHz
NUM1 13C
P1 10.50 usec
PLW1 95.00000000 W

CHANNEL f2
SFO2 600.1724007 MHz
NUM2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
ST 16384
DF 150.9129377 MHz
WDW EM
SSB 0
LB 1.00 Hz
GC 0
PC 1.40
HRMS-spectra of compound 4h
$^1$H-NMR spectra of compound 4i
$^{13}$C-NMR spectra of compound 4i
HRMS spectra of compound 4i
$^1$H-NMR spectra of compound 4j
$^{13}$C-NMR spectra of compound 4j
HRMS-spectra of compound 4j
$^1$H-NMR spectra of compound 4k
$^{13}$C-NMR spectra of compound 4k
HRMS-spectra of compound 4k
$^1$H-NMR spectra of compound 41
$^1$H-NMR spectra of compound 41
1H-NMR spectra of compound 4m
$^{13}$C-NMR spectra of compound 4m
HRMS-spectra of compound 4m
\(^1\)H-NMR spectra of compound 4n
$^{13}$C-NMR spectra of compound 4n

![C-NMR spectra diagram]
$^1$H-NMR spectra of compound 40

$^{13}$C-NMR spectra of compound 40
HRMS-spectra of compound 4o
$^1$H-NMR spectra of compound 4p
$^{13}$C-spectra of compound 4p
HRMS-spectra of compound 4p

救命
$^1$H-NMR spectra of compound 4q
$^{13}$C-NMR spectra of compound 4q
HRMS-spectra of compound 4q
$^1$H-NMR spectra of compound 4r
$^{13}$C-NMR spectra of compound 4r

HRMS-spectra of compound 4r
$^1$H-NMR spectra of compound 4s

$^{13}$C-NMR spectra of compound 4s
HRMS-spectra of compound 4s
$^1$H-NMR spectra of compound 4t
$^{13}$C-NMR spectra of compound 4t
HRMS-spectra of compound 4t
$^1$H-NMR spectra of compound 4u

$^{13}$C-NMR spectra of compound 4u
HRMS-spectra of compound 4u
$^1$H-NMR spectra of compound 4v
$^{13}$C-NMR spectra of compound 4v
HRMS-spectra of compound 4v
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<th>User Name</th>
<th>IRM Calibration Status</th>
<th>Acquired Time</th>
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<td>Comment</td>
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</table>

+ESI Scan (13.8 sec) Frag=175.0V SS-4ME-PY.d

![Chemical Structure]

Counts (%) vs. Mass-to-Charge (m/z)

- Mass 304.1565
- Mass 242.2870


**1H-NMR spectra of compound 6a**

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**Sample Name:** SS-Ph-BA  
**Data Collected on:** IIYU-NMR-mercury400  
**Archive directory:** /home/chem/data/study  
**Sample directory:**  
**HS-CN-Li-S-TER-P1-01**  
**Pulse sequence:** PROTON  
**Solvent:** ddeo  
**Data collected on:** May 20 2014  
**Temp:** 298.1 K  
**Operator:** chem  
**Relax. delay 1.000 sec**  
**Pulse 45.0 degrees**  
**Acq. time 2.561 sec**  
**Width 6398.0 Hz**  
**32 repetitions**  
**RESONANT 31, 399.9528627 MHz**  
**DATA PROCESSING**  
**FT size 32768**  
**Total time 2 min 12 sec**

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\(^{13}\)C-NMR spectra of compound 6a

HRMS-spectra of compound 6a
$^{1}$H-NMR spectra of compound $6b$
$^{13}$C-NMR spectra of compound 6b
HRMS-spectra of compound 6b
$^1$H-NMR spectra of compound 6c
$^{13}$C-NMR spectra of compound 6c

HRMS-spectra of compound 6c
$^1$H-NMR spectra of compound 6d

$^{13}$C-NMR spectra of compound 6d
HRMS-spectra of compound 6d
$^1$H-spectra of compound 6e
$^{13}$C-spectra of compound $6e$
HRMS-spectra of compound 6e
$^1$H-spectra of compound 6f
$^{13}$C-spectra of compound 6f
$^{1}$H-spectra of compound 6g
$^{13}$C-spectra of compound 6g
HRMS-spectra of compound 6g
$^1$H-NMR spectra of compound 6h
$^{13}$C-NMR spectra of compound 6h
HRMS-spectra of compound 6h
1H-NMR spectra of compound 6i
$^{13}$C-NMR spectra of compound 6i
HRMS-spectra of compound 6i
$^1$H-NMR spectra of compound 6j
$^{13}$C-NMR spectra of compound 6j
HRMS-spectra of compound 6j