# Table of Contents

1. Crystallography data of Compound 10  
2. Copies of $^1$H and $^{13}$C NMR Spectra  
3. Copies of HRMS spectra  
4. Copies of HPLC data

## 1. Crystallography data of Compound 10

![Compound 10](image)

<table>
<thead>
<tr>
<th>Identification code</th>
<th>shelxl</th>
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<tbody>
<tr>
<td>Empirical formula</td>
<td>C26 H23 Cl N4 O</td>
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<tr>
<td>Formula weight</td>
<td>442.93</td>
</tr>
<tr>
<td>Temperature</td>
<td>113(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Monoclinic, P2(1)</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>$a = 8.1418(16)$ Å, $alpha = 90$ deg.</td>
</tr>
<tr>
<td></td>
<td>$b = 12.894(3)$ Å, $beta = 105.75(3)$ deg.</td>
</tr>
<tr>
<td></td>
<td>$c = 10.541(2)$ Å, $gamma = 90$ deg.</td>
</tr>
<tr>
<td>Volume</td>
<td>1065.1(4) Å$^3$</td>
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<tr>
<td>Z, Calculated density</td>
<td>2, 1.381 Mg/m$^3$</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>0.207 mm$^{-1}$</td>
</tr>
<tr>
<td>F(000)</td>
<td>464</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.20 x 0.18 x 0.12 mm</td>
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<tr>
<td>Theta range for data collection</td>
<td>2.01 to 28.10 deg.</td>
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<tr>
<td>Limiting indices</td>
<td>-9&lt;=h&lt;=10, -16&lt;=k&lt;=16, -13&lt;=l&lt;=13</td>
</tr>
<tr>
<td>Reflections collected / unique</td>
<td>10819 / 4910 [R(int) = 0.0301]</td>
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<tr>
<td>Completeness to theta = 28.10</td>
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<tr>
<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
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<tr>
<td>Max. and min. transmission</td>
<td>0.9756 and 0.9598</td>
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<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F$^2$</td>
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<tr>
<td>Data / restraints / parameters</td>
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<td>Goodness-of-fit on F$^2$</td>
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<tr>
<td>Final R indices [I&gt;2sigma(I)]</td>
<td>R1 = 0.0312, wR2 = 0.0797</td>
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</table>
R indices (all data)  R1 = 0.0414, wR2 = 0.0828
Absolute structure parameter  -0.01(5)
Largest diff. peak and hole  0.209 and -0.296 eÅ^-3

2. Copies of $^1$H and $^{13}$C NMR Spectra
2. Copies of HRMS spectra

- **7a**

- **7b**
3. Copies of HPLC data

**<Chromatogram>**

Detector A 254nm

<table>
<thead>
<tr>
<th>Peak#</th>
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<th>Height%</th>
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<tbody>
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<td>2218565</td>
<td>216367</td>
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**<Peak Table>**

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