Brandt, SD, Kavanagh, PV, Twamley, B, Westphal, F, Elliott, SP, Wallach, J, Stratford, A, Klein, LM, McCorvy, JD, Nichols, DE and Halberstadt, AL

Return of the lysergamides. Part IV: Analytical and pharmacological characterization of lysergic acid morpholide (LSM-775)

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Article

Citation (please note it is advisable to refer to the publisher’s version if you intend to cite from this work)

Return of the lysergamides. Part IV: Analytical and pharmacological characterization of lysergic acid morpholide (LSM-775)

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e Alere Forensics (Forensics Ltd), Malvern Hills Science Park, Geraldine Road, WR14 3SZ, UK

f Department of Pharmaceutical Sciences, Philadelphia College of Pharmacy, University of the Sciences, 600 South 43rd Street, Philadelphia, PA 19104, USA

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<table>
<thead>
<tr>
<th>Content</th>
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<tbody>
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<td>Photograph of powdered LSM-775 tartrate sample</td>
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<td>S3</td>
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<tr>
<td>Proposed LSM-775 dissociation pathways (QTOF-MS/MS)</td>
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<td>^1H/H COSY of LSM-775 hemitartrate (CD_3OD )</td>
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<td>HMQC of LSM-775 hemitartrate (CD_3OD)</td>
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<td>X-ray data for recrystallized LSM-775</td>
<td>S25–S43</td>
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</table>
Drug Testing and Analysis – Brandt et al. – Supporting Information

LSM-775
Powder - vendor
HPLC-DAD
220 nm

O
N
H

O
N
H

O

0.0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0 18.0 min

5.97 min
LSM-775 hemitartrate
$^1$H NMR / 600 MHz
d$_8$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate

$^1$H NMR / 600 MHz
d$_6$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate

$^1$H NMR / 600 MHz
d$_8$ - DMSO

$\text{TA} = \text{tartaric acid}$

Increased baseline led to inaccurate integration values, particularly between 4.0 and 2.7 ppm
LSM-775 hemitartrate
$^{13}$C NMR / 150 MHz
d$_6$ - DMSO

LSM-775 hemitartrate
DEPTQ / 75 MHz
d$_6$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate
HSQC
600 / 150 MHz
d$_{6}$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate
HSQC
600 / 150 MHz
d$_6$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate
HMBC
600 / 150 MHz
d$_6$ - DMSO

TA = tartaric acid
LSM-77S hemitartrate
HMBC
600 / 150 MHz
d$_9$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate
HMBC
600 / 150 MHz
d$_6$ - DMSO

TA = tartaric acid

Drug Testing and Analysis – Brandt et al. – Supporting Information
LSM-775 hemitartrate
HMBC
600 / 150 MHz
d$_9$ - DMSO

TA = tartaric acid
LSM-775 hemitartrate
HMBC
600 / 150 MHz
d6 - DMSO

TA = tartaric acid
Drugs Testing and Analysis – Brandt et al. – Supporting Information

LSM-775 hemitartrate
$^1$H NMR / 400 MHz
CD$_3$OD

TA = tartaric acid
$^1$H and $^{13}$C NMR data for LSM-775 hemitartrate in CD$_3$OD at 400 / 100 MHz (20 mg/mL).

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<th>No.</th>
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<td>6.99 (d, $J = 1.3$ Hz, 1H)</td>
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<td>3</td>
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<td>26.32</td>
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<td>5</td>
<td>64.09</td>
<td>3.90–3.80 (m, 5β-H, 1H)</td>
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<td>7</td>
<td>55.18</td>
<td>3.47 (dd, $J = 11.8$, 5.1 Hz, 7α-H, 1H) 3.27–3.21 (m, 7β-H, 1H)</td>
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<td>TA $^g$</td>
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$^a$ Overlapping with 22-CH$_2$ and 21-CH$_2$ (4H)

$^b$ Overlapping with 17-CH$_3$ (3H)

$^c$ Overlapping with 4α-H (1H)

$^d$ Overlapping with 2 x 22-CH$_2$ (4H)

$^e$ Overlapping with 4β-H (1H)

$^f$ Overlapping with 1 x 21-CH$_2$ (2H)

$^g$ TA: tartaric acid
LSM-775 hemitartrate
$^{13}$C NMR / 100 MHz
CD$_3$OD

TA = tartaric acid
LSM-775 hemitartrate
COSY
CD$_3$OD
Small Molecule X-ray Facility
School Of Chemistry

Structure Report

Filename: TCD173

Submitted by: Pierce Kavanagh
Reference: PKSBLSM
Group: Kavanagh

Fig. 1. Asymmetric unit of TCD173 showing both molecules with the tartrate anion as well as solvates H$_2$O and EtOH. Displacement ellipsoids shown at 50%.

11/12/14

Brendan Twamley
Figure 2. Packing diagram of TCD173 viewed down the a-axis. Hydrogen atoms omitted for clarity.
Crystal Structure Report for TCD173

A specimen of $C_{46}H_{60}N_6O_{12}$, approximate dimensions 0.060 mm x 0.060 mm x 0.210 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 100(2)K using an Oxford Cryosystems Cobra low temperature device using a MiTeGen micromount. See Table 1 for collection parameters and exposure time. Bruker APEX software was used to correct for Lorentz and polarization effects.

A total of 5863 frames were collected. The total exposure time was 29.31 hours. The integration of the data using an orthorhombic unit cell yielded a total of 57701 reflections to a maximum θ angle of 68.30° (0.83 Å resolution), of which 8027 were independent (average redundancy 7.188, completeness = 99.9%, $R_{int} = 4.44\%$, $R_{sig} = 2.32\%$) and 7723 (96.21%) were greater than 2σ(F²). The final cell constants of $a = 5.9621(2)$ Å, $b = 15.5087(6)$ Å, $c = 47.4811(19)$ Å, volume = 4390.3(3) Å³, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Data were corrected for absorption effects using the numerical method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8490 and 0.9424.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_12_12_1$, with Z = 4 for the formula unit, $C_{46}H_{60}N_6O_{12}$. The final anisotropic full-matrix least-squares refinement on F² with 607 variables converged at R₁ = 3.71\%, for the observed data and wR2 = 9.92\% for all data. The goodness-of-fit was 1.050. The largest peak in the final difference electron density synthesis was 0.557 e/Å³ and the largest hole was -0.395 e/Å³ with an RMS deviation of 0.049 e/Å³. On the basis of the final model, the calculated density was 1.345 g/cm³ and F(000), 1896 e⁻.

**Refinement Note:** All donor hydrogen atoms were located and refined with restraints (SADI). The solvent EtOH molecule C-C distance was also restrained (DFIX). Absolute configuration was established by anomalous-dispersion effects in diffraction measurements on the crystal.

**References:**
Bruker APEX v2012.12-0, Bruker AXS Inc., Madison, Wisconsin, USA.

SADABS (2014/3) Bruker AXS Inc., Madison, Wisconsin, USA; Sheldrick, G. M. University of Göttingen, Germany.


**Acknowledgement:**
Facility funded by PRTLI and ERDF.
Table 1: Data collection details for TCD173.

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<th>Ψ/°</th>
<th>χ/°</th>
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Table 2. Crystal data and structure refinement for TCD173.

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Table 3. Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters (Å²x $10^3$) for TCD173. U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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### Table 4: Bond lengths [Å] and angles [°] for TCD173.

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Table 5. Anisotropic displacement parameters (Å²×10³) for TCD173. The anisotropic displacement factor exponent takes the form: -2π²( h a*²U₁₁ + ... + 2 h k a* b* U₁₂ )

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<td>-1.6(4)</td>
</tr>
<tr>
<td>C(14)-C(16)-C(25)-C(20)</td>
<td>178.0(2)</td>
</tr>
<tr>
<td>C(17)-C(16)-C(25)-C(23)</td>
<td>178.9(3)</td>
</tr>
<tr>
<td>C(14)-C(16)-C(25)-C(23)</td>
<td>-1.5(4)</td>
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N(46)-C(47)-C(48)-C(49) | -173.2(3)
C(47)-C(48)-C(49)-C(38)  -150.8(3)  C(6)-C(5)-N(4)-C(3)  -56.9(3)
C(50)-C(48)-C(49)-C(38)  35.1(3)  C(2)-C(3)-N(4)-C(7)  -118.7(3)
N(36)-C(38)-C(49)-C(48)  -174.4(2)  C(2)-C(3)-N(4)-C(5)  56.8(3)
C(39)-C(38)-C(49)-C(48)  -51.1(3)  C(9)-C(10)-N(11)-C(12)  163.7(2)
N(46)-C(45)-C(50)-C(41)  -176.1(2)  C(9)-C(10)-N(11)-C(13)  -70.8(2)
C(44)-C(45)-C(50)-C(41)  3.6(4)  C(14)-C(13)-N(11)-C(12)  177.5(2)
N(46)-C(45)-C(50)-C(48)  1.8(3)  C(24)-C(13)-N(11)-C(12)  -56.1(3)
C(44)-C(45)-C(50)-C(48)  -178.6(2)  C(14)-C(13)-N(11)-C(10)  53.5(3)
C(42)-C(41)-C(50)-C(45)  -2.9(4)  C(24)-C(13)-N(11)-C(10)  179.9(2)
C(39)-C(41)-C(50)-C(45)  172.9(2)  C(19)-C(20)-N(21)-C(22)  179.7(3)
C(42)-C(41)-C(50)-C(48)  179.7(2)  C(25)-C(20)-N(21)-C(22)  -0.3(3)
C(39)-C(41)-C(50)-C(48)  -4.5(4)  C(23)-C(22)-N(21)-C(20)  -0.7(4)
C(47)-C(48)-C(50)-C(45)  -2.0(3)  O(33)-C(32)-N(29)-C(28)  172.2(3)
C(49)-C(48)-C(50)-C(45)  173.8(2)  C(34)-C(32)-N(29)-C(28)  -11.8(4)
C(47)-C(48)-C(50)-C(41)  175.8(2)  O(33)-C(32)-N(29)-C(30)  1.1(4)
C(49)-C(48)-C(50)-C(41)  -8.5(4)  C(34)-C(32)-N(29)-C(30)  177.0(2)
O(53)-C(52)-C(54)-O(55)  -167.1(2)  C(27)-C(28)-N(29)-C(32)  134.7(3)
O(51)-C(52)-C(54)-O(55)  15.1(3)  C(27)-C(28)-N(29)-C(30)  -53.6(3)
O(53)-C(52)-C(54)-C(56)  71.4(3)  C(31)-C(30)-N(29)-C(32)  -134.6(2)
O(51)-C(52)-C(54)-C(56)  -106.4(2)  C(31)-C(30)-N(29)-C(28)  53.1(3)
O(55)-C(54)-C(56)-O(57)  -72.3(2)  C(34)-C(35)-N(36)-C(37)  165.7(2)
C(52)-C(54)-C(56)-O(57)  49.1(2)  C(34)-C(35)-N(36)-C(38)  -69.6(2)
O(55)-C(54)-C(56)-C(58)  50.9(3)  C(39)-C(38)-N(36)-C(37)  177.78(19)
C(52)-C(54)-C(56)-C(58)  172.3(2)  C(49)-C(38)-N(36)-C(37)  -55.8(3)
O(57)-C(56)-C(58)-O(60)  8.1(3)  C(39)-C(38)-N(36)-C(35)  54.9(2)
C(54)-C(56)-C(58)-O(60)  -112.1(2)  C(49)-C(38)-N(36)-C(35)  -178.63(19)
O(57)-C(56)-C(58)-O(59)  -173.1(2)  C(44)-C(45)-N(46)-C(47)  179.5(3)
C(54)-C(56)-C(58)-O(59)  66.7(3)  C(50)-C(45)-N(46)-C(47)  -0.9(3)
O(8)-C(7)-N(4)-C(5)  1.3(4)  C(48)-C(47)-N(46)-C(45)  -0.4(3)
C(9)-C(7)-N(4)-C(5)  178.6(2)  C(5)-C(6)-O(1)-C(2)  -56.6(3)
O(8)-C(7)-N(4)-C(3)  176.5(2)  C(3)-C(2)-O(1)-C(6)  57.2(3)
C(9)-C(7)-N(4)-C(3)  -6.2(4)  C(30)-C(31)-O(26)-C(27)  60.5(3)
C(6)-C(5)-N(4)-C(7)  119.0(3)  C(28)-C(27)-O(26)-C(31)  -60.2(3)
Table 8. Hydrogen bonds for TCD173 [Å and °].

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>&lt;(DHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(5)-H(5A)...O(33)</td>
<td>0.99</td>
<td>2.45</td>
<td>3.280(3)</td>
<td>141</td>
</tr>
<tr>
<td>C(9)-H(9)...O(53)</td>
<td>1.00</td>
<td>2.60</td>
<td>3.469(3)</td>
<td>145</td>
</tr>
<tr>
<td>C(10)-H(10A)...O(57)</td>
<td>0.99</td>
<td>2.49</td>
<td>3.117(3)</td>
<td>121</td>
</tr>
<tr>
<td>C(12)-H(12A)...O(51)#1</td>
<td>0.98</td>
<td>2.57</td>
<td>3.407(3)</td>
<td>143</td>
</tr>
<tr>
<td>C(22)-H(22)...O(62)#2</td>
<td>0.95</td>
<td>2.58</td>
<td>3.527(5)</td>
<td>177</td>
</tr>
<tr>
<td>C(27)-H(27B)...O(33)#3</td>
<td>0.99</td>
<td>2.37</td>
<td>3.299(3)</td>
<td>156</td>
</tr>
<tr>
<td>C(30)-H(30B)...O(8)</td>
<td>0.99</td>
<td>2.60</td>
<td>3.411(3)</td>
<td>139</td>
</tr>
<tr>
<td>C(35)-H(35A)...O(60)#4</td>
<td>0.99</td>
<td>2.57</td>
<td>3.125(3)</td>
<td>115</td>
</tr>
<tr>
<td>C(44)-H(44)...O(59)#5</td>
<td>0.95</td>
<td>2.44</td>
<td>3.373(3)</td>
<td>169</td>
</tr>
<tr>
<td>C(49)-H(49B)...O(1)#6</td>
<td>0.99</td>
<td>2.40</td>
<td>3.273(3)</td>
<td>147</td>
</tr>
<tr>
<td>C(54)-H(54)...O(60)#3</td>
<td>1.00</td>
<td>2.28</td>
<td>3.181(3)</td>
<td>149</td>
</tr>
<tr>
<td>N(11)-H(11)...O(51)</td>
<td>0.89(2)</td>
<td>1.84(2)</td>
<td>2.729(3)</td>
<td>171(3)</td>
</tr>
<tr>
<td>N(21)-H(21)...O(26)#7</td>
<td>0.90(2)</td>
<td>2.00(3)</td>
<td>2.859(3)</td>
<td>160(4)</td>
</tr>
<tr>
<td>N(36)-H(36)...O(59)#4</td>
<td>0.90(2)</td>
<td>1.73(2)</td>
<td>2.631(3)</td>
<td>179(4)</td>
</tr>
<tr>
<td>N(36)-H(36)...O(60)#4</td>
<td>0.90(2)</td>
<td>2.55(4)</td>
<td>3.109(3)</td>
<td>120(3)</td>
</tr>
<tr>
<td>N(46)-H(46)...O(53)#5</td>
<td>0.89(2)</td>
<td>2.05(2)</td>
<td>2.908(3)</td>
<td>161(3)</td>
</tr>
<tr>
<td>O(55)-H(55)...O(51)</td>
<td>0.84(3)</td>
<td>2.09(3)</td>
<td>2.634(3)</td>
<td>122(3)</td>
</tr>
<tr>
<td>O(57)-H(57)...O(53)#1</td>
<td>0.85(3)</td>
<td>2.10(3)</td>
<td>2.804(3)</td>
<td>141(3)</td>
</tr>
<tr>
<td>O(57)-H(57)...O(60)</td>
<td>0.85(3)</td>
<td>2.23(4)</td>
<td>2.679(3)</td>
<td>113(3)</td>
</tr>
<tr>
<td>O(61)-H(61A)...O(60)</td>
<td>0.94</td>
<td>1.91</td>
<td>2.831(3)</td>
<td>165</td>
</tr>
<tr>
<td>O(61)-H(61B)...O(55)#1</td>
<td>0.90</td>
<td>2.01</td>
<td>2.887(3)</td>
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</tr>
<tr>
<td>O(62)-H(62)...O(61)</td>
<td>0.86</td>
<td>1.95</td>
<td>2.795(4)</td>
<td>169</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z  #2 x-1/2,-y+1/2,-z+2  #3 x-1,y,z  
#4 x,y+1,z  #5 -x,y+1/2,-z+3/2  #6 -x+1,y+1/2,-z+3/2  
#7 x-1/2,-y+3/2,-z+2