CHIR-99021 HNMR Analysis, Solvent = DMSO

MedKoo Cat#: 200774
Name: CHIR-99021
CAS#: 252917-06-9
Lot#: A8T12K19
Chemical Formula: C22H18Cl2N8
Exact Mass: 464.10315
Molecular Weight: 465.34

DMSO, F1: 400.132, F2: 1.000, SW1: 8224, OF1: 2467.9, PTS1d: 32768
EX: zg30, PW: 13.0 usec, PD: 1.0 sec, NA: 8, LB: 0.0

DATE: Tue Dec 18 04:45:28 2018

MedKoo Biosciences
Product Quality Control Data
www.medkoo.com   sales@medkoo.com
**HPLC Analysis Report**

Injection Date: 18 Dec 18  
Sample Name: 252917-06-9  

**Analysis Method:** D:\METHODS\2-POS-15MIN.M  
**Sample Info:** Easy-Access Method: '2-POS-15MIN.M'  
**Method Info:**  
- Column: XBridge C18 (4.6* 50 mm, 3.5 um)  
- Mobile phase: H2O(10 mmol NH4HCO3) (A) / ACN(B)  
- Elution program: Gradient from 10 to 95% of B in 8 min at 1 ml/min  
- Column Temperature: 40 ºC  
- Detection: UV (214, 254, 4 nm)

### Integration Results for DAD1 A, Sig=214,4 Ref=off

<table>
<thead>
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<th>RetTim</th>
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<tr>
<td>7.17</td>
<td>0.04</td>
<td>6770.60</td>
<td>2736.67</td>
<td>98.51</td>
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<td>8.07</td>
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<td>70.69</td>
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### Integration Results for DAD1 B, Sig=254,4 Ref=off

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<td>0.04</td>
<td>49.58</td>
<td>18.40</td>
<td>0.85</td>
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**LC-MS Analytical Report**

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</table>

1. Instrument: Dionex Ultimate 3000 series HPLC system (Thermo, Germering, Germany) and Q-Exactive MS system (Thermo, Bremen, Germany)

2. LC condition:
   1. Mobile phase A (water with 0.1% formic acid) and mobile phase B (acetonitrile with 0.1% formic acid)
   2. Flow rate: 0.2 ml/min.
   3. Column: Phenomenex Gemini 3u C6-phenyl column (2.0 x 100 mm, 3 μm)
   4. Gradient: 0-1 min, 100% A; 10-20 min, 2% A

3. Mass spectrum was acquired in the range of m/z 100 - m/z 700 under positive ESI

**UV chromatogram at 280 nm:**

**Mass spectrum (positive electrospary ionization) from above peak 6.88 min:**