

## Analytical Data Sheet

Lot number **1066897**  
not for drug use

Retest date July 2018  
 Catalog number **Q-2525.0250**  
 Product number **4029066.0250**  
 Product **4, 7, 10- Tri- (t- butyloxycarbonylmethyl) - 1, 4, 7, 10-tetraazacyclododecan- 1- yl- acetic acid hydrobromide salt**  
 Molecular formula  $C_{28}H_{52}N_4O_8$   
 Relative molecular mass 572.74

Tests	Results
Appearance	white crystals
Appearance of solution	clear, colorless solution (50 mg/mL in methanol)
Identification (ESI-MS)	m = 572.7u (average mass)
Identification (TLC)	complies with authentic material
Purity (HPLC)	98.6% (TFA)
Related impurities (HPLC)	0.7% DOTA(OtBu) <sub>2</sub> (OH) <sub>2</sub>
Purity (TLC)	≥ 95%
TLC conditions	chloroform/methanol/acetic acid/H <sub>2</sub> O 85/13/0.5/1.5 chloroform/methanol/acetic acid/H <sub>2</sub> O 45/13/1/2 plate: silicagel 60 F <sub>254</sub> detected by: UV, ninhydrin, TMB
Assay (elemental analysis)	75.2% (Nth 9.78%, Nfd 7.35%)
Water content (KF volumetric)	2.7%
Elemental content (AAS)	<u>sodium content (FAAS)</u> < 0.004%
Acetic acid content (IC)	< 0.020% (limit test)
Residual organic solvents (GC)	chloroform not det. (LOQ 151 mg/kg, LOD 45 mg/kg) hexane not det. (LOQ 52 mg/kg, LOD 16 mg/kg) methanol < LOQ (LOQ 38 mg/kg, LOD 11 mg/kg) acetone not det. (LOQ 33 mg/kg, LOD 10 mg/kg) diisopropyl ether not det. (LOQ 46 mg/kg, LOD 14 mg/kg) 2-methyltetrahydrofuran 557 mg/kg (LOQ 66 mg/kg, LOD 20 mg/kg) MTBE not det. (LOQ 38 mg/kg, LOD 12 mg/kg)

<b>Bromide content (titration)</b>	18.3%
<b>Heavy metals (ICP-OES)</b>	28mg/kg Ca 5mg/kg Mg
<b>Trace metals (ICP-MS)</b>	19mg/kg sum of Cu, Fe, Ni, Pb, Pd, Zn

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Latest update: July 15, 2016

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