Table 1. Drug Substance General Properties

Physical and Chemical Properties	Results
Appearance	white to slightly yellow powder
Solubilities according to PhEur 1.4[a,b]	
purified water	freely soluble (XXX to XXXX mg/mL)[c]
acetone	slightly soluble (X to XX mg/mL)
dimethylsulfoxide (DMSO)	freely soluble (XXX to XXXX mg/mL)
ethanol	soluble (XX to XXX mg/mL)
methanol	freely soluble (XXX to XXXX mg/mL)
methylene chloride	freely soluble (XXX to XXXX mg/mL)
Solubilities at saturation in aqueous medium after 2 hours[a]:	
Purified water	~ XX mg/mL
Glucose solution (5%)	~ XX mg/mL
Saline solution (NaCl 0.9%)	~ XX mg/mL
Solubility as a function of pH in USP buffers[a, d]	
pH = X.X	XX.X mg/mL
pH = 1.2	XX.X mg/mL
pH = X.X	XX.X mg/mL
pH = X.X	XX.X mg/mL
pH = 4.5	XX.X mg/mL
pH = X.X	XX.X mg/mL
pH = X.X	XX.X mg/mL
pH = 6.8	XX.X mg/mL
pH = X.X	XX.X mg/mL

PhEur = European Pharmacopoeia; USP = United States Pharmacopeia

[a] Solubilities expressed as base form; apply conversion factor to the salt to free base form (use appropriate salt conversion).

[b] Solubilities were measured in different solvents by determining the volume of solvent required to dissolve 25 mg of drug substance.

[c] <INN> is freely soluble in purified water, but partly precipitates after 1 hour at room temperature to reach the solubility at saturation.

[d] This behavior is explained in 3.2.S.3.1 (Elucidation of Structure and Other Characteristics).

[e] Heating rate for thermal analysis by differential scanning calorimetry and thermogravimetric analysis was 10°C/min.

[f] According to PhEur 5.11.

Table 1. Drug Substance General Properties

Physical and Chemical Properties	Results
Solubility for the neutral form (B) in 0.15 M KCl[a]	X.X mg/mL
Dissociation constant pKa_1 (amine group)	X.XX
Dissociation constant pKa_2 (phenol group)	X.XX
Partition Coefficient	
Log P octanol/0.1 M KNO_3 (pH = 7.4)	X.XX
Distribution Coefficient	
Log D octanol/0.1 M KNO_3 (pH = X.X)	X.XX
Log D octanol/0.1 M KNO_3 (pH = X.X)	X.XX
Log D octanol/0.1 M KNO_3 (pH = X.X)	X.XX
Log D octanol/0.1 M KNO_3 (pH = X.X)	X.XX
pH in aqueous solution at 10 mg/mL (XX°C)	from X.X to X.X
Optical rotation (10 g/L, DMSO)	$[a]_{365}^{20}$ = +XX°
Thermal Analysis	
Melting point onset temperature (T_m)	XXX.X°C
Glass transition temperature (T_g)	T_g Onset = XXX.X°C T_g Midpoint = XXX.X°C T_g Endpoint = XXX.X°C
Thermogravimetric Analysis (TGA)	Weight loss of X.X% from XX°C to XXX°C
Hygroscopicity	Hygroscopic[d, f]
Crystalline form	Drug substance exists as Form X Naming: free form, # salt and hydration. Additional solid forms exist
Stereochemistry	One asymmetric center and one axis of chirality; (*S,M*) - enantiomer

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