CERTIFICATE OF ANALYSIS

(+)-*cis,trans*-ABSCISIC ACID (ABA)

[S]-5-[1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methyl-[2Z,4E]-pentadienoic acid]

$C_{15}H_{20}O_4$, FW = 264.32

OLCHEMIM CODE: 013 272n
OLCHEMIM BATCH: 272-B
MANUFACTURING DATE: October 2024
EXPIRATION DATE: October 2033
CAS: 21293-29-8
BATCH SIZE: 1250 g

PREPARATION

Prepared by biotechnological bacterial production, extracted and purified by reversed-phase chromatography. Crystallized from water and re-crystallized from ethyl acetate. A colourless, amorphous solid soluble in EtOH, MeOH, DMSO and water (3 g/L, 20ºC). White to nearly white powder (slightly yellow), free of foreign matter.

ANALYSIS

mp 161.0-163.0 ºC (Kofler block)
UV: Determined after drying to constant weight over phosphorus pentoxide in vacuo.
acidic EtOH λ_{max} 262 nm, sh 240 nm (21,500)
basic EtOH λ_{max} 245 nm
TLC (silica-chloroform/MeOH, 85/15), Rf = 0.41. Purity 99+%.
TLC (silica-toluene/EtOAc/AcOH. 5O/3O/4), *cis-trans* isomer Rf = 0.36. Purity 99+%. No *trans-trans* isomer present (Rf 0.41) detectable (< 0.5%).
HPLC (250 x 4.5 mm, 5µm ODS, 40% MeOH/0.1M AcOH, 2 ml/min), Rt 10.5 min. Purity 99+%.
MASS SPETROMETRY: MASS SPETROMETRY: Matches the reference spectrum $[M+H]^+$= 265.1 amu, ZMD 2000 (Waters) single quadrupole electrospray MS.
HPLC: Samples were dissolved in mobile phase (initial conditions) and separated on RP-column (150 mm × 4.6 mm, 5µm) (Microsorb C18; Varian). The elution was performed with a methanolic gradient. The flow rate was 0.6 ml/min. The UV absorbance was scanned between 240 – 300 nm. Rt (ABA) = 11.4 min, λ_{max} 261.8 nm. Purity > 99+%.

STORAGE & STABILITY

LIGHT-SENSITIVE! Store over silica gel in tightly sealed container below 0ºC. No detectable decomposition after 12 months storage under these conditions.

FOR LABORATORY USE BY EXPERIENCED PERSONNEL ONLY; NOT FOR DRUG, HOUSEHOLD OR OTHER USES

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