



Technical Data Sheet:

Compound E

Catalog Number	SML02B
Synonyms	XXI, Compound E (secretase inhibitor), DuPont E, C-E, γ -secretase inhibitor XXI, Gamma-secretase inhibitor XXI
Size	10 mg
Description	Compound E is a potent γ -secretase inhibitor that specifically blocks β -amyloid-40 (IC ₅₀ of 0.24), β -amyloid-42 (IC ₅₀ of 0.37), and cleavage of the Notch domain (IC ₅₀ of 0.32). Compound E has been shown to promote the differentiation of embryonic stem cells (ESCs) to primitive neural precursors in addition to generating a self-renewing progenitor neuroepithelia stem cell population (Li, et al.) when combined with CHIR99021 (Cat. No. SML01B), SB431542 (Cat. No. SML09B), and hLIF. Forebrain GABA interneurons have also been derived from human pluripotent stem cells (PSCs) through the utilization of Compound E (Liu, et al.); additionally, it has shown promising effects in Alzheimer's disease models using iPSC-derived neurons (Yagi, et al.).
Molecular Weight	490.50
Molecular Formula	C ₂₇ H ₂₄ F ₂ N ₄ O ₃
Chemical Name	Benzeneacetamide, N-[[[(1S)-2-[[[(3S)-2,3-dihydro-1-methyl-2-oxo-5-phenyl-1H-1,4-benzodiazepin-3-yl]amino]-1-methyl-2-oxoethyl]-3,5-difluoro-
CAS Number	209986-17-4
Target	γ -secretase
Appearance	White to off-white (Solid)
Purity	≥95% by LCMS
Solubility and Reconstitution	Soluble in DMSO up to 100mM, for example: 10 mg/101.936 mL = 0.098 mg/mL = 0.2 mM 10 mg/20.387 mL = 0.491 mg/mL = 1 mM 10 mg/4.078 mL = 2.452 mg/mL = 5 mM 10 mg/2.0387 mL = 4.905 mg/mL = 10 mM
Storage Temperature and Stability	Powder: -20°C 3 years In solvent: -80°C 6 months -20°C 1 month
References	Li, et al. 2011. Rapid induction and long-term self-renewal of primitive neural precursors from human embryonic stem cells by small molecule inhibitors. PNAS. 108(20): 8299-304. Liu, et al. 2013. Directed differentiation of forebrain GABA interneurons from human pluripotent stem cells. Nature Protocols. 8: 1670-1679. Yagi, et al. 2011. Modeling familial Alzheimer's disease with induced pluripotent stem cells. Human Molecular Genetics. 20(23): 4530-4539.